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Cover image: The figure shows the outgoing scattered field produced by scattering a plane wave, coming from the northwest, off of the (stylized) letters P A A. The total field satisfies the homogeneous Dirichlet condition on the boundary of the letters. It is based on a numerical computation by Mike O'Neil of the Courant Institute.

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RADIALLY SYMMETRIC TRAVELING WAVES FOR THE SCHRÖDINGER EQUATION ON THE HEISENBERG GROUP

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We consider radial solutions to the cubic Schrödinger equation on the Heisenberg group

$$i\partial_t u - \Delta_{\mathbb{H}^1} u = |u|^2 u, \quad \Delta_{\mathbb{H}^1} = \tfrac{1}{4}(\partial_x^2 + \partial_y^2) + (x^2 + y^2)\partial_s^2, \quad (t, x, y, s) \in \mathbb{R} \times \mathbb{H}^1.$$

This equation is a model for totally nondispersive evolution equations. We show existence of ground state traveling waves with speed $\beta \in (-1, 1)$. When the speed β is sufficiently close to 1, we prove their uniqueness up to symmetries and their smoothness along the parameter β. The main ingredient is the emergence of a limiting system as β tends to the limit 1, for which we establish linear stability of the ground state traveling wave.

1. Introduction

Dispersion for nonlinear Schrödinger equations. We consider the cubic focusing Schrödinger equation on the Heisenberg group

$$i\partial_t u - \Delta_{\mathbb{H}^1} u = |u|^2 u, \quad (t, x, y, s) \in \mathbb{R} \times \mathbb{H}^1, \tag{1}$$

where $\Delta_{\mathbb{H}^1}$ denotes the sub-Laplacian on the Heisenberg group. When the solution is radial, in the sense that it only depends on t, $|x + iy|$ and s, the sub-Laplacian becomes

$$\Delta_{\mathbb{H}^1} = \tfrac{1}{4}(\partial_x^2 + \partial_y^2) + (x^2 + y^2)\partial_s^2.$$

The Heisenberg group is a typical case of geometry where dispersive properties of the nonlinear Schrödinger equation disappear. Let us recall the motivation for this setting.

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Fix a Riemannian manifold M, and denote by Δ the Laplace operator associated to the metric g on M. As observed by Burq, Gérard and Tzvetkov [Burq et al. 2005], qualitative properties of the solutions to the nonlinear Schrödinger equation

$$i\partial_t u - \Delta u = |u|^2 u, \quad (t,x) \in \mathbb{R} \times M$$

are strongly influenced by the underlying geometry of the manifold M. When some loss of dispersion occurs, for example in the spherical geometry, a condition for well-posedness of the Cauchy problem in $H^s(M)$ is that s must be larger than a critical parameter.

To take it further, on sub-Riemannian manifolds, Bahouri, Gérard and Xu [Bahouri et al. 2000] noticed that the dispersion properties totally disappear for the sub-Laplacian on the Heisenberg group, leaving the existence and uniqueness of smooth global in time solutions as an open problem. Del Hierro [2005] analyzed the dispersion properties on H-type groups, proving sharp decay estimates for the Schrödinger equation depending on the dimension of the center of the group. More generally, Bahouri, Fermanian and Gallagher [Bahouri et al. 2016] proved optimal dispersive estimates on stratified Lie groups of step 2 under some property of the canonical skew-symmetric form. In contrast, they also give a class of groups without this property displaying total lack of dispersion, which includes the Heisenberg group.

In this spirit, Gérard and Grellier [2010a; 2010b] introduced the cubic Szegő equation on the torus as a simpler model of a nondispersive Hamiltonian equation in order to better understand the situation on the Heisenberg group. The cubic Szegő equation was then studied on the real line by Pocovnicu [2011], where it has the form

$$i\partial_t u = \Pi(|u|^2 u), \quad (t,x) \in \mathbb{R} \times \mathbb{R},$$

$\Pi : L^2(\mathbb{R}) \to L^2_+(\mathbb{R})$ being the Szegő projector onto the space $L^2_+(\mathbb{R})$ of functions in $L^2(\mathbb{R})$ with nonnegative frequencies. The cubic Szegő equation displays a strong link with the mass-critical half-wave equation on the torus [Gérard and Grellier 2012] and on the real line [Krieger et al. 2013]. On the real line, the cubic focusing half-wave equation is written

$$i\partial_t u + |D|u = |u|^2 u, \quad (t,x) \in \mathbb{R} \times \mathbb{R},$$

where $D = -i\partial_x$, $\widehat{|D|f}(\xi) = |\xi|\hat{f}(\xi)$. Some of the interactions between the Szegő equation and the half-wave equation will be discussed below, because they can be transferred to the setting of the Heisenberg group.

Traveling waves and limiting profiles. Constructing traveling wave solutions which are weak global solutions in the energy space can be obtained by a classical variational argument. For example, this technique was used to study the famous focusing mass-critical NLS problem

$$i\partial_t u - \Delta u = |u|^{\frac{4}{n}} u, \quad (t,x) \in \mathbb{R} \times \mathbb{R}^n.$$

From [Weinstein 1982], the existence of a ground state positive solution $Q \in H^1(\mathbb{R}^n)$ to

$$\Delta Q - Q + Q^{1+\frac{4}{n}} = 0$$

leads to a criterion for global existence of solutions in $H^1(\mathbb{R}^n)$. The uniqueness of this ground state (up to symmetries) holds [Gidas et al. 1979; Kwong 1989].

Concerning the half-wave equation, the Cauchy problem is locally well-posed in the energy space $H^{\frac{1}{2}}(\mathbb{R})$ [Gérard and Grellier 2012; Krieger et al. 2013]. Moreover, one also gets a global existence criterion, derived from the existence of a unique [Frank and Lenzmann 2013] ground state positive solution $Q \in H^{\frac{1}{2}}(\mathbb{R})$ to

$$|D|Q + Q - Q^3 = 0.$$

Contrary to the mass-critical Schrödinger equation on $\mathbb{R}^n$, the half-wave equation admits traveling waves with speed $\beta \in (-1, 1)$ (see [Krieger et al. 2013]),

$$u_\beta(t, x) = Q_\beta\Big(\frac{x + \beta t}{1-\beta}\Big)\, \mathrm{e}^{-it}.$$

The profile Q_β is a solution to

$$\frac{|D| - \beta D}{1-\beta} Q_\beta + Q_\beta = |Q_\beta|^2 Q_\beta.$$

Moreover, it satisfies

$$\lim_{\beta\to 0} \|Q_\beta - Q\|_{H^{\frac{1}{2}}}(\mathbb{R}) = 0 \quad \text{and} \quad \|Q_\beta\|_{L^2(\mathbb{R})} < \|Q\|_{L^2(\mathbb{R})}.$$

While the existence of the profiles Q_β follows from a standard variational argument, their uniqueness is more delicate to prove. This can be done through the study of the photonic limit $\beta \to 1$ as follows. It has been shown in [Gérard et al. 2018] that the traveling waves converge as β tends to 1 to a solution of the cubic Szegő equation. More precisely, $(Q_\beta)_\beta$ converges in $H^{\frac{1}{2}}(\mathbb{R})$ to a profile Q_+, which is a ground state solution to

$$DQ_+ + Q_+ = \Pi(|Q_+|^2 Q_+), \quad D = -i\partial_x.$$

From Q_+, we recover a traveling wave solution to the cubic Szegő equation by setting

$$u(t, x) = Q_+(x - t)\, \mathrm{e}^{-it}.$$

But Pocovnicu [2011] showed that the traveling waves u are unique up to symmetries and that Q_+ must have the form

$$Q_+(x) = \frac{2}{2x + i}.$$

Moreover, the linearized operator around Q_+ is coercive [Pocovnicu 2012]; and in particular, the Szegő profile is orbitally stable. Gérard, Lenzmann, Pocovnicu and Raphaël [2018] deduced the invertibility of the linearized operator for the half-wave equation around the profiles Q_β when β is close enough to 1, which leads to their uniqueness up to symmetries. This allowed them to define a smooth map of solutions $\beta \mapsto Q_\beta$ on a neighborhood of 1.

On the Heisenberg group, one can also construct a family of radial traveling waves with speed $\beta \in (-1,1)$ under the form

$$u_\beta(t,x,y,s) = Q_\beta\left(\frac{x}{\sqrt{1-\beta}}, \frac{y}{\sqrt{1-\beta}}, \frac{s+\beta t}{1-\beta}\right). \tag{2}$$

The profile Q_β satisfies the following stationary hypoelliptic equation:

$$-\frac{\Delta_{\mathbb{H}^1}+\beta D_s}{1-\beta} Q_\beta = |Q_\beta|^2 Q_\beta. \tag{3}$$

There exist ground state solutions, constructed as optimizers for some Gagliardo–Nirenberg inequalities derived from the Folland–Stein embedding $\dot{H}^1(\mathbb{H}^1) \hookrightarrow L^4(\mathbb{H}^1)$ [Folland and Stein 1974]. The proof of existence relies on a concentration-compactness argument, which first appeared in the work of Cazenave and Lions [1982] and was refined into a profile decomposition theorem on $\mathbb{R}^n$ by Gérard [1998]. The profile decomposition theorem was then adapted to the Heisenberg group by Benameur [2008]. The family of traveling waves u_β is constructed in the radial setting for simplicity, but it seems realistic to establish the existence of nonradial traveling waves as minimizers for the same Gagliardo–Nirenberg inequalities restricted to some other set of functions.

Our purpose is to show the uniqueness of the profiles Q_β when their speed β is close to 1 up to some symmetries. Following the strategy deployed on the half-wave equation, we derive a limiting system in the photonic limit $\beta \to 1$. We then determine all ground state solutions to the limiting system and prove their linear stability. From the linear stability of the limiting ground states, we recover the uniqueness of the profiles Q_β up to symmetries when their speed β is close to 1.

Main results. Any solution u of the Schrödinger equation on the Heisenberg group (1) enjoys the following symmetries:

- For all $s_0 \in \mathbb{R}$, $(t,x,y,s) \mapsto u(t,x,y,s+s_0)$ is a solution (translation in s).
- For all $\theta \in \mathbb{T}$, $(t,x,y,s) \mapsto e^{i\theta} u(t,x,y,s)$ is a solution (phase multiplication).
- For all $\lambda \in \mathbb{R}$, $(t,x,y,s) \mapsto \lambda u(\lambda^2 t, \lambda x, \lambda y, \lambda^2 s)$ is a solution (scaling).

Our main result is the uniqueness of the ground states Q_β when β is close to 1.

Theorem 1.1. *There exists $\beta_* \in (0,1)$ such that the following holds: For all $\beta \in (\beta_*,1)$, there is a unique ground state up to symmetries to* (3),

$$-\frac{\Delta_{\mathbb{H}^1}+\beta D_s}{1-\beta} Q_\beta = |Q_\beta|^2 Q_\beta.$$

Denote by Q_β this ground state, then the set of all ground state solutions of the above equation can be described as

$$\{T_{s_0,\theta,\alpha} Q_\beta : (x,y,s) \mapsto e^{i\theta} \alpha Q_\beta(\alpha x, \alpha y, \alpha^2(s+s_0)) \mid (s_0,\theta,\alpha) \in \mathbb{R} \times \mathbb{T} \times \mathbb{R}_+^*\}.$$

For $\beta \in (\beta_*,1)$, Q_β can be chosen such that, as β tends to 1, *it tends to the profile*

$$Q_+ : (x, y, s) \in \mathbb{H}^1 \mapsto \frac{\sqrt{2}i}{s + i(x^2 + y^2) + i}$$

and so that the map $\beta \in (\beta_*, 1) \mapsto Q_\beta \in \dot{H}^1(\mathbb{H}^1)$ *is smooth. Moreover, for all* $\gamma \in (0, \frac{1}{4})$ *and all* $k \in [1, \infty)$*,* Q_β *lies in* $\dot{H}^k(\mathbb{H}^1)$*, and as* β *tends to* 1*,*

$$\|Q_\beta - Q_+\|_{\dot{H}^k(\mathbb{H}^1)} = \mathcal{O}((1-\beta)^\gamma).$$

We refer to Theorem 5.14 for a more precise statement.

Note that the energy of the traveling waves u_β, which have been defined in (2), vanishes as β goes to 1, indeed, $\|u_\beta\|_{\dot{H}^1(\mathbb{H}^1)} = \sqrt{1-\beta}\|Q_\beta\|_{\dot{H}^1(\mathbb{H}^1)} \to 0$. This is similar to the cubic half-wave equation, for which the critical norm $\|u_\beta\|_{L^2(\mathbb{R})}$ vanishes as β goes to 1 [Krieger et al. 2013].

We now briefly present the emergence of the profile Q_+ as a ground state solution to a limiting system and the key ingredient for the proof of Theorem 1.1, which relies on the study of the limiting geometry.

We are interested in radial solutions with values in the homogeneous energy space $\dot{H}^1(\mathbb{H}^1)$, which is a Hilbert space endowed with the real scalar product

$$(u, v)_{\dot{H}^1(\mathbb{H}^1)} = \operatorname{Re}\left(\int_{\mathbb{H}^1} -\Delta_{\mathbb{H}^1} u(x, y, s)\overline{v(x, y, s)}\, \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}s\right).$$

For $u \in \dot{H}^{-1}(\mathbb{H}^1)$ and $v \in \dot{H}^1(\mathbb{H}^1)$, we will also make use of the duality product

$$(u, v)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} = \operatorname{Re}\left(\int_{\mathbb{H}^1} u(x, y, s)\overline{v(x, y, s)}\, \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}s\right).$$

Up to the three symmetries (translation, phase multiplication, scaling), one can show convergence as β tends to 1 of the profiles Q_β to some profile Q_+ in $\dot{H}^1(\mathbb{H}^1)$. Then, Q_+ is a ground state solution to

$$D_s Q_+ = \Pi_0^+(|Q_+|^2 Q_+), \quad D_s = -i\partial_s. \tag{4}$$

The operator Π_0^+ is an orthogonal projector from $L^2(\mathbb{H}^1)$ onto a subspace $L^2(\mathbb{H}^1) \cap V_0^+$, which will be defined in Section 2B. In order to study this projector and the space $L^2(\mathbb{H}^1) \cap V_0^+$, we introduce a link between the space $L^2(\mathbb{H}^1) \cap V_0^+$ and the Bergman space $L^2(\mathbb{C}_+) \cap \operatorname{Hol}(\mathbb{C}_+)$ on the complex upper half-plane [Békollé et al. 2004]. The orthogonal projection Π_0^+ from $L^2(\mathbb{H}^1)$ onto $L^2(\mathbb{H}^1) \cap V_0^+$ then matches with a Bergman projector. This projection is a simplification of the usual Cauchy–Szegő projector for the Heisenberg group in the radial case.

A salutary fact is that the profile Q_+ can be determined explicitly and is unique up to symmetry (see Section 3C):

$$Q_+(x, y, s) = \frac{\sqrt{2}i}{s + i(x^2 + y^2) + i}.$$

Our key result is the coercivity of the linearized operator $\mathcal{L}$ around Q_+ on the orthogonal of a finite-dimensional manifold in some subspace $\dot{H}^1(\mathbb{H}^1) \cap V_0^+$ of $\dot{H}^1(\mathbb{H}^1)$ (see Section 2B). On $\dot{H}^1(\mathbb{H}^1) \cap V_0^+$, the linearized operator $\mathcal{L}$ around Q_+ is defined by

$$\mathcal{L}h = D_s h - 2\Pi_0^+(|Q_+|^2 h) - \Pi_0^+(Q_+^2 \bar{h}).$$

Theorem 1.2. *For some constant $c > 0$, the following holds: Let $h \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+$, and suppose h is orthogonal to the directions $Q_+, iQ_+, \partial_s Q_+$ and $i\partial_s Q_+$ in the Hilbert space $\dot{H}^1(\mathbb{H}^1)$. Then*

$$(\mathcal{L}h, h)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} \geq c\|h\|^2_{\dot{H}^1(\mathbb{H}^1)}.$$

In particular, the linearized operator $\mathcal{L}$ is nondegenerate in the sense that its kernel is composed only of three directions coming from the three symmetries of the equation

$$\operatorname{Ker}(\mathcal{L}) = \operatorname{Vect}_{\mathbb{R}}(\partial_s Q_+, iQ_+, Q_+ + 2i\partial_s Q_+).$$

Following the approach employed in the study of the half-wave equation [Gérard et al. 2018], one can then prove the invertibility of the linearized operators $\mathcal{L}_{Q_\beta}$ for the Schrödinger equation around the profiles Q_β for β close enough to 1. In order to do so, we need to combine the above coercivity result with some regularity estimates and decay properties for Q_β. This enables us to achieve our goal, which is the uniqueness of these profiles up to symmetries for β close to 1.

Stereographic projection and Cayley transform. Conclusive information on the linearized operator $\mathcal{L}$ around Q_+ is not easy to obtain directly. Indeed, the operator $\mathcal{L}$ is self-adjoint acting on $L^2(\mathbb{H}^1)$, but the space we consider is the Hilbert space $\dot{H}^1(\mathbb{H}^1)$. In order to get a coercivity estimate, we rely on a conformal invariance between the Heisenberg group $\mathbb{H}^1$ and the CR sphere $\mathbb{S}^3$ in $\mathbb{C}^2$ called the Cayley transform

$$\mathcal{C}: \mathbb{H}^1 \to \mathbb{S}^3 \setminus (0,-1), \quad (w,s) \mapsto \left(\frac{2w}{1+|w|^2+is}, \frac{1-|w|^2-is}{1+|w|^2+is}\right),$$

where $\mathbb{H}^1$ is parametrized by the complex number $w = x+iy$ and by s.

This transformation links estimates for the linearized operator $\mathcal{L}$ to the spectrum of the sub-Laplacian on the CR sphere, which is explicit [Stanton 1989]. Potential negative eigenvalues are discarded by the orthogonality conditions from Theorem 1.2. This latter step follows from technical but direct calculations.

For the n-dimensional Heisenberg group $\mathbb{H}^n$, the Cayley transform gives an equivalence between $\mathbb{H}^n$ and the CR sphere $\mathbb{S}^{2n+1}$ in $\mathbb{C}^n$. This transform is the counterpart of the stereographic projection, which links the space $\mathbb{R}^n$ with the euclidean sphere $\mathbb{S}^n$ in $\mathbb{R}^{n+1}$. Both transformations have been a useful tool in the study of fractional Folland–Stein inequalities on $\mathbb{H}^n$ and fractional Sobolev inequalities in $\mathbb{R}^n$, as we will now recall.

On the space $\mathbb{R}^n$, Lieb [1983] characterized all optimizers for the fractional Sobolev embeddings $\dot{H}^k(\mathbb{R}^n) \hookrightarrow L^p(\mathbb{R}^n)$, $0 < k < n/2$, $p = 2n/(n-2k)$, as the set of functions which, up to translation, dilation and multiplication by a nonzero constant, coincide with

$$U(x) = \frac{1}{(1+|x|^2)^{(n-2k)/2}}, \quad U \in \dot{H}^k(\mathbb{R}^n).$$

Stereographic projection appears in Lieb's paper in order to show that these functions are actually optimizers. The formula for U was first established with different methods for $k = 2$ and $n = 3$ by Rosen [1971], and then for $k = 1$ and arbitrary n by Aubin [1976] and Talenti [1976].

Stereographic projection also appears in the proofs of nondegeneracy of the optimizers for the critical Sobolev embeddings, indeed, this transformation provides a simpler form of the eigenvalue problem when transferred to the unit sphere $\mathbb{S}^n$. In this spirit, Dávila, Del Pino and Sire [2013] proved the nondegeneracy of the linearized operator for the critical equation corresponding to the fractional Sobolev embeddings. Chen, Frank and Weth [2013] showed a quadratic estimate for the remainder terms for the equivalent fractional Hardy–Littlewood–Sobolev inequalities.

On the Heisenberg group $\mathbb{H}^n$, Frank and Lieb [2012b] determined the optimizers for the fractional Folland–Stein embeddings $\dot{H}^k(\mathbb{H}^n) \hookrightarrow L^p(\mathbb{H}^n)$, $0 < k < Q/2$, $p = 2Q/(Q-2k)$, $Q = 2n+2$, with the use of the Cayley transform. These optimizers are the functions equal, up to translations, dilations and multiplication by a constant, to

$$H(u) = \frac{1}{\big((1+\|w\|^2)^2+\|s\|^2\big)^{(Q-2k)/4}}, \quad H \in \dot{H}^k(\mathbb{H}^n).$$

Here, the notation $u = (w, s)$ uses the identification of $\mathbb{H}^n$ with $\mathbb{C}^n \times \mathbb{R}^n$. In [Frank and Lieb 2012a], the same authors proved that a similar approach with stereographic projection on $\mathbb{R}^n$ enables one to characterize the optimizers of the fractional Sobolev embeddings on $\mathbb{R}^n$. Liu and Zhang [2015] then carried the study of the remainder term to the complex sphere $\mathbb{S}^{2n+1}$ by using the Cayley transform. When $k = 1$, the optimizers were first determined by Jerison and Lee [1988], who already made use of the Cayley transform. One can notice that fixing $n = k = 1$, $u = (x, y, s) \in \mathbb{H}^1$, we get

$$H(u) = \frac{1}{\big((1+x^2+y^2)^2+s^2\big)^{\frac{1}{2}}}.$$

Therefore, up to multiplication by a constant, H coincides with $|Q_+|$, where Q_+ is the ground state we are interested in. In fact, the profile Q_+ is an optimizer for the Folland–Stein inequality $\dot{H}^1(\mathbb{H}^1) \hookrightarrow L^4(\mathbb{H}^1)$ restricted to the subspace $\dot{H}^1(\mathbb{H}^1) \cap V_0^+$.

Plan of the paper. In Section 3, we prove the existence of the profiles Q_β and their convergence to a ground state solution to the limiting system (4). We then determine all the limiting profiles (Section 3C); in particular, we show that they are unique up to symmetries. In Section 4, we focus on the linear stability of the limiting profile Q_+. After recalling some results about orthogonal projections on Bergman spaces (Section 4A) and about the spectrum of the sub-Laplacian on the CR sphere (Section 4C), we prove the coercivity of the linearized operator around Q_+. Finally, in Section 5, we retrieve the uniqueness of the profiles Q_β up to symmetries for β close to 1. In order to do so, we first need to collect some regularity properties and decay estimates on the profiles Q_β, which come from the theory of elliptic and hypoelliptic equations (Section 5A).

2. Notation

2A. ***The Heisenberg group.*** We recall some facts about the Heisenberg group. We identify the Heisenberg group $\mathbb{H}^1$ with $\mathbb{R}^3$. The group multiplication is given by

$$(x, y, s) \cdot (x', y', s') = \big(x + x', y + y', s + s' + 2(x'y - xy')\big).$$

The Lie algebra of left-invariant vector fields on $\mathbb{H}^1$ is spanned by the vector fields $X = \partial_x + 2y\partial_s$, $Y = \partial_y - 2x\partial_s$ and $T = \partial_s = \frac{1}{4}[Y, X]$. The sub-Laplacian is defined as

$$\mathcal{L}_0 := \tfrac{1}{4}(X^2 + Y^2) = \tfrac{1}{4}(\partial_x^2 + \partial_y^2) + (x^2 + y^2)\partial_s^2 + (y\partial_x - x\partial_y)\partial_s.$$

When u is a radial function, the sub-Laplacian coincides with the operator

$$\Delta_{\mathbb{H}^1} := \tfrac{1}{4}(\partial_x^2 + \partial_y^2) + (x^2 + y^2)\partial_s^2.$$

The space $\mathbb{H}^1$ is endowed with a smooth left invariant measure, the Haar measure, which in the coordinate system (x, y, s) is the Lebesgue measure $d\lambda_3(x, y, s)$. Sobolev spaces of positive order can then be constructed on $\mathbb{H}^1$ from powers of the operator $-\Delta_{\mathbb{H}^1}$; for example, $\dot{H}^1(\mathbb{H}^1)$ is the completion of the Schwarz space $\mathscr{S}(\mathbb{H}^1)$ for the norm

$$\|u\|_{\dot{H}^1(\mathbb{H}^1)} := \|(-\Delta_{\mathbb{H}^1})^{\frac{1}{2}} u\|_{L^2(\mathbb{H}^1)}.$$

The distance between two points (x, y, s) and (x', y', s') in $\mathbb{H}^1$ is defined as

$$d((x, y, s), (x', y', s')) := \big(((x - x')^2 + (y - y')^2)^2 + (s - s' + 2(x'y - xy'))^2\big)^{\frac{1}{4}}.$$

For convenience, the distance to the origin is denoted by

$$\rho(x, y, s) := \big((x^2 + y^2)^2 + s^2\big)^{\frac{1}{4}}.$$

2B. ***Decomposition along the Hermite functions.*** In order to study radial functions valued on the Heisenberg group $\mathbb{H}^1$, it is convenient to use their decomposition along Hermite-type functions (see, for example, [Stein 1993], Chapters 12 and 13). The Hermite functions

$$h_m(x) = \frac{1}{\pi^{\frac{1}{4}} 2^{\frac{m}{2}} (m!)^{\frac{1}{2}}} (-1)^m \, e^{\frac{x^2}{2}} \partial_x^m (e^{-x^2}), \quad x \in \mathbb{R}, m \in \mathbb{N},$$

form an orthonormal basis of $L^2(\mathbb{R})$. In $L^2(\mathbb{R}^2)$, the family of products of two Hermite functions $(h_m(x)h_p(y))_{m,p\in\mathbb{N}}$ diagonalizes the two-dimensional harmonic oscillator: for all $m, p \in \mathbb{N}$,

$$(-\Delta_{x,y} + x^2 + y^2)h_m(x)h_p(y) = 2(m + p + 1)h_m(x)h_p(y).$$

Given $u \in \mathscr{S}(\mathbb{H}^1)$, we will denote by $\hat{u}$ its usual Fourier transform under the variable s, with corresponding variable σ:

$$\hat{u}(x, y, \sigma) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-is\sigma} u(x, y, s) \, ds.$$

For $m, p \in \mathbb{N}$, set $\hat{h}_{m,p}(x, y, \sigma) := h_m(\sqrt{2|\sigma|}\, x) h_p(\sqrt{2|\sigma|}\, y)$. Then

$$\widehat{\Delta_{\mathbb{H}^1} h_{m,p}} = -(m + p + 1)\, |\sigma| \, \hat{h}_{m,p}.$$

Let $k \in \{-1, 0, 1\}$, and denote by $\dot{H}^k(\mathbb{H}^1) \cap V_n^{\pm}$ the subspace of functions in $\dot{H}^k(\mathbb{H}^1)$ spanned by $\{h_{m,p} : m, p \in \mathbb{N}, m + p = n\}$. A function $u_n^{\pm} \in \dot{H}^k(\mathbb{H}^1)$ belongs to $\dot{H}^k(\mathbb{H}^1) \cap V_n^{\pm}$ if there exist functions $f^{\pm}_{m,p}$ such that

$$\hat{u}^{\pm}_n(x,y,\sigma) = \sum_{\substack{m,p\in\mathbb{N}\\ m+p=n}} f^{\pm}_{m,p}(\sigma)\hat{h}_{m,p}(x,y,\sigma)\mathbb{1}_{\sigma\gtrless 0}.$$

For $u^{\pm}_n \in \dot{H}^k(\mathbb{H}^1)\cap V^{\pm}_n$, the $\dot{H}^k$ norm of $u^{\pm}_n$ has the form

$$\begin{aligned}\|u^{\pm}_n\|^2_{\dot{H}^k(\mathbb{H}^1)} &= \int_{\mathbb{R}_\pm}((n+1)|\sigma|)^k \int_{\mathbb{R}^2} |\hat{u}^{\pm}_n(x,y,\sigma)|^2\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}\sigma \\ &= \sum_{\substack{m,p\in\mathbb{N}\\ m+p=n}} \int_{\mathbb{R}_\pm}((n+1)|\sigma|)^k |f^{\pm}_{m,p}(\sigma)|^2 \frac{\mathrm{d}\sigma}{2|\sigma|}.\end{aligned}$$

Any function $u\in\dot{H}^k(\mathbb{H}^1)$ admits a decomposition along the orthogonal sum of subspaces $\dot{H}^k(\mathbb{H}^1)\cap V^{\pm}_n$. Let us write $u=\sum_{\pm}\sum_{n\in\mathbb{N}} u^{\pm}_n$, where $u^{\pm}_n\in\dot{H}^k(\mathbb{H}^1)\cap V^{\pm}_n$ for all $(n,\pm)$. Then

$$\|u\|^2_{\dot{H}^k(\mathbb{H}^1)} = \sum_{\pm}\sum_{n\in\mathbb{N}} \|u^{\pm}_n\|^2_{\dot{H}^k(\mathbb{H}^1)}.$$

Note that rotations of the (x,y) variable commute with $-\Delta_{\mathbb{H}^1}$, so $u\in\dot{H}^k(\mathbb{H}^1)$ is radial if and only if for all $(n,\pm)$, $u^{\pm}_n$ is radial. Moreover, $u\in\dot{H}^k(\mathbb{H}^1)$ belongs to $\dot{H}^k(\mathbb{H}^1)\cap V^{\pm}_n$ if and only if $-\Delta_{\mathbb{H}^1}u$ belongs to $\dot{H}^{k-2}(\mathbb{H}^1)\cap V^{\pm}_n$, and the same holds for $D_s u$.

For $k=0$, we get an orthogonal decomposition of the space $L^2(\mathbb{H}^1)$, and denote by $\Pi^{\pm}_n$ the associated orthogonal projectors.

The particular space $\dot{H}^k(\mathbb{H}^1)\cap V^+_0$ will be especially interesting in our discussion below. This space is spanned by a unique radial function h^+_0, satisfying

$$\hat{h}^+_0(x,y,\sigma) = \frac{1}{\sqrt{\pi}}\,\mathrm{e}^{-(x^2+y^2)\sigma}\mathbb{1}_{\sigma\geq 0}.$$

Set $u\in\dot{H}^k(\mathbb{H}^1)\cap V^+_0$, then there exists f such that

$$\hat{u}(x,y,s) = f(\sigma)\hat{h}^+_0(x,y,\sigma),$$

and in this case

$$\|u\|^2_{\dot{H}^k(\mathbb{H}^1)} = \int_{\mathbb{R}_+} |f(\sigma)|^2\frac{\mathrm{d}\sigma}{2\sigma^{1-k}}.$$

3. Existence of traveling waves and limiting profile

In this subsection we prove the existence of ground states Q_β for equation (3) with speed $\beta\in(-1,1)$ (Section 3A), and we will show the convergence in $\dot{H}^1(\mathbb{H}^1)$ of the profiles Q_β to a limiting profile Q_+ as β tends to 1 (Section 3B). The profile Q_+ is a ground state solution of equation (4), which will be determined explicitly (Section 3C).

3A. ***Existence of traveling waves with speed $\beta \in (-1,1)$.*** A family of traveling wave solutions to the Schrödinger equation on the Heisenberg group (1) can be found under the form

$$u(t,x,y,s) = Q_\beta\left(\frac{x}{\sqrt{1-\beta}}, \frac{y}{\sqrt{1-\beta}}, \frac{s+\beta t}{1-\beta}\right),$$

with Q_β satisfying the equation

$$-\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} Q_\beta = |Q_\beta|^2 Q_\beta.$$

The Q_β are constructed as minimizers of some Gagliardo–Nirenberg inequalities. We will be adapting the proofs of Krieger, Lenzmann and Raphaël [Krieger et al. 2013] which concern the L^2-critical half-wave equation on the real line. Our starting point is the Folland–Stein embedding:

Theorem 3.1 [Folland and Stein 1974]. *Let $p \in (1,4)$, and set $p^* = \dfrac{4p}{4-p}$. Then there exists $C_p > 0$ such that for $u \in \mathcal{C}_c^\infty(\mathbb{H}^1)$,*

$$\left(\int_{\mathbb{H}^1} |u(x,y,s)|^{p^*}\,dx\,dy\,ds\right)^{\frac{1}{p^*}} \le C_p\left(\int_{\mathbb{H}^1} |(-\Delta_{\mathbb{H}^1})^{\frac12} u(x,y,s)|^p\,dx\,dy\,ds\right)^{\frac1p}.$$

In particular, from the embedding $\dot H^1(\mathbb{H}^1) \hookrightarrow L^4(\mathbb{H}^1)$, we deduce some Gagliardo–Nirenberg inequalities.

Proposition 3.2 (Gagliardo–Nirenberg). *Set $\beta \in (-1,1)$. Then there exists some constant $C > 0$ such that for every $u \in \dot H^1(\mathbb{H}^1)$,*

$$\|u\|_{L^4(\mathbb{H}^1)}^4 \le C(-(\Delta_{\mathbb{H}^1} + \beta D_s)u, u)^2_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)}.$$

Proof. Fix $u \in \dot H^1(\mathbb{H}^1)$, and decompose u along the spaces $V_n^+ \cup V_n^-$ as $u = \sum_{n\in\mathbb{N}} u_n$, where $u_n = u_n^+ + u_n^-$. Then

$$(-(\Delta_{\mathbb{H}^1} + \beta D_s)u, u)_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)} = \sum_{n\in\mathbb{N}} \int_{\mathbb{R}^3} \big((n+1)|\sigma| - \beta\sigma\big)|\hat u_n(x,y,\sigma)|^2\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}\sigma,$$

$$\|u\|^2_{\dot H^1(\mathbb{H}^1)} = \sum_{n\in\mathbb{N}} \int_{\mathbb{R}^3} (n+1)|\sigma|\,|\hat u_n(x,y,\sigma)|^2\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}\sigma.$$

We deduce the equivalence of norms

$$(1-|\beta|)\|u\|^2_{\dot H^1(\mathbb{H}^1)} \le (-(\Delta_{\mathbb{H}^1} + \beta D_s)u, u)_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)} \le (1+|\beta|)\|u\|^2_{\dot H^1(\mathbb{H}^1)}. \tag{5}$$

The result follows from the Folland–Stein embedding $\dot H^1(\mathbb{H}^1) \hookrightarrow L^4(\mathbb{H}^1)$. □

From the Gagliardo–Nirenberg inequalities, one knows that the infimum over nonzero radial functions $u \in \dot H^1(\mathbb{H}^1)$ of the functional

$$J_\beta(u) := \frac{(-(\Delta_{\mathbb{H}^1} + \beta D_s)u, u)^2_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)}}{\|u\|^4_{L^4}}$$

is positive. Let us denote by I_β the minimal value of J_β. We want to show that it is attained by some $Q_\beta \in \dot{H}^1(\mathbb{H}^1)$. We consider a minimizing sequence for J_β. Then this sequence converges to a minimizer for J_β thanks to the following profile decomposition theorem:

Definition 3.3. The scaling-core pairs $((\tilde{h}_i)_{i\in\mathbb{N}}, (\tilde{s}_i)_{i\in\mathbb{N}})$ and $((h_i)_{i\in\mathbb{N}}, (s_i)_{i\in\mathbb{N}})$ of $(\mathbb{R}_+^*)^{\mathbb{N}} \times \mathbb{R}^{\mathbb{N}}$ are said to be *strange* if

$$\left(\left|\log \frac{\tilde{h}_n}{h_n}\right| \underset{n\to\infty}{\longrightarrow} \infty\right) \text{ or } \left((\tilde{h}_n)_n = (h_n)_n \text{ and } \frac{|\tilde{s}_n - s_n|}{h_n^2} \underset{n\to\infty}{\longrightarrow} \infty\right).$$

Theorem 3.4 (concentration-compactness). *Fix a bounded sequence $\underline{u} = (u_n)_{n\in\mathbb{N}}$ of radial functions in $\dot{H}^1(\mathbb{H}^1)$. Then there exist a subsequence $(u_{n_i})_{i\in\mathbb{N}}$ of $\underline{u}$ and sequences of cores $(s_{n_i}^{(j)})_{i,j\in\mathbb{N}} \subset \mathbb{R}$, scalings $(h_{n_i}^{(j)})_{i,j\in\mathbb{N}} \subset \mathbb{R}$, and radial functions $(U^{(j)})_{j\in\mathbb{N}} \subset \dot{H}^1(\mathbb{H}^1)$ satisfying these conditions*:

(1) *The pairs $\big((h_{n_i}^{(j)})_i, (s_{n_i}^{(j)})_i\big)$, $j \in \mathbb{N}$, are pairwise strange.*

(2) *Let* $r_{n_i}^{(l)}(x, y, s) = u_{n_i}(x, y, s) - \sum_{j=1}^{l} \frac{1}{h_{n_i}^{(j)}} U^{(j)}\left(\frac{x}{h_{n_i}^{(j)}}, \frac{y}{h_{n_i}^{(j)}}, \frac{s - s_{n_i}^{(j)}}{(h_{n_i}^{(j)})^2}\right)$. *Then*

$$\lim_{l\to\infty} \limsup_{i\to\infty} \|r_{n_i}^{(l)}\|_{L^4(\mathbb{H}^1)} = 0.$$

Moreover, for all $l \geq 1$, one has the following orthogonality relations as i goes to ∞:

$$\|u_{n_i}\|^2_{\dot{H}^1(\mathbb{H}^1)} = \sum_{j=1}^{l} \|U^{(j)}\|^2_{\dot{H}^1(\mathbb{H}^1)} + \|r_{n_i}^{(l)}\|^2_{\dot{H}^1(\mathbb{H}^1)} + o(1),$$

$$(D_s u_{n_i}, u_{n_i})_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} = \sum_{j=1}^{l} (D_s U^{(j)}, U^{(j)})_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} + (D_s r_{n_i}^{(l)}, r_{n_i}^{(l)})_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} + o(1),$$

$$\|u_{n_i}\|^4_{L^4(\mathbb{H}^1)} \underset{i\to\infty}{\longrightarrow} \sum_{j=1}^{\infty} \|U^{(j)}\|^4_{L^4(\mathbb{H}^1)}.$$

This result is an adaptation of a concentration-compactness argument from [Cazenave and Lions 1982], which was refined into a profile decomposition theorem as above by Gérard [1998] for Sobolev spaces on $\mathbb{R}^n$. One can find a proof of this profile decomposition theorem for Sobolev spaces on the Heisenberg group in [Benameur 2008], which is here restricted to the subspace of radial functions.

3B. *The limit $\beta \to 1^-$.* In this section, we study the behavior of the traveling waves Q_β as β tends to the limit 1^-. We show that these traveling waves converge up to symmetries to a limiting profile. The strategy is similar to [Gérard et al. 2018] for the half-wave equation.

For $\beta \in (-1, 1)$, let Q_β be a minimizer of J_β: $I_\beta = J_\beta(Q_\beta)$. Up to a change of functions $Q_\beta \rightsquigarrow \alpha Q_\beta$, one can choose Q_β such that

$$\frac{(-(\Delta_{\mathbb{H}^1} + \beta D_s) Q_\beta, Q_\beta)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}}{1-\beta} = \|Q_\beta\|^4_{L^4(\mathbb{H}^1)},$$

so that Q_β is a solution to (3).

Definition 3.5 (minimizers in $\mathcal{Q}_\beta$). For all $\beta \in (-1,1)$, denote by $\mathcal{Q}_\beta$ the set of minimizers Q_β of $J_\beta : u \mapsto (-(\Delta_{\mathbb{H}^1} + \beta D_s)u, u)^2_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} / \|u\|^4_{L^4}$ which satisfy

$$\frac{(-(\Delta_{\mathbb{H}^1} + \beta D_s)Q_\beta, Q_\beta)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}}{1-\beta} = \|Q_\beta\|^4_{L^4} = \frac{I_\beta}{(1-\beta)^2}, \quad I_\beta = J_\beta(Q_\beta). \tag{6}$$

Note that equation (3) is satisfied for $Q_\beta \in \mathcal{Q}_\beta$.

Definition 3.6 (minimizers in $\mathcal{Q}_+$). For all radial functions $u \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+ \setminus \{0\}$ whose Fourier transform has a nonzero component only along the Hermite-type function $\hat{h}_0^+$, define

$$J_+(u) := \frac{\|u\|^4_{\dot{H}^1(\mathbb{H}^1)}}{\|u\|^4_{L^4(\mathbb{H}^1)}}$$

(note that $-\Delta_{\mathbb{H}^1} = D_s$ on the space $\dot{H}^1(\mathbb{H}^1) \cap V_0^+$). Denote by I_+ its infimum:

$$I_+ := \inf\{J_+(u) : u \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+ \setminus \{0\}\}.$$

Let $\mathcal{Q}_+$ be the set of minimizers Q_+ of J_+ such that

$$\|Q_+\|^2_{\dot{H}^1(\mathbb{H}^1)} = \|Q_+\|^4_{L^4(\mathbb{H}^1)} = I_+, \quad I_+ = J_+(Q_+).$$

Then any $Q_+ \in \mathcal{Q}_+$ is a solution to (4):

$$D_s Q_+ = \Pi_0^+(|Q_+|^2 Q_+).$$

The minimum I_+ is attained and positive. The proof is similar to the one for I_β; we just need to restrict the profile decomposition theorem to the closed subspace $\dot{H}^1(\mathbb{H}^1) \cap V_0^+$ of $\dot{H}^1(\mathbb{H}^1)$.

The term $\Pi_0^+(|Q_+|^2 Q_+)$ may not seem suitable since $|Q_+|^2 Q_+$ belongs to $L^{\frac{4}{3}(\mathbb{H}^1)} \hookrightarrow \dot{H}^{-1}(\mathbb{H}^1)$, whereas Π_0^+ is a projector defined on $L^2(\mathbb{H}^1)$. Later arguments, however, will show that things work out: we will see in Section 3C that $|Q_+|^2 Q_+ \in L^2(\mathbb{H}^1)$, and in Theorem 4.6. that the projector Π_0^+ extends to $L^p(\mathbb{H}^1)$ for all $p > 1$.

The convergence result is as follows:

Theorem 3.7 (convergence). *For all $\beta \in (-1,1)$, fix $Q_\beta \in \mathcal{Q}_\beta$. Then, there exist a subsequence $\beta_n \to 1^-$, scalings $(\alpha_n)_{n\in\mathbb{N}} \in (\mathbb{R}_+^*)^{\mathbb{N}}$, cores $(s_n)_{n\in\mathbb{N}} \in \mathbb{R}^{\mathbb{N}}$ and a function $Q_+ \in \mathcal{Q}_+$ such that*

$$\left\|\alpha_n Q_{\beta_n}(\alpha_n \cdot, \alpha_n \cdot, \alpha_n^2(\cdot + s_n)) - Q_+\right\|_{\dot{H}^1(\mathbb{H}^1)} \underset{n\to\infty}{\longrightarrow} 0.$$

We introduce the quantity $\delta(u)$, which quantifies the gap between the norms of a function u in $\dot{H}^1(\mathbb{H}^1)$ and those of the profiles $Q_+ \in \mathcal{Q}_+$. We prove that $\delta(Q_\beta)$ is small and then show that $\delta(u)$ controls the distance up to symmetries from u to the profiles Q_+ in $\mathcal{Q}_+$.

Definition 3.8. For $u \in \dot{H}^1(\mathbb{H}^1)$, define

$$\delta(u) = \left|\|u\|^2_{\dot{H}^1(\mathbb{H}^1)} - I_+\right| + \left|\|u\|^4_{L^4(\mathbb{H}^1)} - I_+\right|.$$

We first show a lemma about $\delta(Q_\beta)$, $Q_\beta \in \mathcal{Q}_\beta$.

Lemma 3.9. *There exist $C > 0$ and $\beta_* \in (0,1)$ such that the following holds: For all $\beta \in (\beta_*, 1)$ fix $Q_\beta \in \mathcal{Q}_\beta$, and decompose Q_β along the Hermite-type functions from Section 2B,*

$$Q_\beta = Q_\beta^+ + R_\beta,$$

where $Q_\beta^+ \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+$ and $R_\beta \in \dot{H}^1(\mathbb{H}^1) \cap \bigoplus_{(n,\pm)\neq(0,+)} V_n^\pm$. Then $\|R_\beta\|_{\dot{H}^1(\mathbb{H}^1)} \le C(1-\beta)^{\frac{1}{2}}$, $\delta(Q_\beta^+) \le C(1-\beta)^{\frac{1}{2}}$ and $\delta(Q_\beta) \le C(1-\beta)^{\frac{1}{2}}$.

Proof. Fix $u \in \dot{H}^1(\mathbb{H}^1)$. Thanks to inequality (5), one knows that $I_\beta \ge (1-\beta)^2 I_0$ when $\beta \in (0,1)$. Furthermore, let $Q_+ \in \mathcal{Q}_+$. Then, using the fact that $-\Delta_{\mathbb{H}^1} Q_+ = D_s Q_+$,

$$I_\beta \le J_\beta(Q_+) = \frac{(1-\beta)^2 (D_s Q_+, Q_+)^2_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}}{\|Q_+\|^4_{L^4}} = (1-\beta)^2 I_+.$$

Consequently, $\left(\frac{I_\beta}{(1-\beta)^2}\right)_\beta$ is bounded above and below:

$$I_0 \le \frac{I_\beta}{(1-\beta)^2} \le I_+.$$

We will show that actually $\frac{I_\beta}{(1-\beta)^2} \to I_+$ as β tends to 1.

Let us decompose a minimizer $Q_\beta \in \mathcal{Q}_\beta$ along the Hermite-type functions from Section 2B:

$$Q_\beta = Q_\beta^+ + R_\beta,$$

where $Q_\beta^+ \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+$ and $R_\beta \in \dot{H}^1(\mathbb{H}^1) \cap \bigoplus_{(n,\pm)\neq(0,+)} V_n^\pm$ is a remainder term which will go to zero.

Multiplying (3) by $\overline{R_\beta}$, we get that for all n,

$$\left(-\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} Q_\beta, R_\beta\right)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} = (|Q_\beta|^2 Q_\beta, R_\beta)_{L^{\frac{4}{3}}(\mathbb{H}^1)\times L^4(\mathbb{H}^1)}.$$

Since the operators $\Delta_{\mathbb{H}^1}$ and D_s let invariant the spaces $V_n^\pm$, we can replace Q_β by R_β in the left term of the equality

$$\left(-\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} R_\beta, R_\beta\right)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} = (|Q_\beta|^2 Q_\beta, R_\beta)_{L^{\frac{4}{3}}(\mathbb{H}^1)\times L^4(\mathbb{H}^1)}.$$

Applying Hölder's inequality, we deduce that

$$\left(-\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} R_\beta, R_\beta\right)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} \le \|Q_\beta\|^3_{L^4(\mathbb{H}^1)} \|R_\beta\|_{L^4(\mathbb{H}^1)}. \tag{7}$$

We now write more precisely the equivalence between the norms

$$\|u\|_{\dot{H}^1(\mathbb{H}^1)} \quad \text{and} \quad (-(\Delta_{\mathbb{H}^1} + \beta D_s)u, u)^{\frac{1}{2}}_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}.$$

The left inequality in (5) can be controlled with sharper constants which do not depend on β when we require the function $u \in \dot{H}^1(\mathbb{H}^1)$ to have a zero component u_0^+. Indeed, we have $n+1-\beta \geq n \geq \frac{n+1}{2}$ when $n \geq 1$, and $n+1+\beta \geq n+1 \geq \frac{n+1}{2}$ when $n \geq 0$. We deduce that for all $u \in \dot{H}^1(\mathbb{H}^1) \cap \bigoplus_{(n,\pm)\neq(0,+)} V_n^\pm$, decomposing u as $u = \sum_{(n,\pm)\neq(0,+)} u_n^\pm, u_n^\pm \in \dot{H}^1(\mathbb{H}^1) \cap V_n^\pm$,

$$\begin{aligned}(-(\Delta_{\mathbb{H}^1} + \beta D_s)u, u)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} &= \sum_{(n,\pm)\neq(0,0)} \int_{\mathbb{R}^3} \big((n+1)|\sigma| - \beta\sigma\big)\, |\hat{u}_n^\pm(x,y,\sigma)|^2 \,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}\sigma \\ &\geq \frac{1}{2} \sum_{(n,\pm)\neq(0,0)} \int_{\mathbb{R}^3} (n+1)|\sigma|\, |\hat{u}_n^\pm(x,y,\sigma)|^2 \,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}\sigma.\end{aligned}$$

This implies the inequality

$$\|u\|^2_{\dot{H}^1(\mathbb{H}^1)} \leq 2(-(\Delta_{\mathbb{H}^1} + \beta D_s)u, u)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}, \quad u \in \dot{H}^1(\mathbb{H}^1) \cap \bigoplus_{(n,\pm)\neq(0,+)} V_n^\pm, \tag{8}$$

which we can use for $u = R_\beta$. Combining this inequality and the Folland–Stein inequality $\|u\|_{L^4(\mathbb{H}^1)} \leq C\|u\|_{\dot{H}^1(\mathbb{H}^1)}$ in (7) , we get

$$\begin{aligned}&\Big(-\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} R_\beta, R_\beta\Big)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} \\ &\qquad\leq C\|Q_\beta\|^3_{L^4(\mathbb{H}^1)} \bigg(2(1-\beta)\Big(-\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} R_\beta, R_\beta\Big)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}\bigg)^{\frac{1}{2}},\end{aligned}$$

so

$$\Big(-\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} R_\beta, R_\beta\Big)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} \leq 2C^2(1-\beta)\|Q_\beta\|^6_{L^4(\mathbb{H}^1)}.$$

Since $(\|Q_\beta\|_{L^4(\mathbb{H}^1)})_\beta$ is bounded independently of β thanks to the norm conditions (6) and the boundedness of $\big(\frac{I_\beta}{(1-\beta)^2}\big)_\beta$, we deduce that as β goes to 1,

$$\Big(-\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} R_\beta, R_\beta\Big)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} = \mathcal{O}(1-\beta).$$

This implies immediately that $\|R_\beta\|_{\dot{H}^1}(\mathbb{H}^1)^2 = \mathcal{O}(1-\beta)$ and $\|R_\beta\|^2_{L^4(\mathbb{H}^1)} = \mathcal{O}(1-\beta)$. Using the orthogonal decomposition $Q_\beta = Q_\beta^+ + R_\beta$ in $\dot{H}^1(\mathbb{H}^1)$ and the fact that $-\Delta_{\mathbb{H}^1} = D_s$ on $\dot{H}^1(\mathbb{H}^1) \cap V_0^+$, we get

$$\begin{aligned}\|Q_\beta^+\|^2_{\dot{H}^1(\mathbb{H}^1)} &= \Big(-\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} Q_\beta^+, Q_\beta^+\Big)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} \\ &= \Big(-\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} Q_\beta, Q_\beta\Big)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} + \mathcal{O}(1-\beta) \\ &= \frac{I_\beta}{(1-\beta)^2} + \mathcal{O}(1-\beta),\end{aligned}$$

$$\|Q_\beta^+\|^4_{L^4(\mathbb{H}^1)} = \|Q_\beta\|^4_{L^4(\mathbb{H}^1)} + \mathcal{O}((1-\beta)^{\frac{1}{2}}) = \frac{I_\beta}{(1-\beta)^2} + \mathcal{O}((1-\beta)^{\frac{1}{2}}).$$

We can now prove that $\frac{I_\beta}{(1-\beta)^2} \to I_+$ as $\beta \to 1^-$. From the definition of I_+ as a minimum on

$\dot{H}^1(\mathbb{H}^1) \cap V_0^+$,

$$I_+ \le \frac{\|Q_\beta^+\|^4_{\dot{H}^1(\mathbb{H}^1)}}{\|Q_\beta^+\|^4_{L^4(\mathbb{H}^1)}} = \frac{\left(\frac{I_\beta}{(1-\beta)^2} + \mathcal{O}(1-\beta)\right)^2}{\frac{I_\beta}{(1-\beta)^2} + \mathcal{O}((1-\beta)^{\frac{1}{2}})} = \frac{I_\beta}{(1-\beta)^2}\left(1 + \mathcal{O}((1-\beta)^{\frac{1}{2}})\right).$$

We already know that $\frac{I_\beta}{(1-\beta)^2} \le I_+$ for all β, so we conclude that

$$\frac{I_\beta}{(1-\beta)^2} \underset{\beta \to 1^-}{\longrightarrow} I_+.$$

Therefore, the norms of Q_β^+ can be written as $\|Q_\beta^+\|^2_{\dot{H}^1(\mathbb{H}^1)} = I_+ + \mathcal{O}((1-\beta)^{\frac{1}{2}})$ and $\|Q_\beta^+\|^4_{L^4(\mathbb{H}^1)} = I_+ + \mathcal{O}((1-\beta)^{\frac{1}{2}})$. We conclude that

$$\delta(Q_\beta^+) = \mathcal{O}((1-\beta)^{\frac{1}{2}}) \quad \text{and} \quad \delta(Q_\beta) = \delta(Q_\beta^+ + R_\beta) = \mathcal{O}((1-\beta)^{\frac{1}{2}}). \qquad \square$$

The following stability result allows us to complete the proof of Theorem 3.7:

Proposition 3.10. *Fix a sequence $(u_n)_{n\in\mathbb{N}}$ of radial functions in $\dot{H}^1(\mathbb{H}^1) \cap V_0^+$. Suppose that $\delta(u_n) \to 0$ as $n \to \infty$. Then, up to a subsequence, there exist scalings $(\alpha_n)_{n\in\mathbb{N}} \in (\mathbb{R}_+^*)^{\mathbb{N}}$, cores $(s_n)_{n\in\mathbb{N}} \in \mathbb{R}^{\mathbb{N}}$ and a ground state $Q_+ \in \mathcal{Q}_+$ optimizing*

$$I_+ = \inf\left\{ J_+(u) = \frac{\|u\|^4_{\dot{H}^1(\mathbb{H}^1)}}{\|u\|^4_{L^4(\mathbb{H}^1)}} : u \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+ \setminus \{0\} \right\}$$

such that $\left\|\alpha_n u_n(\alpha_n \cdot, \alpha_n \cdot, \alpha_n^2(\cdot + s_n)) - Q_+\right\|_{\dot{H}^1(\mathbb{H}^1)} \to 0$ as $n \to \infty$.

Proof. Let $(u_n)_{n\in\mathbb{N}} \in (\dot{H}^1(\mathbb{H}^1) \cap V_0^+)^{\mathbb{N}}$ such that $\delta(u_n) \to 0$ as $n \to \infty$. Since $\dot{H}^1(\mathbb{H}^1) \cap V_0^+$ is a closed subspace of $\dot{H}^1(\mathbb{H}^1)$, one can restrict the concentration-compactness Theorem 3.4 to this subspace. In consequence, one can assume that the profiles $U^{(j)}$ from the theorem lie in $\dot{H}^1(\mathbb{H}^1) \cap V_0^+$. Hence, up to a subsequence, there exist a core sequence $(s_n^{(j)})_{n,j\in\mathbb{N}} \subset \mathbb{R}$, a scaling sequence $(h_n^{(j)})_{n,j\in\mathbb{N}} \subset \mathbb{R}$ and radial functions $(U^{(j)})_{j\in\mathbb{N}} \subset \dot{H}^1(\mathbb{H}^1) \cap V_0^+$ satisfying these conditions:

- For all $j, k \in \mathbb{N}$, $j \neq k$, the pairs $((h_n^{(j)})_n, (s_n^{(j)})_n)$ are pairwise strange.
- Let $r_n^{(l)}(x, y, s) = u_n(x, y, s) - \sum_{j=1}^{l} \frac{1}{h_n^{(j)}} U^{(j)}\left(\frac{x}{h_n^{(j)}}, \frac{y}{h_n^{(j)}}, \frac{s - s_n^{(j)}}{(h_n^{(j)})^2}\right)$, then

$$\lim_{l\to\infty} \limsup_{n\to\infty} \|r_n^{(l)}\|_{L^4(\mathbb{H}^1)} = 0.$$

Moreover, for all l, as n goes to ∞,

$$\|u_n\|^2_{\dot{H}^1(\mathbb{H}^1)} = \sum_{j=1}^{l} \|U^{(j)}\|^2_{\dot{H}^1(\mathbb{H}^1)} + \|r_n\|^2_{\dot{H}^1(\mathbb{H}^1)} + o(1) \tag{9}$$

and

$$\|u_n\|^4_{L^4(\mathbb{H}^1)} \underset{n\to\infty}{\longrightarrow} \sum_{j=1}^{\infty} \|U^{(j)}\|^4_{L^4(\mathbb{H}^1)}.$$

By construction, since $\delta(u_n)\to 0$, we have $\sum_{j=1}^{\infty}\|U^{(j)}\|^4_{\dot H^1(\mathbb{H}^1)}=I_+$ and $\sum_{j=1}^{\infty}\|U^{(j)}\|^2_{\dot H^1(\mathbb{H}^1)}\le I_+$, and $\|u_n\|^4_{\dot H^1(\mathbb{H}^1)}/\|u_n\|^4_{L^4(\mathbb{H}^1)}$ tends to I_+. But from the definition of I_+ as a minimum,

$$I_+^2\ge\Big(\sum_{j=1}^{\infty}\|U^{(j)}\|^2_{\dot H^1(\mathbb{H}^1)}\Big)^2\ge\sum_{j=1}^{\infty}\|U^{(j)}\|^4_{\dot H^1(\mathbb{H}^1)}\ge I_+\sum_{j=1}^{\infty}\|U^{(j)}\|^4_{\dot H^1(\mathbb{H}^1)}\ge I_+\sum_{j=1}^{\infty}\|U^{(j)}\|^4_{L^4(\mathbb{H}^1)}=I_+^2.$$

All the above inequalities must then be equalities.

In particular, only one of the profiles $U^{(j)}$ is allowed to be nonzero, we denote this profile by Q_+, and by r_n, h_n and s_n the corresponding rests, scalings and cores. Then Q_+ must be a ground state of the functional J_+, and

$$u_n(x,y,s)=\frac{1}{h_n}Q_+\Big(\frac{x}{h_n},\frac{y}{h_n},\frac{s-s_n}{h_n^2}\Big)+r_n(x,y,s).$$

From relation (9), as n goes to ∞,

$$\|u_n\|^2_{\dot H^1(\mathbb{H}^1)}=\|Q_+\|^2_{\dot H^1(\mathbb{H}^1)}+\|r_n\|^2_{\dot H^1(\mathbb{H}^1)}+o(1).$$

Since $\|u_n\|^2_{\dot H^1(\mathbb{H}^1)}$ must converge to $\|Q_+\|^2_{\dot H^1(\mathbb{H}^1)}$ because the inequalities turned to equalities, we get $\|r_n\|^2_{\dot H^1(\mathbb{H}^1)}\to 0$ as $n\to\infty$, and the sequence $h_nu_n(h_n\cdot,h_n\cdot,h_n^2(\cdot+s_n))$ converges to Q_+ in $\dot H^1(\mathbb{H}^1)$. □

Proof of Theorem 3.7. Consider the sequence $(Q_\beta^+)_{\beta\in(-1,1)}$ from Lemma 3.9. We know that $\delta(Q_\beta^+)=\mathcal{O}((1-\beta)^{\frac12})$. Applying Proposition 3.10, there exist a subsequence $(Q_{\beta_n}^+)_{n\in\mathbb{N}}$ with $\beta_n\to 1^-$ as $n\to\infty$, a core sequence $(s_n)_{n\in\mathbb{N}}\in\mathbb{R}^{\mathbb{N}}$, a scaling sequence $(\alpha_n)_{n\in\mathbb{N}}\in(\mathbb{R}_+^*)^{\mathbb{N}}$ and a ground state $Q_+\in\mathcal{Q}_+$ such that

$$\|\alpha_nQ_{\beta_n}^+(\alpha_n\cdot,\alpha_n\cdot,\alpha_n^2(\cdot+s_n))-Q_+\|_{\dot H^1(\mathbb{H}^1)}\underset{n\to\infty}{\longrightarrow}0.$$

To conclude, since $R_{\beta_n}=Q_{\beta_n}-Q_{\beta_n}^+$ satisfies $\|R_{\beta_n}\|_{\dot H^1(\mathbb{H}^1)}\to 0$ as $n\to\infty$, and since the $\dot H^1$ norm is invariant by translation and scaling, we deduce that

$$\|\alpha_nQ_{\beta_n}(\alpha_n\cdot,\alpha_n\cdot,\alpha_n^2(\cdot+s_n))-Q_+\|_{\dot H^1(\mathbb{H}^1)}\underset{n\to\infty}{\longrightarrow}0. \qquad \square$$

3C. *Ground state solutions to the limiting equation.* We now show that the optimizers for

$$I_+:=\inf\left\{\frac{\|u\|^4_{\dot H^1(\mathbb{H}^1)}}{\|u\|^4_{L^4(\mathbb{H}^1)}}:u\in\dot H^1(\mathbb{H}^1)\cap V_0^+\setminus\{0\}\right\}$$

are unique up to symmetries (translation, phase multiplication and scaling).

Proposition 3.11. *The minimum I_+ is equal to π^2. Moreover*:

- *The set composed of all minimizing functions for I_+ is*

$$\left\{(x,y,s)\in\mathbb{H}^1\mapsto\frac{C}{s+s_0+i(x^2+y^2)+i\alpha}:(s_0,C,\alpha)\in\mathbb{R}\times\mathbb{C}\times\mathbb{R}_+^*\right\}.$$

- *The set $\mathcal{Q}_+$ composed of all minimizing functions for I_+ which satisfy*

$$\|Q_+\|^2_{\dot{H}^1(\mathbb{H}^1)} = \|Q_+\|^4_{L^4(\mathbb{H}^1)} = I_+$$

(*so that Q_+ is a solution to* (4)) *is*

$$\mathcal{Q}_+ = \Big\{(x,y,s) \in \mathbb{H}^1 \mapsto \frac{i\, e^{i\theta}\sqrt{2\alpha}}{s + s_0 + i(x^2+y^2) + i\alpha} : (s_0,\theta,\alpha) \in \mathbb{R}\times\mathbb{T}\times\mathbb{R}^*_+\Big\}.$$

Proof. Let $U \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+$. Let us transform the expression of the L^4 norm of U as follows:

$$\|U\|^4_{L^4(\mathbb{H}^1)} = \|U^2\|^2_{L^2(\mathbb{H}^1)} = \|\widehat{U^2}\|^2_{L^2(\mathbb{H}^1)} = \frac{1}{2\pi}\|\hat{U} * \hat{U}\|^2_{L^2(\mathbb{H}^1)}.$$

Let f be the function associated to U in the decomposition along $\hat{h}_0^+$:

$$\hat{U}(x,y,s) = f(\sigma)\frac{1}{\sqrt{\pi}}\,\mathrm{e}^{-(x^2+y^2)\sigma}.$$

Then

$$\|U\|^2_{\dot{H}^1(\mathbb{H}^1)} = \frac{1}{2}\int_0^\infty |f(\sigma)|^2\,\mathrm{d}\sigma,$$

$$\begin{aligned}\|U\|^4_{L^4(\mathbb{H}^1)} &= \frac{1}{2\pi}\int_{\mathbb{R}_+}\int_{\mathbb{R}}\int_{\mathbb{R}}\left|\int_0^\sigma f(\sigma-\sigma')\frac{\mathrm{e}^{-(x^2+y^2)(\sigma-\sigma')}}{\sqrt{\pi}} f(\sigma')\frac{\mathrm{e}^{-(x^2+y^2)\sigma'}}{\sqrt{\pi}}\,\mathrm{d}\sigma'\right|^2 \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}\sigma\\ &= \frac{1}{2\pi^2}\int_{\mathbb{R}_+}\left|\int_0^\sigma f(\sigma-\sigma')f(\sigma')\,\mathrm{d}\sigma'\right|^2\frac{\mathrm{d}\sigma}{2\sigma}.\end{aligned}$$

Applying Cauchy–Schwarz's inequality,

$$\begin{aligned}\|U\|^4_{L^4(\mathbb{H}^1)} &\le \frac{1}{4\pi^2}\int_0^\infty\int_0^\sigma |f(\sigma-\sigma')f(\sigma')|^2\,\mathrm{d}\sigma'\int_0^\sigma 1\,\mathrm{d}\sigma'\frac{\mathrm{d}\sigma}{\sigma}\\ &= \frac{1}{4\pi^2}\int_0^\infty\int_0^\sigma |f(\sigma-\sigma')f(\sigma')|^2\,\mathrm{d}\sigma'\,\mathrm{d}\sigma = \frac{1}{4\pi^2}\|f\|^4_{L^2(\mathbb{R}_+)} = \frac{1}{\pi^2}\|U\|^4_{\dot{H}^1(\mathbb{H}^1)}.\end{aligned}$$

Consequently, $I_+ \ge \pi^2$.

Equality holds if and only if there is equality in Cauchy–Schwarz's inequality, that is to say, for almost every $\sigma > 0$ and almost every $\sigma' \in]0,\sigma[$,

$$f(\sigma')f(\sigma-\sigma') = C(\sigma).$$

Fix an open interval I contained in $]0,\sigma[$ with positive length $|I|$. Then

$$\int_I f(\sigma')f(\sigma-\sigma')\,\mathrm{d}\sigma' = |I|\,C(\sigma).$$

Therefore, C is continuous on $\mathbb{R}^*_+$ as a product of two L^2 functions. Since f is not identically zero, one can find an interval $J \subset \mathbb{R}^*_+$ such that $\int_J f(\zeta)\,\mathrm{d}\zeta \neq 0$. Integrating the equality

$$f(\sigma)f(\zeta) = C(\sigma+\zeta), \quad (\sigma,\zeta) \in (\mathbb{R}^*_+)^2 \tag{10}$$

along the ζ variable, one gets that for all $\sigma \in \mathbb{R}_+^*$,

$$f(\sigma)\int_J f(\zeta)\,\mathrm{d}\zeta = \int_J C(\sigma+\zeta)\,\mathrm{d}\zeta = \int_{J+\sigma} C(\zeta)\,\mathrm{d}\zeta.$$

Therefore, f has $\mathcal{C}^1$ regularity on $\mathbb{R}_+^*$, so C also has $\mathcal{C}^1$ regularity on $\mathbb{R}_+^*$. Fix $\zeta > 0$ such as $f(\zeta) \neq 0$. Letting $\sigma \to 0^+$ in (10), one knows that f admits a finite limit as $\sigma \to 0^+$ which is equal to

$$f(0^+) = \frac{C(\zeta)}{f(\zeta)}.$$

Likewise, computing the derivative along the variable σ of (10), $f'(\sigma)f(\zeta) = C'(\sigma+\zeta)$, one gets that f' admits a finite limit at 0^+ which is equal to

$$f'(0^+) = \frac{C'(\zeta)}{f(\zeta)}.$$

We deduce that f satisfies the differential equation

$$f'(\sigma)f(0^+) = f(\sigma)f'(0^+) = C'(\sigma), \quad \sigma \in \mathbb{R}_+^*.$$

Let us show that $f(0^+) \neq 0$. Supposing $f(0^+) = 0$, we would get that for all $\sigma > 0$, $C'(\sigma) = 0$. Then C would be a constant function, so f would be constant too since

$$f(\sigma) = \frac{C(\sigma+\zeta)}{f(\zeta)}.$$

As f is in $L^2(\mathbb{R}_+)$, this would imply that f is identically zero, which is a contradiction.

Therefore, solving the differential equation, there exist some constants K and α such that, for all $\sigma \geq 0$,

$$f(\sigma) = K\,\mathrm{e}^{-\alpha\sigma}.$$

The assumption $f \in L^2(\mathbb{R}_+)$ implies that $\mathrm{Re}(\alpha) > 0$.

Computing the inverse Fourier transform leads to

$$U(x,y,s) = \frac{1}{\sqrt{2\pi}}\int_0^\infty \mathrm{e}^{is\sigma} f(\sigma)\frac{1}{\sqrt{\pi}}\,\mathrm{e}^{-(x^2+y^2)\sigma}\,\mathrm{d}\sigma = \frac{K}{\pi\sqrt{2}}\int_0^\infty \mathrm{e}^{is\sigma-\alpha\sigma-(x^2+y^2)\sigma}\,\mathrm{d}\sigma,$$

so

$$U(x,y,s) = \frac{K}{\pi\sqrt{2}}\frac{1}{x^2+y^2+\alpha-is}.$$

This is the first point of the proposition. Let us now prove the second point.

Since the equation and the result we want to show are both invariant under translation of the variable s, up to translating of a factor s_0, we will assume from now on that α is a (positive) real number.

Now,

$$\|U\|^2_{\dot{H}^1(\mathbb{H}^1)} = \frac{1}{2}|K|^2\int_0^\infty \mathrm{e}^{-2\alpha\sigma}\,\mathrm{d}\sigma = \frac{1}{2}\frac{|K|^2}{2\alpha},$$

$$\|U\|^4_{L^4(\mathbb{H}^1)} = \frac{1}{4\pi^2}|K|^4\int_0^\infty \left|\int_0^\sigma \mathrm{e}^{-\alpha(\sigma-\sigma')}\,\mathrm{e}^{-\alpha\sigma'}\,\mathrm{d}\sigma'\right|^2\frac{\mathrm{d}\sigma}{\sigma} = \frac{1}{4\pi^2}|K|^4\int_0^\infty \sigma\,\mathrm{e}^{-2\alpha\sigma}\,\mathrm{d}\sigma = \frac{1}{4\pi^2}\frac{|K|^4}{(2\alpha)^2},$$

so U satisfies $\|U\|^2_{\dot{H}^1(\mathbb{H}^1)} = \|U\|^4_{L^4(\mathbb{H}^1)} = I_+$ if and only if $|K|^2 = 4\pi^2\alpha$. In this case, write $K = 2\pi\sqrt{\alpha}\,\mathrm{e}^{i\theta}$ for some $\theta \in \mathbb{T}$, then

$$U(s,x,y) = \frac{K}{\pi\sqrt{2}}\frac{1}{x^2+y^2+\alpha-is} = \frac{\mathrm{e}^{i\theta}\sqrt{2\alpha}}{x^2+y^2+\alpha-is}. \qquad \square$$

We proved that up to the symmetries of the equation, there is a unique minimizer Q_+ in $\mathcal{Q}_+$, which is equal with the choice of parameters $(s_0,\theta,\alpha) = (0,0,1)$ to

$$Q_+(s,x,y) = \frac{i\sqrt{2}}{s+i(x^2+y^2)+i},$$

with Fourier transform

$$\hat{Q}_+(x,y,\sigma) = 2\pi\,\mathrm{e}^{-\sigma}\hat{h}_0^+(x,y,\sigma).$$

Note that the profile Q_+ has infinite mass.

4. The limiting problem

We now focus on the stability of Q_+, which is the unique ground state solution up to symmetry to (4). Let us study the linearized operator $\mathcal{L}$ close to Q_+:

$$\mathcal{L}h = -\Delta_{\mathbb{H}^1}h - 2\Pi_0^+(|Q_+|^2h) - \Pi_0^+(Q_+^2\bar{h}), \quad h \in \dot{H}^1(\mathbb{H}^1)\cap V_0^+.$$

We first study the linearized operator on the real subspace spanned by $(Q_+, iQ_+, \partial_s Q_+, i\partial_s Q_+)$ with the help of the correspondence with Bergman spaces (Sections 4A and 4B). Then, on the orthogonal of this subspace in $\dot{H}^1(\mathbb{H}^1)\cap V_0^+$, we prove the coercivity of $\mathcal{L}$ by using the spectral properties of the sub-Laplacian on the CR sphere via the Cayley transform (Sections 4C and 4D). We conclude this section with some estimates about the invertibility of the linearized operator $\mathcal{L}$ (Section 4E).

4A. ***Bergman spaces on the upper half plane.*** In order to better understand the spaces $\dot{H}^k(\mathbb{H}^1)\cap V_0^+$, $k \in \{-1,0,1\}$, we need to introduce their link with Bergman spaces on the upper half-plane $\mathbb{C}_+$. The space $\dot{H}^k(\mathbb{H}^1)\cap V_0^+$ is the subspace of $\dot{H}^k(\mathbb{H}^1)$ spanned (after a Fourier transform under the variable s) by $\hat{h}_0^+(x,y,\sigma) = \frac{1}{\sqrt{\pi}}\exp(-(x^2+y^2)\sigma)\mathbb{1}_{\sigma\geq 0}$ such that $u \in \dot{H}^k(\mathbb{H}^1)\cap V_0^+$ if $u \in \dot{H}^k(\mathbb{H}^1)$ and

$$\hat{u}(x,y,s) = f(\sigma)\hat{h}_0^+(x,y,\sigma),$$

where

$$\|u\|^2_{\dot{H}^k(\mathbb{H}^1)} = \big\|(-\Delta_{\mathbb{H}^1})^{\frac{k}{2}}u\big\|^2_{L^2(\mathbb{H}^1)} = \int_{\mathbb{R}_+}|f(\sigma)|^2\,\frac{\mathrm{d}\sigma}{2\sigma^{1-k}}.$$

Definition 4.1 (weighted Bergman spaces). Given $k < 1$ and $p \in [1,\infty)$, the weighted Bergman space A^p_{1-k} is the subspace of $L^p_{1-k} := L^p(\mathbb{C}_+, \mathrm{Im}(z)^{-k}\,\mathrm{d}\lambda(z))$ composed of holomorphic functions of the complex upper half-plane $\mathbb{C}_+$:

$$A^p_{1-k} := \left\{F \in \mathrm{Hol}(\mathbb{C}_+) : \|F\|^p_{L^p_{1-k}} := \int_0^\infty\int_{\mathbb{R}}|F(s+it)|^p\,\mathrm{d}s\,\frac{\mathrm{d}t}{t^k} < \infty\right\}.$$

Thanks to the following Paley–Wiener theorem on weighted Bergman spaces [Békollé et al. 2004], one can associate to each element of $\dot{H}^k(\mathbb{H}^1) \cap V_0^+$ a function of the weighted Bergman space A^2_{1-k}:

Theorem 4.2 (Paley–Wiener). *Let $k < 1$. Then for every $f \in L^2(\mathbb{R}_+, \sigma^{k-1}\, d\sigma)$, the integral*

$$F(z) = \frac{1}{\sqrt{2\pi}} \int_0^\infty e^{iz\sigma} f(\sigma)\, d\sigma \tag{11}$$

is absolutely convergent on $\mathbb{C}_+$ and defines a function $F \in A^2_{1-k}$ which satisfies

$$\|F\|^2_{L^2_{1-k}} = \frac{\Gamma(1-k)}{2^{1-k}} \int_0^\infty |f(\sigma)|^2 \frac{d\sigma}{\sigma^{1-k}}. \tag{12}$$

Conversely, for every $F \in A^2_{1-k}$, there exists $f \in L^2(\mathbb{R}_+, \sigma^{k-1}\, d\sigma)$ such that (11) *and* (12) *hold.*

When dealing with functions from the space $\dot{H}^1(\mathbb{H}^1)$, we use the Paley–Wiener theorem [Rudin 1966].

Definition 4.3. The Hardy space $\mathcal{H}^2(\mathbb{C}_+)$ is the space of holomorphic functions of the upper half-plane $\mathbb{C}_+$ such that the following norm is finite:

$$\|F\|^2_{\mathcal{H}^2(\mathbb{C}_+)} := \sup_{t>0} \int_{\mathbb{R}} |F(s+it)|^2\, \mathrm{d}s < \infty.$$

Theorem 4.4 (Paley–Wiener). *For every $f \in L^2(\mathbb{R}_+)$, the integral*

$$F(z) = \frac{1}{\sqrt{2\pi}} \int_0^\infty e^{iz\sigma} f(\sigma)\, d\sigma \tag{13}$$

is absolutely convergent on $\mathbb{C}_+$ and defines a function F in the Hardy space $\mathcal{H}^2(\mathbb{C}_+)$ which satisfies

$$\|F\|^2_{\mathcal{H}^2(\mathbb{C}_+)} = \int_0^\infty |f(\sigma)|^2\, d\sigma. \tag{14}$$

Conversely, for every $F \in \mathcal{H}^2(\mathbb{C}_+)$, there exists $f \in L^2(\mathbb{R}_+)$ such that (13) *and* (14) *hold.*

Given any $h \in \dot{H}^k(\mathbb{H}^1)$ radial, one can define

$$F_h(s + i(x^2+y^2)) := h(x, y, s).$$

If $h \in \dot{H}^k(\mathbb{H}^1) \cap V_0^+$, $k \in \{-1, 0, 1\}$, then F_h is holomorphic, since the holomorphic representation given by the suitable Paley–Wiener theorem is given by $\sqrt{\pi} F_h$. Note that

$$F_{-\Delta_{\mathbb{H}^1} h} = -iF_{\partial_s h} = -iF'_h, \quad h \in \dot{H}^k(\mathbb{H}^1) \cap V_0^+,$$
$$F_{gh} = F_g F_h, \quad g, h \in \dot{H}^k(\mathbb{H}^1) \cap V_0^+.$$

Moreover, if $h \in L^2(\mathbb{H}^1)$,

$$\|h\|^2_{L^2(\mathbb{H}^1)} = \pi \|F_h\|^2_{L^2(\mathbb{C}_+)}. \tag{15}$$

For example, the holomorphic representation in the Hardy space $\mathcal{H}^2(\mathbb{C}_+)$ of

$$Q_+(x, y, s) = \frac{i\sqrt{2}}{i(x^2+y^2)+i+s}$$

is

$$F_{Q_+}(z) = \frac{i\sqrt{2}}{z+i}.$$

One can now identify the orthogonal projector Π_0^+ from the Hilbert space $L^2(\mathbb{H}^1)$ onto its closed subspace $L^2(\mathbb{H}^1) \cap V_0^+$ as a projector P_0 from $L^2(\mathbb{C}_+)$ to $A_1^2 = L^2(\mathbb{C}_+) \cap \mathrm{Hol}(\mathbb{C}_+)$. More generally, for $k < 1$, the orthogonal projector from the Hilbert space $\dot{H}^k(\mathbb{H}^1)$ onto its closed subspace $\dot{H}^k(\mathbb{H}^1) \cap V_0^+$ corresponds to the Bergman projector P_k from L^2_{1-k} onto A^2_{1-k}. For general $k < 1$, the Bergman projector P_k can be expressed as a convolution through a reproducing kernel, called the Bergman kernel [Békollé et al. 2004]. We are here interested in the case $k = 0$.

Proposition 4.5. *For all $F \in L^2(\mathbb{C}_+)$,*

$$P_0(F)(z) = -\frac{1}{\pi}\int_{\mathbb{C}_+} \frac{1}{(z-s+it)^2} F(s+it)\, ds\, dt.$$

For $h \in L^2(\mathbb{H}^1)$, the holomorphic function $F_{\Pi_0^+(h)}$ is the projection of F_h on the subspace A_1^2 of $L^2(\mathbb{C}_+)$:

$$F_{\Pi_0^+(h)}(z) = P_0(F_h)(z).$$

Hence

$$F_{\Pi_0^+(h)}(z) = -\frac{1}{\pi}\int_{\mathbb{C}_+} \frac{1}{(z-s+it)^2} F_h(s+it)\, \mathrm{d}s\, \mathrm{d}t.$$

For $p \in (1, \infty)$, the orthogonal projector P_0 can be extended as a bounded operator from the space $L^p(\mathbb{C}_+, \mathrm{d}\lambda(z))$ onto the Bergman space A_1^p [Békollé et al. 2004].

Theorem 4.6. *Let $p \in [1, \infty)$. Then the Bergman projector P_0 is a bounded operator in $L^p(\mathbb{C}_+)$ if and only if $p > 1$.*

One has $\|h\|^p_{L^p(\mathbb{H}^1)} = \pi \|F_h\|^p_{L^p(\mathbb{C}_+)}$ when this quantity is finite. Therefore, if h_1, h_2, h_3 lie in $\dot{H}^1(\mathbb{H}^1)$ (which embeds in $L^4(\mathbb{H}^1)$), it makes sense to consider $\Pi_0^+(h_1 h_2 h_3)$.

4B. *Symmetries of the equation and orthogonality conditions.* In this subsection, we focus on the linearized operator $\mathcal{L}$ around Q_+

$$\mathcal{L}h = -\Delta_{\mathbb{H}^1} h - 2\Pi_0^+(|Q_+|^2 h) - \Pi_0^+(Q_+^2 \bar{h}), \quad h \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+.$$

This operator is self-adjoint acting on $L^2(\mathbb{H}^1)$, but we are interested in elements of $\dot{H}^1(\mathbb{H}^1)$ endowed with its own scalar product. After studying the action of $\mathcal{L}$ on the real subspace V spanned by $(Q_+, iQ_+, \partial_s Q_+, i\partial_s Q_+)$, we will try to find a new form for $(\mathcal{L}h, h)_{\dot{H}^{-1}(\mathbb{H}^1)\times \dot{H}^1(\mathbb{H}^1)}$ on the orthogonal of V in $\dot{H}^1(\mathbb{H}^1)$ which is more suitable for a spectral study.

Proposition 4.7. *In the real subspace V of $\dot{H}^1(\mathbb{H}^1) \cap V_0^+$ spanned by the orthogonal basis of vectors $(\partial_s Q_+, iQ_+ - \partial_s Q_+, Q_+ + 2i\partial_s Q_+, Q_+)$, the linearized operator $\mathcal{L}$ has the form*

$$\mathcal{L}_{|V} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{16}$$

Proof. We define

$$\tilde{\mathcal{L}}(F) := -iF' - 2P_0(|F_{Q_+}|^2 F_h) - P_0(F_{Q_+}^2 \overline{F_h}), \quad F \in \mathcal{H}^2(\mathbb{C}_+).$$

For $h \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+$, the holomorphic function $F_h \in \mathcal{H}^2(\mathbb{C}_+)$ satisfies

$$\tilde{\mathcal{L}}(F_h) = F_{\mathcal{L}h}.$$

We study $\tilde{L}$ on $\mathcal{H}^2(\mathbb{C}_+)$. For $F \in \mathcal{H}^2(\mathbb{C}_+)$, define

$$\mathscr{F}(F) := -iF' - P_0(|F|^2 F).$$

Let U be a $\mathcal{C}^1$ function defined on a neighborhood of $t = 0$, valued in $\mathcal{H}^2(\mathbb{C}_+)$, and satisfying $U(0) = F_{Q_+}$ and $U'(0) = F$. Then

$$\tilde{\mathcal{L}}F = \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} \mathscr{F}(U(t)).$$

Thanks to the invariance under translation in the variable s, we consider $U : s_0 \in \mathbb{R} \mapsto F_{Q_+}(\cdot + s_0)$. For all $s_0 \in \mathbb{R}$, $\mathscr{F}(U(s_0)) = 0$, so

$$\tilde{\mathcal{L}}(F'_{Q_+}) = 0 = \mathcal{L}(\partial_s Q_+).$$

Following the same pattern, the invariance under phase multiplication gives, with $U : \theta \in \mathbb{R} \mapsto \mathrm{e}^{i\theta} F_{Q_+}$, that $\mathscr{F}(U(\theta)) = 0$ for all θ, so

$$\tilde{\mathcal{L}}(iF_{Q_+}) = 0 = \mathcal{L}(iQ_+).$$

Finally, let $U : \lambda \in \,]-1, 1[\, \mapsto (1+\lambda)F_{Q_+}((1+\lambda)^2 \cdot)$, then $\mathscr{F}(U(\lambda)) = 0$ for all λ thanks to the scaling invariance, so

$$\tilde{\mathcal{L}}(F_{Q_+} + 2zF'_{Q_+}) = 0.$$

Remark that

$$zF'_{Q_+} = -\frac{i\sqrt{2}z}{(z+i)^2} = -F_{Q_+} - iF'_{Q_+}.$$

Consequently,

$$\mathcal{L}(Q_+ + 2i\partial_s Q_+) = 0.$$

In order to determine $\mathcal{L}$ entirely on the subspace V, it is sufficient to calculate $\mathcal{L}(Q_+)$. Yet

$$\mathcal{L}(Q_+) = -i\partial_s Q_+ - 3\Pi_0^+(|Q_+|^2 Q_+) = 2i\partial_s Q_+.$$

We have proved that in the orthogonal basis $(\partial_s Q_+, iQ_+ - \partial_s Q_+, Q_+ + 2i\partial_s Q_+, Q_+)$ of V, $\mathcal{L}$ admits the matrix representation (16). □

We want now to work on the orthogonal of V, so we will study the orthogonality conditions. For this section, it is more natural to work with the complex scalar product in $\dot{H}^1(\mathbb{H}^1)$

$$\langle h_1, h_2 \rangle_{\dot{H}^1(\mathbb{H}^1)} = \int_{\mathbb{H}^1} (-\Delta_{\mathbb{H}^1} h_1)\overline{h_2}\, \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}s = \langle -\Delta_{\mathbb{H}^1} h_1, h_2 \rangle_{\dot{H}^{-1}(\mathbb{H}^1) \times \dot{H}^1(\mathbb{H}^1)}.$$

We have

$$\langle h, Q_+ \rangle_{\dot{H}^1(\mathbb{H}^1)} = (h, Q_+)_{\dot{H}^1(\mathbb{H}^1)} + i(h, iQ_+)_{\dot{H}^1(\mathbb{H}^1)}.$$

Proposition 4.8. *Let* $h \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+$, $F_h(s + i(x^2 + y^2)) = h(x, y, s)$ *its holomorphic counterpart. Then*

$$\langle h, Q_+ \rangle_{\dot{H}^1(\mathbb{H}^1)} = \sqrt{2}\,\pi^2 F_h(i).$$

Consequently:

- *h is orthogonal to* Q_+ *and* iQ_+ *in* $\dot{H}^1(\mathbb{H}^1)$ *if and only if* $F_h(i) = 0$.
- *h is orthogonal to* $\partial_s Q_+$ *and* $i\partial_s Q_+$ *if and only if* $F_h'(i) = 0$.

This proposition enables us to check easily that the basis $(\partial_s Q_+, iQ_+ - \partial_s Q_+, Q_+ + 2i\partial_s Q_+, Q_+)$ of V is orthogonal in $\dot{H}^1(\mathbb{H}^1)$.

Proof. We study the duality bracket in $\dot{H}^{-1}(\mathbb{H}^1) \times \dot{H}^1(\mathbb{H}^1)$ between $-\Delta_{\mathbb{H}^1} Q_+ = D_s Q_+$ and h, for which we use the holomorphic function F_h. Knowing that

$$F_{\partial_s Q_+}(z) = F'_{Q_+}(z) = -\frac{i\sqrt{2}}{(z+i)^2},$$

equality (15) leads to

$$\langle h, \partial_s Q_+ \rangle_{\dot{H}^1(\mathbb{H}^1) \times \dot{H}^{-1}(\mathbb{H}^1)} = \pi \int_{\mathbb{C}_+} \frac{i\sqrt{2}}{(\overline{z+i})^2} F_h(z)\,\mathrm{d}\lambda(z).$$

Let $t > 0$, and define $f_t : z \mapsto F_h(z + it)$ on $\{z \in \mathbb{C} : \operatorname{Im}(z) > -t\}$. Applying the residue formula to $z \mapsto \frac{1}{(z-it-i)^2} f_t(z)$, which is holomorphic on $\{z \in \mathbb{C} : \operatorname{Im}(z) > -t\} \setminus \{it + i\}$ with a simple pole at $it + i$, we get that on every rectangle $\mathscr{R} := [-a, a] + i[0, b]$ containing $it + i$,

$$\int_{\partial\mathscr{R}} \frac{1}{(z-it-i)^2} f_t(z)\,\mathrm{d}z = 2i\pi f_t'(it + i) = 2i\pi F_h'(2it + i). \tag{17}$$

Since the integral of $z \mapsto \frac{1}{(z-it-i)^2} f_t(z)$ is absolutely convergent on $\{z \in \mathbb{C};\ \operatorname{Im}(z) > -t\}$, there are some sequences $(a_j)_{j\in\mathbb{N}}$ and $(b_j)_{j\in\mathbb{N}}$ of real numbers converging to ∞ that satisfy

$$\int_{\mathbb{R}_+} \frac{1}{(-a_j + it' - it - i)^2} f_t(-a_j + it')\,\mathrm{d}t' \to 0,$$

$$\int_{\mathbb{R}_+} \frac{1}{(a_j + it' - it - i)^2} f_t(a_j + it')\,\mathrm{d}t' \to 0,$$

$$\int_{\mathbb{R}} \frac{1}{(s + ib_j - it - i)^2} f_t(s + ib_j)\,\mathrm{d}s \to 0.$$

Applying (17) to the rectangles $[-a_j, a_j] \times [0, b_j]$ and passing to the limit $j \to \infty$, one gets

$$\int_{\mathbb{R}} \frac{1}{(s-it-i)^2} f_t(s)\,\mathrm{d}s = 2i\pi F_h'(2it + i).$$

Consequently,

$$\langle h, \partial_s Q_+ \rangle_{\dot{H}^1(\mathbb{H}^1) \times \dot{H}^{-1}(\mathbb{H}^1)} = i\pi\sqrt{2}\,2i\pi \int_{\mathbb{R}_+} F_h'(2it + i)\,\mathrm{d}t = -i\pi^2\sqrt{2}\,F_h(i),$$

since $F_h(it)$ goes to 0 as t goes to ∞. This latter fact can be established by using the function $f \in L^2(\mathbb{R}_+)$ associated to F_h, which satisfies for all $t \in \mathbb{R}_+^*$

$$F_h(it) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \mathrm{e}^{-t\sigma} f(\sigma)\,\mathrm{d}\sigma.$$

Indeed,

$$|F_h(it)| \le \frac{1}{\sqrt{2\pi}} \left(\int_0^\infty \mathrm{e}^{-2t\sigma}\,\mathrm{d}\sigma \right)^{\frac{1}{2}} \left(\int_0^\infty |f(\sigma)|^2\,\mathrm{d}\sigma \right)^{\frac{1}{2}} = \frac{1}{2\sqrt{\pi t}} \|f\|_{L^2},$$

which goes to 0 as t goes to ∞.

We have shown, as wanted, that

$$\langle h, Q_+ \rangle_{\dot{H}^1(\mathbb{H}^1)} = \langle h, -i\partial_s Q_+ \rangle_{\dot{H}^1(\mathbb{H}^1)\times \dot{H}^{-1}(\mathbb{H}^1)} = \sqrt{2}\,\pi^2 F_h(i).$$

In particular,

$$\langle h, \partial_s Q_+ \rangle_{\dot{H}^1(\mathbb{H}^1)} = -\langle \partial_s h, -i\partial_s Q_+ \rangle_{\dot{H}^1(\mathbb{H}^1)\times \dot{H}^{-1}(\mathbb{H}^1)} = -\sqrt{2}\,\pi^2 F_h'(i). \qquad \square$$

We now check that $\mathcal{L}h$, $h \in \dot{H}^1(\mathbb{H}^1)$ decomposes in the Hilbert space $\dot{H}^{-1}(\mathbb{H}^1)$ as an orthogonal sum $\mathcal{L}h = \mathcal{L}_{|V} h + \mathcal{L}_{|V^\perp} h$, where $V^\perp$ is the orthogonal of V in $\dot{H}^1(\mathbb{H}^1)$.

Corollary 4.9. *Let $h \in \dot{H}^1(\mathbb{H}^1)$ and decompose h as $h = h_0 + h_- + h_+$, where*

$$\begin{aligned} &h_0 \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+ \cap \mathrm{Vect}_{\mathbb{R}}(\partial_s Q_+, iQ_+, Q_+ + 2i\partial_s Q_+), \\ &h_- \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+ \cap \mathrm{Vect}_{\mathbb{R}}(Q_+), \\ &h_+ \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+ \cap (Q_+, iQ_+, \partial_s Q_+, i\partial_s Q_+)^{\perp, \dot{H}^1(\mathbb{H}^1)}. \end{aligned}$$

Then

$$(\mathcal{L}h, h)_{\dot{H}^{-1}(\mathbb{H}^1)\times \dot{H}^1(\mathbb{H}^1)} = (\mathcal{L}h_+, h_+)_{\dot{H}^{-1}(\mathbb{H}^1)\times \dot{H}^1(\mathbb{H}^1)} + (\mathcal{L}h_-, h_-)_{\dot{H}^{-1}(\mathbb{H}^1)\times \dot{H}^1(\mathbb{H}^1)}$$

and

$$\|\mathcal{L}h\|^2_{\dot{H}^{-1}(\mathbb{H}^1)} = \|\mathcal{L}h_+\|^2_{\dot{H}^{-1}(\mathbb{H}^1)} + \|\mathcal{L}h_-\|^2_{\dot{H}^{-1}(\mathbb{H}^1)}.$$

Proof. We decompose $\mathcal{L}h$ as $\mathcal{L}h = \mathcal{L}h_+ + \mathcal{L}h_-$.

Let us show that $\mathcal{L}h_+$ is orthogonal to Q_+, iQ_+, $\partial_s Q_+$ and $i\partial_s Q_+$ for the duality product space $\dot{H}^{-1}(\mathbb{H}^1) \times \dot{H}^1(\mathbb{H}^1)$. We treat separately each term of

$$\mathcal{L}h_+ = -\Delta_{\mathbb{H}^1} h_+ - 2\Pi_0^+(|Q_+|^2 h_+) - \Pi_0^+(Q_+^2 \overline{h_+}).$$

By assumption on h_+, $-\Delta_{\mathbb{H}^1} h_+ = D_s h_+$ and

$$\begin{aligned} \langle D_s h_+, Q_+ \rangle_{\dot{H}^{-1}(\mathbb{H}^1)\times \dot{H}^1(\mathbb{H}^1)} &= \langle h_+, Q_+ \rangle_{\dot{H}^1(\mathbb{H}^1)} = 0, \\ \langle D_s h_+, \partial_s Q_+ \rangle_{\dot{H}^{-1}(\mathbb{H}^1)\times \dot{H}^1(\mathbb{H}^1)} &= \langle h_+, \partial_s Q_+ \rangle_{\dot{H}^1(\mathbb{H}^1)} = 0. \end{aligned}$$

Moreover, using Proposition 4.8,

$$\begin{aligned}\langle \Pi_0^+(|Q_+|^2 h_+), Q_+\rangle_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)} &= \langle Q_+ h_+, Q_+^2\rangle_{L^2(\mathbb{H}^1)\times L^2(\mathbb{H}^1)}\\ &= \langle Q_+ h_+, -i\sqrt{2}\,\partial_s Q_+\rangle_{L^2(\mathbb{H}^1)\times L^2(\mathbb{H}^1)} = 2\pi^2 F_{Q_+h_+}(i) = 0,\end{aligned}$$

since $F_{Q_+h_+} = F_{Q_+}F_{h_+}$ and $F_{h_+}(i) = 0$. In the same way,

$$\langle \Pi_0^+(Q_+^2\overline{h^+}), Q_+\rangle_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)} = \langle Q_+^2, Q_+ h_+\rangle_{L^2(\mathbb{H}^1)\times L^2(\mathbb{H}^1)} = 0.$$

Finally,

$$\begin{aligned}\langle \Pi_0^+(|Q_+|^2 h_+), \partial_s Q_+\rangle_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)} &= \tfrac{1}{2}\langle Q_+ h_+, \partial_s(Q_+^2)\rangle_{L^2(\mathbb{H}^1)\times L^2(\mathbb{H}^1)}\\ &= -\tfrac{1}{2}\langle \partial_s(Q_+ h_+), Q_+^2\rangle_{\dot H^{-2}(\mathbb{H}^1)\times \dot H^2(\mathbb{H}^1)}\\ &= -\tfrac{1}{2}\langle \partial_s(Q_+ h_+), -i\sqrt{2}\,\partial_s Q_+\rangle_{\dot H^{-2}(\mathbb{H}^1)\times \dot H^2(\mathbb{H}^1)}\\ &= -\pi^2 F_{Q_+h_+}(i) = 0,\end{aligned}$$

and in the same way,

$$\langle \Pi_0^+(Q_+^2\overline{h^+}), \partial_s Q_+\rangle_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)} = \langle Q_+^2, \partial_s(Q_+)h_+\rangle_{L^2(\mathbb{H}^1)\times L^2(\mathbb{H}^1)} = 2\pi^2\overline{F_{\partial_s(Q_+)h_+}(i)} = 0.$$

Therefore, $\mathcal{L}h_+ \in \dot H^{-1}(\mathbb{H}^1)\cap V_0^+\cap (Q_+, iQ_+, \partial_s Q_+, i\partial_s Q_+)^{\perp, L^2(\mathbb{H}^1)}$, where the orthogonal is taken for the duality product $\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)$. In particular,

$$(\mathcal{L}h_+, h)_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)} = (\mathcal{L}h_+, h_+)_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)}.$$

Now, since $\mathcal{L}h_-$ is in $\mathrm{Vect}_{\mathbb{R}}(i\partial_s Q_+)$, write $\mathcal{L}h_- = \lambda i\partial_s Q_+ = \lambda\Delta_{\mathbb{H}^1}Q_+$ for some real number λ. One has

$$(\mathcal{L}h_-, h)_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)} = -\lambda(Q_+, h)_{\dot H^1(\mathbb{H}^1)} = -\lambda(Q_+, h_-)_{\dot H^1(\mathbb{H}^1)} = (\mathcal{L}h_-, h_-)_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)},$$

which gives the first part of the proposition.

Then,

$$(\mathcal{L}h_+, \mathcal{L}h_-)_{\dot H^{-1}(\mathbb{H}^1)} = (\mathcal{L}h_+, -\lambda Q_+)_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)} = 0,$$

so we conclude that

$$\|\mathcal{L}h\|^2_{\dot H^{-1}(\mathbb{H}^1)} = \|\mathcal{L}h_+\|^2_{\dot H^{-1}(\mathbb{H}^1)} + \|\mathcal{L}h_-\|^2_{\dot H^{-1}(\mathbb{H}^1)}.$$ □

We now give a simplified expression of $(\mathcal{L}h, h)_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)}$ when h is orthogonal to Q_+ and iQ_+.

Proposition 4.10. *For $h \in \dot H^1(\mathbb{H}^1)\cap V_0^+\cap \mathrm{Vect}_{\mathbb{R}}(Q_+, iQ_+)^{\perp, \dot H^1(\mathbb{H}^1)}$, the following identity is true*:

$$(\mathcal{L}h, h)_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)} = \langle -\Delta_{\mathbb{H}^1}h - 2|Q_+|^2 h, h\rangle_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)}$$

Note that it is more convenient to switch to a complex scalar product, because $-\Delta_{\mathbb{H}^1}h - 2|Q_+|^2 h$ is a complex linear operator of the variable h.

Proof. We only have to show that $(\Pi_0^+(Q_+^2\bar{h}),h)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}$ is zero. We calculate

$$\begin{aligned}(\Pi_0^+(Q_+^2\bar{h}),h)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} &= (Q_+^2\bar{h},h)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}\\ &= (Q_+^2,h^2)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}\\ &= (-i\sqrt{2}\,\partial_s Q_+,h^2)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}\\ &= 2\pi^2\,\mathrm{Re}(F_{h^2}(i)).\end{aligned}$$

Now, $F_{h^2}=F_h^2$. Therefore, $F_{h^2}(i)=0$ as soon as $h\in\dot{H}^1(\mathbb{H}^1)\cap V_0^+\cap\mathrm{Vect}_{\mathbb{R}}(Q_+,iQ_+)^{\perp,\dot{H}^1(\mathbb{H}^1)}$. □

4C. ***Study of the limiting profile through the Cayley transform.*** We will now study the spectrum of $-\Delta_{\mathbb{H}^1}-2|Q_+|^2$, which is natural since we are searching for a coercivity estimate on $\mathcal{L}$ and we just proved in Proposition 4.10 that

$$(\mathcal{L}h,h)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}=\langle-\Delta_{\mathbb{H}^1}h-2|Q_+|^2h,h\rangle_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}.$$

This spectrum can be determined via the equivalence between the Heisenberg group $\mathbb{H}^1$ and the CR sphere $\mathbb{S}^3$ in $\mathbb{C}^2$, called the Cayley transform. We rely on [Branson et al. 2013] in order to introduce this equivalence and its spectral consequences. In this subsection, we will denote by (w,s) the elements of the Heisenberg group, bearing in mind that $w=x+iy$ in the former notation. The Cayley transform is

$$\mathcal{C}:\mathbb{H}^1\to\mathbb{S}^3\setminus(0,-1),\quad (w,s)\mapsto\Big(\frac{2w}{1+|w|^2+is},\frac{1-|w|^2-is}{1+|w|^2+is}\Big).$$

The inverse of $\mathcal{C}$ is given by $\mathcal{C}^{-1}(\zeta_1,\zeta_2)=\big(\frac{\zeta_1}{1+\zeta_2},\mathrm{Im}\,\frac{1-\zeta_2}{1+\zeta_2}\big)$. The Jacobian of the Cayley transform is

$$|J_{\mathcal{C}}(w,s)|=\frac{8}{\big((1+|w|^2)^2+s^2\big)^2}.$$

Notice that $|J_{\mathcal{C}}|$ is linked to Q_+ as follows:

$$|J_{\mathcal{C}}(x+iy,s)|=2|Q_+(x,y,s)|^4.$$

For any integrable function F on $\mathbb{S}^3$, we have the relation

$$\int_{\mathbb{S}^3}F\,\mathrm{d}\zeta=\int_{\mathbb{H}^1}(F\circ\mathcal{C})|J_{\mathcal{C}}|\,\mathrm{d}\lambda_3(w,s).$$

Here, $\mathrm{d}\zeta$ denotes the standard euclidean volume element of $\mathbb{S}^3$. We consider the complex scalar product on $L^2(\mathbb{S}^3)$

$$\langle F,G\rangle_{L^2(\mathbb{S}^3)}=\int_{\mathbb{S}^3}F\overline{G}\,\mathrm{d}\zeta,\quad F,G\in L^2(\mathbb{S}^3).$$

One can notice that

$$\int_{\mathbb{S}^3}|F|^2\,\mathrm{d}\zeta=\int_{\mathbb{H}^1}|F\circ\mathcal{C}|^2|J_{\mathcal{C}}|\,\mathrm{d}\lambda_3(w,s).$$

In particular, $|J_C|=2|Q_+|^4$ is in $L^2(\mathbb{H}^1)$, so if a function F is such that $F\circ\mathcal{C}$ belongs to $L^4(\mathbb{H}^1)$ (for example if $F\circ\mathcal{C}\in\dot{H}^1(\mathbb{H}^1)$), then $|F\circ\mathcal{C}|^2$ belongs to $L^2(\mathbb{H}^1)$, and therefore F is in $L^2(\mathbb{S}^3)$.

On the standard sphere $\mathbb{S}^3$, let

$$\mathcal{R} = \zeta_1 \partial_{\zeta_1} + \zeta_2 \partial_{\zeta_2}.$$

Then the vector fields

$$T_i = \partial_{\zeta_i} - \overline{\zeta_i}\mathcal{R}, \quad i = 1, 2,$$

generate the holomorphic tangent space to $\mathbb{S}^3$.

The conformal sub-Laplacian is defined as

$$\mathcal{D} = -\tfrac{1}{2}\sum_{i=1}^{2}(T_i \overline{T_i} + \overline{T_i} T_i) + \tfrac{1}{4},$$

where $\mathcal{D} - \frac{1}{4}$ is the sub-Laplacian. One can construct the Sobolev space

$$H^1(\mathbb{S}^3) := \{ v \in L^2(\mathbb{S}^3) : \|v\|_{H^1(\mathbb{S}^3)} := \|\mathcal{D}^{\frac{1}{2}} v\|_{L^2(\mathbb{S}^3)} < \infty \}.$$

The operator $\mathcal{D}$ on the sphere has a direct link with the sub-Laplacian on the Heisenberg group via the Cayley transform: for any radial function $F \circ \mathcal{C}$ in $\dot{H}^1(\mathbb{H}^1)$,

$$-\Delta_{\mathbb{H}^1}\big((2|J_{\mathcal{C}}|)^{\frac{1}{4}}(F \circ \mathcal{C})\big) = (2|J_{\mathcal{C}}|)^{\frac{3}{4}}(\mathcal{D}F) \circ \mathcal{C}.$$

Notice that a function in $\dot{H}^1(\mathbb{H}^1)$ maps to a function in $H^1(\mathbb{S}^3)$ via the following transformation:

Proposition 4.11. *Let h be a function on $\mathbb{H}^1$, and define a function v_h on $\mathbb{S}^3$ by*

$$h(x, y, s) = (2|J_{\mathcal{C}}|)^{\frac{1}{4}}(v_h \circ \mathcal{C})(x + iy, s) = \sqrt{2}\,|Q_+|(v_h \circ \mathcal{C})(x + iy, s). \tag{18}$$

Then for radial h,

$$\langle \mathcal{D}v_h, v_h\rangle_{L^2(\mathbb{S}^3)} = \tfrac{1}{2}\langle -\Delta_{\mathbb{H}^1} h, h\rangle_{\dot{H}^{-1}(\mathbb{H}^1)\times \dot{H}^1(\mathbb{H}^1)} \quad \text{and} \quad \langle v_h, v_h\rangle_{L^2(\mathbb{S}^3)} = \int_{\mathbb{H}^1} |h|^2 |Q_+|^2 \, d\lambda_3.$$

Therefore, v_h defines a function in $H^1(\mathbb{S}^3)$ if and only if h is in $\dot{H}^1(\mathbb{H}^1)$.

Proof. Fix a radial function h, and define v_h by (18). Then

$$(-\Delta_{\mathbb{H}^1} h) \cdot \bar{h} = (2|J_{\mathcal{C}}|)^{\frac{3}{4}}(\mathcal{D}v_h) \circ \mathcal{C} \cdot \overline{(2|J_{\mathcal{C}}|)^{\frac{1}{4}}(v_h \circ \mathcal{C})} = 2|J_{\mathcal{C}}|(\mathcal{D}v_h) \circ \mathcal{C} \cdot \overline{v_h \circ \mathcal{C}},$$

so

$$\langle -\Delta_{\mathbb{H}^1} h, h\rangle_{\dot{H}^{-1}(\mathbb{H}^1)\times \dot{H}^1(\mathbb{H}^1)} = 2\langle \mathcal{D}v_h, v_h\rangle_{L^2(\mathbb{S}^3)}.$$

Moreover, when $h \in L^4(\mathbb{H}^1)$, we have $v_h \in L^2(\mathbb{S}^3)$ and

$$\begin{aligned}\langle v_h, v_h\rangle_{L^2(\mathbb{S}^3)} &= \int_{\mathbb{S}^3} |v_h|^2 \, \mathrm{d}\zeta = \int_{\mathbb{H}^1} |v_h \circ \mathcal{C}|^2 |J_{\mathcal{C}}| \, \mathrm{d}\lambda_3(w, s) \\ &= \frac{1}{\sqrt{2}} \int_{\mathbb{H}^1} |h|^2 |J_{\mathcal{C}}|^{\frac{1}{2}} \, \mathrm{d}\lambda_3(w, s) = \int_{\mathbb{H}^1} |h|^2 |Q_+|^2 \, \mathrm{d}\lambda_3.\end{aligned}$$

□

Propositions 4.10 and 4.11 combined imply the following corollary:

Corollary 4.12. *Let h in $\dot{H}^1(\mathbb{H}^1) \cap V_0^+ \cap (Q_+, iQ_+)^{\perp, \dot{H}^1(\mathbb{H}^1)}$. Then*

$$(\mathcal{L}h, h)_{\dot{H}^{-1}(\mathbb{H}^1)\times \dot{H}^1(\mathbb{H}^1)} = 2\langle \mathcal{D}v_h, v_h\rangle_{L^2(\mathbb{S}^3)} - 2\langle v_h, v_h\rangle_{L^2(\mathbb{S}^3)}.$$

The spectrum of the operator $\mathcal{D}$ on $H^1(\mathbb{S}^3)$ is well known. Indeed, the space $L^2(\mathbb{S}^3)$ endowed with the inner product $\langle F, G\rangle_{L^2(\mathbb{S}^3)} = \int_{\mathbb{S}^3} F\overline{G}\,\mathrm{d}\zeta$ admits the orthogonal decomposition

$$L^2(\mathbb{S}^3) = \bigoplus_{j,k\geq 0} \mathrm{Ha}_{j,k},$$

where $\mathrm{Ha}_{j,k}$ is the space of harmonic polynomials on $\mathbb{C}^2$ that are homogeneous of degree j in ζ_1, ζ_2 and k in $\overline{\zeta_1}, \overline{\zeta_2}$, restricted to the sphere $\mathbb{S}^3$. Fix $j, k \geq 0$, then the dimension of $\mathrm{Ha}_{j,k}$ is

$$m_{j,k} := \dim(\mathrm{Ha}_{j,k}) = j + k + 1.$$

The spectrum of $\mathcal{D}$ is as follows:

Proposition 4.13 [Stanton 1989]. *Let $\lambda_j = j + \frac{1}{2}$. Then for all $Y_{j,k} \in \mathrm{Ha}_{j,k}$,*

$$\mathcal{D}Y_{j,k} = \lambda_j \lambda_k Y_{j,k}.$$

In particular, the smallest eigenvalue of $\mathcal{D} - \mathrm{Id}$ is $\lambda_{0,0} - 1 = -\frac{3}{4}$, with multiplicity 1 and eigenvectors the constant functions on $\mathbb{S}^3$. The second one is also negative, equal to $\lambda_{1,0} - 1 = \lambda_{0,1} - 1 = -\frac{1}{4}$, with eigenvectors spanned by $\zeta_1, \zeta_2, \overline{\zeta_1}, \overline{\zeta_2}$. The third one is positive, equal to $\lambda_{2,0} - 1 = \lambda_{0,2} - 1 = \frac{1}{4}$.

Let us study the radial property on $\mathbb{S}^3$. Let $h \in \dot{H}^1(\mathbb{H}^1)$ be a radial function and let v_h be as in (18). Since h and $|J_{\mathcal{C}}|$ only depend on $|x+iy|$ and s, so does $v_h \circ \mathcal{C}$, which means that v_h only depends on $|\zeta_1|$, ζ_2 and $\overline{\zeta_2}$. This discards the eigenfunctions ζ_1 and $\overline{\zeta_1}$ in the above orthogonal decomposition of v_h.

The last step is to treat the remaining eigenvectors with negative eigenvalues for the operator $\mathcal{D} - \mathrm{Id}$, in order to find a lower bound in the quadratic form

$$(\mathcal{L}h, h)_{\dot{H}^{-1}(\mathbb{H}^1)\times \dot{H}^1(\mathbb{H}^1)} = 2\langle \mathcal{D}v_h, v_h\rangle_{L^2(\mathbb{S}^3)} - 2\langle v_h, v_h\rangle_{L^2(\mathbb{S}^3)}$$

for $h \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+ \cap \mathrm{Vect}_{\mathbb{R}}(Q_+, iQ_+, \partial_s Q_+, i\partial_s Q_+)^{\perp, \dot{H}^1(\mathbb{H}^1)}$. These eigenvectors are the constant function $e_1 = \mathbb{1}$ (with eigenvalue $-\frac{3}{4}$) and the harmonic polynomials $e_2 = \overline{\zeta_2}$ and $e_3 = \zeta_2$ (with eigenvalue $-\frac{1}{4}$). In order to do so, we reformulate the above spectral study back to the setting of holomorphic functions of the upper complex plane.

For fractional Sobolev embeddings on $\mathbb{R}^n$ and fractional Folland–Stein embeddings on $\mathbb{H}^n$ [Chen et al. 2013; Liu and Zhang 2015], the potential negative eigenvalues are naturally discarded by the orthogonality conditions, since they correspond to the tangent space to the manifold of functions equal, up to translation, dilation and multiplication by a nonzero constant, to the respective optimizers U and H:

$$\mathcal{M}(\mathbb{R}^n) = \left\{ cU\left(\frac{\cdot - x_0}{\varepsilon}\right) : c \in \mathbb{R}^*, x_0 \in \mathbb{R}^n, \varepsilon > 0 \right\},$$
$$\mathcal{M}(\mathbb{H}^1) = \{cH(\delta(u \cdot)) : c \in \mathbb{R}^*, u \in \mathbb{H}^n, \delta > 0\}.$$

4D. ***Coercivity of the linearized operator.*** We now use the spectrum of $\mathcal{D}$ on the CR sphere in order to get a coercivity estimate on $\mathcal{L}$. The lowest eigenvalues of $\mathcal{D} - \mathrm{Id}$ are, in increasing order,

$$\lambda_{0,0} - 1 = -\tfrac{3}{4} < \lambda_{0,1} - 1 = \lambda_{1,0} - 1 = -\tfrac{1}{4} < \lambda_{0,2} - 1 = \lambda_{2,0} - 1 = \tfrac{1}{4}.$$

The negative eigenfunctions are $e_1 = \mathbb{1}$ (for $\lambda_{0,0}$), $e_2 = \overline{\zeta_2}$ (for $\lambda_{0,1}$) and $e_3 = \zeta_2$ (for $\lambda_{1,0}$).

Let $h \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+ \cap \mathrm{Vect}_{\mathbb{R}}(Q_+, iQ_+, \partial_s Q_+, i\partial_s Q_+)^{\perp, \dot{H}^1(\mathbb{H}^1)}$ and let v be as in (18). Decompose v as

$$v = v_+ + \frac{\langle v, e_1\rangle_{L^2(\mathbb{S}^3)}}{\langle e_1, e_1\rangle_{L^2(\mathbb{S}^3)}} e_1 + \frac{\langle v, e_2\rangle_{L^2(\mathbb{S}^3)}}{\langle e_2, e_2\rangle_{L^2(\mathbb{S}^3)}} e_2 + \frac{\langle v, e_1\rangle_{L^2(\mathbb{S}^3)}}{\langle e_3, e_3\rangle_{L^2(\mathbb{S}^3)}} e_3, \quad v_+ \in \mathrm{Vect}_{\mathbb{C}}(e_1, e_2, e_3)^{\perp}.$$

Since $e_1 \in \mathrm{Ha}_{0,0}$, $e_2 \in \mathrm{Ha}_{0,1}$ and $e_3 \in \mathrm{Ha}_{1,0}$, these three vectors are pairwise orthogonal in $L^2(\mathbb{S}^3)$, and they are orthogonal to $\bigoplus_{(j,k)\notin\{(0,0),(0,1),(1,0)\}} \mathrm{Ha}_{j,k}$. The knowledge of the eigenvalues of $\mathcal{D} - \mathrm{Id}$ enables us to say that

$$\begin{aligned}\frac{1}{2}(\mathcal{L}h, h)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} &= \langle \mathcal{D}v, v\rangle_{L^2(\mathbb{S}^3)} - \langle v, v\rangle_{L^2(\mathbb{S}^3)} \\ &\geq \frac{1}{4}\|v_+\|^2_{L^2(\mathbb{S}^3)} - \frac{1}{4}\frac{|\langle v, e_1\rangle_{L^2(\mathbb{S}^3)}|^2}{\langle e_1, e_1\rangle_{L^2(\mathbb{S}^3)}} - \frac{3}{4}\frac{|\langle v, e_2\rangle_{L^2(\mathbb{S}^3)}|^2}{\langle e_2, e_2\rangle_{L^2(\mathbb{S}^3)}} - \frac{3}{4}\frac{|\langle v, e_3\rangle_{L^2(\mathbb{S}^3)}|^2}{\langle e_3, e_3\rangle_{L^2(\mathbb{S}^3)}}.\end{aligned}$$

But

$$\|v\|^2_{L^2(\mathbb{S}^3)} = \|v_+\|^2_{L^2(\mathbb{S}^3)} + \frac{|\langle v, e_1\rangle_{L^2(\mathbb{S}^3)}|^2}{\langle e_1, e_1\rangle_{L^2(\mathbb{S}^3)}} + \frac{|\langle v, e_2\rangle_{L^2(\mathbb{S}^3)}|^2}{\langle e_2, e_2\rangle_{L^2(\mathbb{S}^3)}} + \frac{|\langle v, e_3\rangle_{L^2(\mathbb{S}^3)}|^2}{\langle e_3, e_3\rangle_{L^2(\mathbb{S}^3)}},$$

so

$$\frac{1}{2}(\mathcal{L}h, h)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} \geq \frac{1}{4}\|v\|^2_{L^2(\mathbb{S}^3)} - \frac{1}{2}\frac{\|\langle v, e_1\rangle_{L^2(\mathbb{S}^3)}|^2}{\langle e_1, e_1\rangle_{L^2(\mathbb{S}^3)}} - \frac{|\langle v, e_2\rangle_{L^2(\mathbb{S}^3)}|^2}{\langle e_2, e_2\rangle_{L^2(\mathbb{S}^3)}} - \frac{|\langle v, e_3\rangle_{L^2(\mathbb{S}^3)}|^2}{\langle e_3, e_3\rangle_{L^2(\mathbb{S}^3)}}.$$

Let us replace these last terms by their expression on the Heisenberg group. We define

$$f_j = \sqrt{2}\,|Q_+| e_j \circ \mathcal{C}, \quad j = 1, 2, 3.$$

From the identity $\zeta_2 \circ \mathcal{C}(w, s) = \dfrac{1 - |w|^2 - is}{1 + |w|^2 + is} = \sqrt{2}\,\overline{Q_+}(w, s) - \mathbb{1}$, we get

$$f_1 = \sqrt{2}\,|Q_+|, \quad f_2 = \sqrt{2}\,|Q_+|(\sqrt{2}\,Q_+ - 1) \quad \text{and} \quad f_3 = \sqrt{2}\,|Q_+|(\sqrt{2}\,\overline{Q_+} - 1).$$

Thanks to Proposition 4.11, one knows that $\langle v, v\rangle_{L^2(\mathbb{S}^3)} = \langle hQ_+, hQ_+\rangle_{L^2(\mathbb{H}^1)}$, so

$$\begin{aligned}&(\mathcal{L}h, h)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} \\ &\quad\geq \frac{1}{2}\|hQ_+\|^2_{L^2(\mathbb{H}^1)} - \frac{|\langle hQ_+, f_3 Q_+\rangle_{L^2(\mathbb{H}^1)}|^2}{\|f_3 Q_+\|^2_{L^2(\mathbb{H}^1)}} - \frac{|\langle hQ_+, f_2 Q_+\rangle_{L^2(\mathbb{H}^1)}|^2}{\|f_2 Q_+\|^2_{L^2(\mathbb{H}^1)}} - 2\frac{|\langle hQ_+, f_1 Q_+\rangle_{L^2(\mathbb{H}^1)}|^2}{\|f_1 Q_+\|^2_{L^2(\mathbb{H}^1)}}.\end{aligned}$$

For $h \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+ \cap \mathrm{Vect}_{\mathbb{R}}(Q_+, iQ_+, \partial_s Q_+, i\partial_s Q_+)^{\perp, \dot{H}^1(\mathbb{H}^1)}$, let us consider the space where F_{hQ_+} lies.

Since $h \in \dot{H}^1(\mathbb{H}^1)$, from the embedding $\dot{H}^1(\mathbb{H}^1) \hookrightarrow L^4(\mathbb{H}^1)$, one knows that hQ_+ is in $L^2(\mathbb{H}^1)$ so F_{hQ_+} belongs to $L^2(\mathbb{C}_+)$.

From Section 4A, h being in $\dot{H}^1(\mathbb{H}^1) \cap V_0^+$, F_h (defined by $h(x, y, s) = F_h(s + i|x + iy|^2)$ for $(x, y, s) \in \mathbb{H}^1$) is a holomorphic function (F_h lies in the Hardy space $\mathcal{H}^2(\mathbb{C}_+)$). This implies that the function $F_{hQ_+} = F_h F_{Q_+}$ is holomorphic too: we have shown that F_h is in the Bergman space $A_1^2 = L^2(\mathbb{C}_+) \cap \mathrm{Hol}(\mathbb{C}_+)$.

Moreover, the fact that h is orthogonal to $\mathrm{Vect}_{\mathbb{R}}(Q_+, iQ_+, \partial_s Q_+, i\partial_s Q_+)$ in $\dot{H}^1(\mathbb{H}^1)$ is equivalent by Proposition 4.8 to $F_h(i) = F_h'(i) = 0$. But then, $F_{hQ_+} = F_h F_{Q_+}$ has a double zero at i. Proposition 4.8 again implies that

$$\langle hQ_+, \partial_s Q_+\rangle_{L^2(\mathbb{H}^1)} = \langle hQ_+, \partial_s^2 Q_+\rangle_{L^2(\mathbb{H}^1)} = 0,$$

which is equivalent to

$$\langle F_{hQ_+}, F'_{Q_+}\rangle_{L^2(\mathbb{C}_+)} = \langle F_{hQ_+}, F''_{Q_+}\rangle_{L^2(\mathbb{C}_+)} = 0.$$

Now, define $W := A_1^2 \cap \mathrm{Vect}_{\mathbb{C}}(F'_{Q_+}, F''_{Q_+})^{\perp, L^2(\mathbb{C}_+)}$, and denote by P_W the orthogonal projection from $L^2(\mathbb{C}_+)$ onto W. We have shown that if $h \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+ \cap \mathrm{Vect}_{\mathbb{R}}(Q_+, iQ_+, \partial_s Q_+, i\partial_s Q_+)^{\perp, \dot{H}^1(\mathbb{H}^1)}$, then $F_{hQ_+} \in W$. In particular, for $u \in L^2(\mathbb{H}^1)$,

$$\langle hQ_+, u\rangle_{L^2(\mathbb{H}^1)} = \pi \langle F_{hQ_+}, F_u\rangle_{L^2(\mathbb{C}_+)} = \pi \langle F_{hQ_+}, P_W(F_u)\rangle_{L^2(\mathbb{C}_+)}.$$

Back to the quadratic form, we deduce that

$$(\mathcal{L}h, h)_{\dot{H}^{-1}(\mathbb{H}^1)\times \dot{H}^1(\mathbb{H}^1)} \geq \pi\Bigg(\frac{1}{2}\|F_{hQ_+}\|^2_{L^2(\mathbb{C}_+)} - \frac{|\langle F_{hQ_+}, P_W(F_{f_3Q_+})\rangle_{L^2(\mathbb{C}_+)}|^2}{\|F_{f_3Q_+}\|^2_{L^2(\mathbb{C}_+)}} - \frac{|\langle F_{hQ_+}, P_W(F_{f_2Q_+})\rangle_{L^2(\mathbb{C}_+)}|^2}{\|F_{f_2Q_+}\|^2_{L^2(\mathbb{C}_+)}} - 2\frac{|\langle F_{hQ_+}, P_W(F_{f_1Q_+})\rangle_{L^2(\mathbb{C}_+)}|^2}{\|F_{f_1Q_+}\|^2_{L^2(\mathbb{C}_+)}}\Bigg).$$

Let us denote

$$X_j = \frac{P_W(F_{f_jQ_+})}{\|F_{f_jQ_+}\|_{L^2(\mathbb{C}_+)}} = \frac{P_W(F_1)}{\|F_1\|_{L^2(\mathbb{C}_+)}}, \quad j = 1, 2, 3,$$

with

$$F_1(z) = \frac{1}{|z+i|(z+i)}, \quad F_2(z) = \frac{1}{|z+i|(z+i)}\Big(\frac{2i}{z+i} - 1\Big) \quad \text{and} \quad F_3(z) = \frac{1}{|z+i|(z+i)}\Big(\frac{-2i}{\bar{z}-i} - 1\Big).$$

We try to find an upper bound on the quadratic form on $L^2(\mathbb{C}_+)$

$$q(F) := 2|\langle F, X_1\rangle_{L^2(\mathbb{C}_+)}|^2 + |\langle F, X_2\rangle_{L^2(\mathbb{C}_+)}|^2 + |\langle F, X_3\rangle_{L^2(\mathbb{C}_+)}|^2, \quad F \in L^2(\mathbb{C}_+).$$

In particular, we want to show that this upper bound is strictly less than $\frac{1}{2}$.

Let us first write explicitly the orthogonal projector P_W from $L^2(\mathbb{C}_+)$ onto the subspace $W = A_1^2 \cap \mathrm{Vect}_{\mathbb{C}}(F'_{Q_+}, F''_{Q_+})^{\perp, L^2(\mathbb{C}_+)}$ We start by finding an orthogonal basis of $\mathrm{Vect}_{\mathbb{C}}(F'_{Q_+}, F''_{Q_+})$ for the scalar product on $L^2(\mathbb{C}_+)$. We know by Proposition 4.8 that

$$\langle u, \partial_s Q_+\rangle_{L^2(\mathbb{H}^1)} = -i\sqrt{2}\pi^2 F_u(i), \quad u \in L^2(\mathbb{H}^1),$$

so

$$\langle F, F'_{Q_+}\rangle_{L^2(\mathbb{C}_+)} = -i\sqrt{2}\pi F(i), \quad F \in L^2(\mathbb{C}_+).$$

Using the equalities

$$F_Q(z) = \frac{i\sqrt{2}}{z+i}, \quad F'_Q(z) = \frac{-i\sqrt{2}}{(z+i)^2}, \quad F''_Q(z) = \frac{2i\sqrt{2}}{(z+i)^3} \quad F'''_{Q_+}(z) = -\frac{6i\sqrt{2}}{(z+i)^4},$$

we obtain

$$F_{Q_+}(i)=\frac{1}{\sqrt{2}},\quad F'_{Q_+}(i)=\frac{i}{2\sqrt{2}},\quad F''_{Q_+}(i)=-\frac{1}{2\sqrt{2}}\quad F'''_{Q_+}(i)=\frac{3i}{4\sqrt{2}}.$$

Therefore,

$$\langle F''_{Q_+},F'_{Q_+}\rangle_{L^2(\mathbb{C}_+)}=-i\sqrt{2}\,\pi F''_{Q_+}(i)=i\frac{\pi}{2}.$$

In the same way,

$$\langle F'_{Q_+},F'_{Q_+}\rangle_{L^2(\mathbb{C}_+)}=-i\sqrt{2}\,\pi F'_{Q_+}(i)=\frac{\pi}{2},$$

so $\tilde{F}:=F'_{Q_+}-\dfrac{\langle F'_{Q_+},F'_{Q_+}\rangle_{L^2(\mathbb{C}_+)}}{\langle F''_{Q_+},F'_{Q_+}\rangle_{L^2(\mathbb{C}_+)}}F''_{Q_+}=F'_{Q_+}+iF''_{Q_+}$ is orthogonal to F'_{Q_+}:

$$\langle \tilde{F},F'_{Q_+}\rangle_{L^2(\mathbb{C}_+)}=0.$$

Moreover,

$$\langle \tilde{F},\tilde{F}\rangle_{L^2(\mathbb{C}_+)}=\langle \tilde{F},F'_{Q_+}\rangle_{L^2(\mathbb{C}_+)}+\langle \tilde{F},iF''_{Q_+}\rangle_{L^2(\mathbb{C}_+)}=0+\langle i\tilde{F}',F'_{Q_+}\rangle_{L^2(\mathbb{C}_+)}=\sqrt{2}\,\pi\tilde{F}'(i).$$

Since $\tilde{F}'(i)=F''_{Q_+}(i)+iF'''_{Q_+}(i)=\frac{1}{4\sqrt{2}}$, $\tilde{F}$ is of norm

$$\langle \tilde{F},\tilde{F}\rangle_{L^2(\mathbb{C}_+)}=\frac{\pi}{4}.$$

The orthogonal projection on $\mathrm{Vect}_{\mathbb{C}}(F'_{Q_+},F''_{Q_+})^{\perp,L^2(\mathbb{C}_+)}$ in $L^2(\mathbb{C}_+)$ is then written

$$F\in L^2(\mathbb{C}_+)\mapsto F-\frac{2}{\pi}\langle F,F'_{Q_+}\rangle_{L^2(\mathbb{C}_+)}F'_{Q_+}-\frac{4}{\pi}\langle F,F'_{Q_+}+iF''_{Q_+}\rangle_{L^2(\mathbb{C}_+)}(F'_{Q_+}+iF''_{Q_+}).$$

Besides, from Proposition 4.5, we know that the orthogonal projection P_0 from $\in L^2(\mathbb{C}_+)$ onto A^2_1 is given by

$$P_0F(s+it)=-\frac{1}{\pi}\int_{\mathbb{C}_+}\frac{1}{(s-u+it+iv)^2}F(u+iv)\,\mathrm{d}u\,\mathrm{d}v,\qquad F\in L^2(\mathbb{C}_+).$$

Therefore, the orthogonal projection P_W on the space $W=A^2_1\cap\mathrm{Vect}_{\mathbb{C}}(F'_{Q_+},F''_{Q_+})^{\perp,L^2(\mathbb{C}_+)}$, for $F\in L^2(\mathbb{C}_+)$, is written

$$P_WF(s+it)=-\frac{1}{\pi}\int_{\mathbb{C}_+}\frac{1}{(s-u+it+iv)^2}F(u+iv)\,\mathrm{d}u\,\mathrm{d}v-\frac{2}{\pi}\langle F,F'_{Q_+}\rangle_{L^2(\mathbb{C}_+)}F'_{Q_+}(s+it)$$
$$-\frac{4}{\pi}\langle F,F'_{Q_+}+iF''_{Q_+}\rangle_{L^2(\mathbb{C}_+)}(F'_{Q_+}+iF''_{Q_+})(s+it).$$

We use the following estimates of $\langle \pi P_0F_j,F_j\rangle_{L^2(\mathbb{C}_+)}$, $j=1,2,3$:

Lemma 4.14. *If* $\varepsilon=10^{-10}$, *then*

$$|\langle \pi P_0F_1,F_1\rangle_{L^2(\mathbb{C}_+)}-2|\le\varepsilon,$$
$$|\langle \pi P_0F_2,F_2\rangle_{L^2(\mathbb{C}_+)}-\tfrac{10}{9}|\le\varepsilon,$$
$$|\langle \pi P_0F_3,F_3\rangle_{L^2(\mathbb{C}_+)}-0.1303955989|\le\varepsilon.$$

The proof of this lemma is rather technical and is postponed to the appendix. It involves simplifying the integrals defining P_0F_j, $j=1,2,3$: we determine explicitly the holomorphic function which coincides with P_0F_j on $\mathbb{C}_+$ thanks to a massive use of the residue formula. This part is necessary in order to compute numerically $\langle P_0F_j, F_j\rangle_{L^2(\mathbb{C}_+)}$. Without this preliminary work, there is a four-dimensional numerical integration to perform and the error estimate is big with a naive approach.

A direct calculation gives

$$\begin{aligned}
&\langle F_1,F_1\rangle_{L^2(\mathbb{C}_+)}=\frac{\pi}{4}, && \langle F_2,F_2\rangle_{L^2(\mathbb{C}_+)}=\langle F_3,F_3\rangle_{L^2(\mathbb{C}_+)}=\frac{\pi}{8}, \\
&\langle F_1,F'_{Q_+}\rangle_{L^2(\mathbb{C}_+)}=-\frac{2\sqrt{2}}{3}, && \langle F_2,F'_{Q_+}\rangle_{L^2(\mathbb{C}_+)}=-\frac{2\sqrt{2}}{9}, && \langle F_3,F'_{Q_+}\rangle_{L^2(\mathbb{C}_+)}=\frac{2\sqrt{2}}{15}, \\
&\langle F_1,\tilde{F}\rangle_{L^2(\mathbb{C}_+)}=-\frac{2\sqrt{2}}{15}, && \langle F_2,\tilde{F}\rangle_{L^2(\mathbb{C}_+)}=\frac{14\sqrt{2}}{45}, && \langle F_3,\tilde{F}\rangle_{L^2(\mathbb{C}_+)}=\frac{2\sqrt{2}}{35}.
\end{aligned}$$

We deduce that

$$\left|2\frac{\langle P_WF_1,F_1\rangle_{L^2(\mathbb{C}_+)}}{\langle F_1,F_1\rangle_{L^2(\mathbb{C}_+)}}+\frac{\langle P_WF_2,F_2\rangle_{L^2(\mathbb{C}_+)}}{\langle F_2,F_2\rangle_{L^2(\mathbb{C}_+)}}+\frac{\langle P_WF_3,F_3\rangle_{L^2(\mathbb{C}_+)}}{\langle F_3,F_3\rangle_{L^2(\mathbb{C}_+)}}-0.2046049976\right|\le 24\varepsilon.$$

This enables us to get a sufficiently precise estimate for the quadratic form. Indeed, we want to show that the norm of the following quadratic form is smaller that $\frac{1}{2}$:

$$q(F)=2|\langle F,X_1\rangle_{L^2(\mathbb{C}_+)}|^2+|\langle F,X_2\rangle_{L^2(\mathbb{C}_+)}|^2+|\langle F,X_3\rangle_{L^2(\mathbb{C}_+)}|^2,\quad F\in L^2(\mathbb{C}_+).$$

Applying Cauchy–Schwarz's inequality, for $F\in W$,

$$\begin{aligned}
q(F)&=2\left|\frac{\langle F,F_1\rangle_{L^2(\mathbb{C}_+)}}{\|F_1\|_{L^2(\mathbb{C}_+)}}\right|^2+\left|\frac{\langle F,F_2\rangle_{L^2(\mathbb{C}_+)}}{\|F_2\|_{L^2(\mathbb{C}_+)}}\right|^2+\left|\frac{\langle F,F_3\rangle_{L^2(\mathbb{C}_+)}}{\|F_3\|_{L^2(\mathbb{C}_+)}}\right|^2 \\
&\le \|F\|^2_{L^2(\mathbb{C}_+)}\left(2\frac{\langle P_WF_1,F_1\rangle_{L^2(\mathbb{C}_+)}}{\|F_1\|^2_{L^2(\mathbb{C}_+)}}+\frac{\langle P_WF_2,F_2\rangle_{L^2(\mathbb{C}_+)}}{\|F_2\|^2_{L^2(\mathbb{C}_+)}}+\frac{\langle P_WF_3,F_3\rangle_{L^2(\mathbb{C}_+)}}{\|F_3\|^2_{L^2(\mathbb{C}_+)}}\right).
\end{aligned}$$

But we just estimated

$$C:=2\frac{\langle P_WF_1,F_1\rangle_{L^2(\mathbb{C}_+)}}{\|F_1\|^2_{L^2(\mathbb{C}_+)}}+\frac{\langle P_WF_2,F_2\rangle_{L^2(\mathbb{C}_+)}}{\|F_2\|^2_{L^2(\mathbb{C}_+)}}+\frac{\langle P_WF_3,F_3\rangle_{L^2(\mathbb{C}_+)}}{\|F_3\|^2_{L^2(\mathbb{C}_+)}}$$

as $C\approx 0.2046049976<\frac{1}{2}$. Going back to h in $\dot{H}^1(\mathbb{H}^1)\cap V_0^+\cap \mathrm{Vect}_{\mathbb{R}}(Q_+,iQ_+,\partial_sQ_+,i\partial_sQ_+)^{\perp,\dot{H}^1(\mathbb{H}^1)}$,

$$\begin{aligned}
(\mathcal{L}h,h)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}&\ge\pi\left(\tfrac{1}{2}\|F_{hQ_+}\|^2_{L^2(\mathbb{C}_+)}-q(F_{hQ_+})\right) \\
&\ge\pi\left(\tfrac{1}{2}\|F_{hQ_+}\|^2_{L^2(\mathbb{C}_+)}-C\|F_{hQ_+}\|^2_{L^2(\mathbb{C}_+)}\right) \\
&=\frac{1-2C}{2}\|hQ_+\|^2_{L^2(\mathbb{H}^1)}=\frac{1-2C}{2}\|v_h\|^2_{L^2(\mathbb{S}^3)}.
\end{aligned}$$

But $\frac{1}{2}(\mathcal{L}h,h)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}=\langle\mathcal{D}v_h,v_h\rangle_{L^2(\mathbb{S}^3)}-\langle v_h,v_h\rangle_{L^2(\mathbb{S}^3)}$, so

$$\langle \mathcal{D}v_h, v_h\rangle_{L^2(\mathbb{S}^3)} \geq \Big(1+\frac{1-2C}{4}\Big)\langle v_h, v_h\rangle_{L^2(\mathbb{S}^3)},$$

$$\langle \mathcal{D}v_h, v_h\rangle_{L^2(\mathbb{S}^3)} - \langle v_h, v_h\rangle_{L^2(\mathbb{S}^3)} \geq \Big(1-\frac{1}{1+(1-2C)/4}\Big)\langle \mathcal{D}v_h, v_h\rangle_{L^2(\mathbb{S}^3)}.$$

Set $\delta = 2\big(1-\frac{1}{1+(1-2C)/4}\big)$. Since $\langle \mathcal{D}v_h, v_h\rangle_{L^2(\mathbb{S}^3)} = \|h\|^2_{\dot{H}^1(\mathbb{H}^1)}$, the following theorem holds:

Theorem 4.15. *The linearized operator $\mathcal{L}$ around Q_+*

$$\mathcal{L}h = -\Delta_{\mathbb{H}^1}h - 2\Pi_0^+(|Q_+|^2h) - \Pi_0^+(Q_+^2\bar{h})$$

is coercive outside the finite-dimensional subspace spanned by Q_+, iQ_+, $\partial_s Q_+$ and $i\partial_s Q_+$: there exists $\delta > 0$ such that for all h in $\dot{H}^1(\mathbb{H}^1)\cap V_0^+ \cap (Q_+, iQ_+, \partial_s Q_+, i\partial_s Q_+)^{\perp,\dot{H}^1(\mathbb{H}^1)}$, then

$$(\mathcal{L}h, h)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} \geq \delta\|h\|^2_{\dot{H}^1(\mathbb{H}^1)}.$$

For the Szegő equation, Pocovnicu [2012] proved that the linearized operator is coercive in directions which are symplectically orthogonal to the manifold of solitons

$$\Big\{\frac{\alpha\mu\, \mathrm{e}^{i\theta}}{\mu(x-a)+i} : \mu\in\mathbb{R}_+^*, \alpha\in\mathbb{R}_+^*, \theta\in\mathbb{T}, a\in\mathbb{R}\Big\}.$$

The nondegeneracy follows from this theorem and the study of $\mathcal{L}$ on the finite-dimensional subspace $V = \dot{H}^1(\mathbb{H}^1)\cap V_0^+\cap \mathrm{Vect}_{\mathbb{R}}(Q_+, iQ_+, \partial_s Q_+, i\partial_s Q_+)$ (Section 4B).

Corollary 4.16. *The linearized operator $\mathcal{L}$ is nondegenerate*:

$$\mathrm{Ker}(\mathcal{L}) = \mathrm{Vect}_{\mathbb{R}}(\partial_s Q_+, iQ_+, Q_+ + 2i\partial_s Q_+).$$

4E. *Invertibility of $\mathcal{L}$.* The following corollaries of Theorem 4.15 make precise the invertibility of $\mathcal{L}$ and the linear stability up to symmetries of the ground state Q_+. These estimates will be useful in order to prove the invertibility of the linearized operators $\mathcal{L}_{Q_\beta}$ around Q_β in Section 5.

Corollary 4.17. *There exists $c > 0$ such that for all $h\in\dot{H}^1(\mathbb{H}^1)\cap V_0^+$,*

$$\|\mathcal{L}h\|_{\dot{H}^{-1}(\mathbb{H}^1)} + |(h,\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(h, iQ_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(h, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}| \geq c\|h\|_{\dot{H}^1(\mathbb{H}^1)}.$$

Proof. Let $h\in\dot{H}^1(\mathbb{H}^1)\cap V_0^+$. We decompose h into three orthogonal components $h = h_0 + h_- + h_+$, where $h_0\in\dot{H}^1(\mathbb{H}^1)\cap V_0^+\cap\mathrm{Vect}_{\mathbb{R}}(\partial_s Q_+, iQ_+, Q_+ + 2i\partial_s Q_+)$, $h_-\in\dot{H}^1(\mathbb{H}^1)\cap V_0^+\cap\mathrm{Vect}_{\mathbb{R}}(Q_+)$ and $h_+\in\dot{H}^1(\mathbb{H}^1)\cap V_0^+\cap\mathrm{Vect}_{\mathbb{R}}(Q_+, iQ_+, \partial_s Q_+, i\partial_s Q_+)^{\perp,\dot{H}^1(\mathbb{H}^1)}$. Then $\mathcal{L}h_0 = 0$, and $\mathcal{L}h_+$ satisfies the above coercivity estimate Theorem 4.15: for some $\delta > 0$,

$$\|\mathcal{L}h_+\|_{\dot{H}^{-1}(\mathbb{H}^1)} \geq \delta\|h_+\|_{\dot{H}^1(\mathbb{H}^1)}.$$

Write $h_- = \lambda Q_+$ for some real number λ. Then $\mathcal{L}h_- = 2\lambda i\partial_s Q_+$, so

$$(\mathcal{L}h_-, h_-)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} = 2\lambda^2(i\partial_s Q_+, Q_+)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}.$$

But

$$\|h_-\|^2_{\dot{H}^1(\mathbb{H}^1)} = (-i\lambda\partial_s Q_+, \lambda Q_+)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)},$$

so $(\mathcal{L}h_-, h)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} = -2\|h_-\|^2_{\dot{H}^1(\mathbb{H}^1)}$. In particular, $\|\mathcal{L}h_-\|_{\dot{H}^{-1}(\mathbb{H}^1)} \geq 2\|h_-\|_{\dot{H}^1(\mathbb{H}^1)}$.

Thanks to Corollary 4.9, we deduce that

$$\begin{aligned}\|\mathcal{L}h\|^2_{\dot{H}^{-1}(\mathbb{H}^1)} &= \|\mathcal{L}h_-\|^2_{\dot{H}^{-1}(\mathbb{H}^1)} + \|\mathcal{L}h_+\|^2_{H^{-1}(\mathbb{H}^1)} \\ &\geq 4\|h_-\|^2_{\dot{H}^1(\mathbb{H}^1)} + \delta^2\|h_+\|^2_{H^1(\mathbb{H}^1)} \geq (\min(2,\delta))^2\|h_- + h_+\|^2_{\dot{H}^1(\mathbb{H}^1)}.\end{aligned}$$

Moreover, since h_0 is in the space spanned by $\partial_s Q_+$, iQ_+ and $Q_+ + 2iQ_+$, there exists some constant $0 < c \leq \min(2,\delta)$ such that

$$|(h, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(h, iQ_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(h, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}| \geq c\|h_0\|_{\dot{H}^1(\mathbb{H}^1)}.$$

Therefore,

$$\|\mathcal{L}h\|_{H^{-1}(\mathbb{H}^1)} + |(h, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(h, iQ_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(h, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}| \geq c\|h\|_{\dot{H}^1(\mathbb{H}^1)}. \quad \square$$

Let us recall that for $h \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+$, we have set in Definition 3.8

$$\delta(u) = \left|\|u\|^2_{\dot{H}^1(\mathbb{H}^1)} - \|Q_+\|^2_{\dot{H}^1(\mathbb{H}^1)}\right| + \left|\|u\|^4_{L^4(\mathbb{H}^1)} - \|Q_+\|^4_{L^4(\mathbb{H}^1)}\right|.$$

Corollary 4.18. *There exists $\varepsilon_0 > 0$ and $c > 0$ such that for all $u \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+$, if $\|u - Q_+\|_{\dot{H}^1(\mathbb{H}^1)} \leq \varepsilon_0$, then*

$$\delta(u) + |(u, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(u, iQ_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(u, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}| \geq c\|u - Q_+\|^2_{\dot{H}^1(\mathbb{H}^1)}.$$

Proof. Let $u \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+$ and set $h = u - Q_+$. We decompose h as above in three orthogonal parts $h = h_0 + h_- + h_+$, where $h_0 \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+ \cap \mathrm{Vect}_{\mathbb{R}}(\partial_s Q_+, iQ_+, Q_+ + 2i\partial_s Q_+)$, $h_- \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+ \cap \mathrm{Vect}_{\mathbb{R}}(Q_+)$ and $h_+ \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+ \cap (Q_+, iQ_+, \partial_s Q_+, i\partial_s Q_+)^{\perp, \dot{H}^1(\mathbb{H}^1)}$.

The link between $\delta(u)$ and the linearized operator $\mathcal{L}$ appears through the functional

$$E(u) := \|u\|^2_{\dot{H}^1(\mathbb{H}^1)} - \tfrac{1}{2}\|u\|^4_{L^4(\mathbb{H}^1)}.$$

Indeed,

$$|E(u) - E(Q_+)| \leq \delta(u),$$

but since Q_+ is a solution to $D_s Q_+ = \Pi_0^+(|Q_+|^2 Q_+)$ and h belongs to $\dot{H}^1(\mathbb{H}^1) \cap V_0^+$, we have the Taylor expansion

$$E(u) - E(Q_+) = (\mathcal{L}h, h)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} + \mathcal{O}(\|h\|^3_{\dot{H}^1(\mathbb{H}^1)}).$$

Therefore,

$$\delta(u) \geq (\mathcal{L}h, h)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} - \mathcal{O}(\|h\|^3_{\dot{H}^1(\mathbb{H}^1)}).$$

From Corollary 4.9, we know that

$$(\mathcal{L}h, h)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} = (\mathcal{L}h_+, h_+)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} + (\mathcal{L}h_-, h_-)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}.$$

Consequently, the coercivity estimate on $\mathcal{L}$ implies that for some constants $c_1, C_1 > 0$,

$$\delta(u) \geq c_1\|h_+\|^2_{\dot{H}^1(\mathbb{H}^1)} - C_1(\|h_-\|^2_{\dot{H}^1(\mathbb{H}^1)} + \|h\|^3_{\dot{H}^1(\mathbb{H}^1)}). \tag{19}$$

Let us focus on the term $\|h_-\|^2_{\dot{H}^1(\mathbb{H}^1)}$. We use the fact that

$$\begin{aligned}\delta(u) &\geq |(Q_+ + h, Q_+ + h)_{\dot{H}^1(\mathbb{H}^1)} - (Q_+, Q_+)_{\dot{H}^1(\mathbb{H}^1)}| \\ &\geq 2|(Q_+, h)_{\dot{H}^1(\mathbb{H}^1)}| - \|h\|^2_{\dot{H}^1(\mathbb{H}^1)} = 2\|Q_+\|_{\dot{H}^1(\mathbb{H}^1)}\|h_-\|_{\dot{H}^1(\mathbb{H}^1)} - \|h\|^2_{\dot{H}^1(\mathbb{H}^1)},\end{aligned}$$

so

$$\delta(u)^2 \geq 4\|Q_+\|^2_{\dot{H}^1(\mathbb{H}^1)}\|h_-\|^2_{\dot{H}^1(\mathbb{H}^1)} - \mathcal{O}(\|h\|^3_{\dot{H}^1(\mathbb{H}^1)}).$$

We use this estimate to control $\|h_-\|^2_{\dot{H}^1(\mathbb{H}^1)}$ in the lower bound (19) of $\delta(u)$. Up to decreasing ε_0, one can absorb the term $\delta(u)^2$ into the term $\delta(u)$: there exist $c_2, C_2 > 0$ and $\varepsilon_0 > 0$ such that if $\|h\|_{\dot{H}^1(\mathbb{H}^1)} = \|u - Q_+\|_{\dot{H}^1(\mathbb{H}^1)} \leq \varepsilon_0$,

$$2\delta(u) \geq \delta(u) + C_2\delta(u)^2 \geq c_2\|h_+\|^2_{\dot{H}^1(\mathbb{H}^1)} + c_2\|h_-\|^2_{\dot{H}^1(\mathbb{H}^1)} - C_2\|h\|^3_{\dot{H}^1(\mathbb{H}^1)}.$$

We now control $\|h_0\|^2_{\dot{H}^1(\mathbb{H}^1)}$. If $\varepsilon_0 \leq 1$, we have an upper bound

$$\|h_0\|^2_{\dot{H}^1(\mathbb{H}^1)} \leq \|h_0\|_{\dot{H}^1(\mathbb{H}^1)} \leq C(|(h, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(h, iQ_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(h, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}|).$$

In the end, there exist $c_3 > 0$ and $C_3 > 0$ such that for all $u \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+$,

$$\begin{aligned}&\delta(u) + |(h, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(h, iQ_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(h, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}| \\ &\quad\geq c_3\big(\|h_+\|^2_{\dot{H}^1(\mathbb{H}^1)} + \|h_-\|^2_{\dot{H}^1(\mathbb{H}^1)} + \|h_0\|^2_{\dot{H}^1(\mathbb{H}^1)}\big) - C_3\|h\|^3_{\dot{H}^1(\mathbb{H}^1)} = c_3\|h\|^2_{\dot{H}^1(\mathbb{H}^1)} - C_3\|h\|^3_{\dot{H}^1(\mathbb{H}^1)}.\end{aligned}$$

Up to decreasing ε_0 again, we can absorb the term $\|h\|^3_{\dot{H}^1(\mathbb{H}^1)}$ into the term $\|h\|^2_{\dot{H}^1(\mathbb{H}^1)}$. Note that Q_+ is orthogonal in $\dot{H}^1(\mathbb{H}^1)$ to $\partial_s Q_+, iQ_+$ and $Q_+ + 2i\partial_s Q_+$, therefore $(h, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)} = (u, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}$, $(h, iQ_+)_{\dot{H}^1(\mathbb{H}^1)} = (u, iQ_+)_{\dot{H}^1(\mathbb{H}^1)}$ and $(h, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)} = (u, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}$. □

We now control the distance of a function $u \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+$ to the profile Q_+ up to symmetries by the difference of their norms $\delta(u)$.

Definition 4.19. Fix $h \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+$, $s_0 \in \mathbb{R}$, $\theta \in \mathbb{T}$ and $\alpha \in \mathbb{R}_+^*$. We denote by $T_{s_0,\theta,\alpha}h$ the function in $\dot{H}^1(\mathbb{H}^1) \cap V_0^+$ defined by

$$T_{s_0,\theta,\alpha}h(x, y, s) := \mathrm{e}^{i\theta}\alpha h(\alpha x, \alpha y, \alpha^2(s + s_0)), \quad (x, y, s) \in \mathbb{H}^1.$$

Corollary 4.20. *There exist* $\delta_0 > 0$ *and* $C > 0$ *such that for all* $u \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+$, *if* $\delta(u) \leq \delta_0$, *then*

$$\inf_{(s_0,\theta,\alpha)\in\mathbb{R}\times\mathbb{T}\times\mathbb{R}_+^*} \|T_{s_0,\theta,\alpha}u - Q_+\|^2_{\dot{H}^1(\mathbb{H}^1)} \leq C\delta(u).$$

Proof. Assume by contradiction that there exists a sequence $(u_n)_{n\in\mathbb{N}} \subset \dot{H}^1(\mathbb{H}^1) \cap V_0^+$ such that $\delta(u_n) \to 0$, but

$$\frac{1}{\delta(u_n)} \inf_{(s_0,\theta,\alpha)\in\mathbb{R}\times\mathbb{T}\times\mathbb{R}_+^*} \|T_{s_0,\theta,\alpha}u_n - Q_+\|^2_{\dot{H}^1(\mathbb{H}^1)} \underset{n\to\infty}{\longrightarrow} \infty.$$

According to the consequence of the profile decomposition theorem stated in Proposition 3.10, since $\delta(u_n) \to 0$; then, up to a subsequence, there exist cores $(s_n)_{n\in\mathbb{N}} \in \mathbb{R}^{\mathbb{N}}$, an angle $\theta_0 \in \mathbb{T}$ and scalings $(\alpha_n)_{n\in\mathbb{N}} \in (\mathbb{R}_+^*)^{\mathbb{N}}$ such that

$$\|T_{s_n,\theta_0,\alpha_n}u_n - Q_+\|_{\dot{H}^1(\mathbb{H}^1)} \underset{n\to\infty}{\longrightarrow} 0.$$

We will make use of the implicit function theorem in order to apply Corollary 4.18 with some functions $T_{s_n,\theta_n,\alpha_n}u_n$ orthogonal to $\partial_s Q_+, iQ_+$ and $Q_+ + 2i\partial_s Q_+$ and get a contradiction. Consider the maps

$$F : \dot{H}^1(\mathbb{H}^1) \cap V_0^+ \to \mathbb{R}^3, \quad u \mapsto \big((u, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}, (u, iQ_+)_{\dot{H}^1(\mathbb{H}^1)}, (u, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}\big),$$
$$G : \mathbb{R} \times \mathbb{T} \times \mathbb{R}_+^* \times (\dot{H}^1(\mathbb{H}^1) \cap V_0^+) \to \mathbb{R}^3, \quad (s, \theta, \alpha, u) \mapsto F(T_{s,\theta,\alpha}u).$$

Then $F(Q_+) = 0$, so $G(0, 0, 1, Q_+) = 0$. Moreover, G is smooth in (s, θ, α), and the Jacobian $\mathrm{d}_{s,\theta,\alpha}G(0, 0, 1, Q_+)$ of this application along (s, θ, α) at $(s, \theta, \alpha, u) = (0, 0, 1, Q_+)$ is equal to

$$\begin{pmatrix} \|\partial_s Q_+\|^2_{\dot{H}^1(\mathbb{H}^1)} & (iQ_+, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)} & (Q_+ + 2i\partial_s Q_+, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)} \\ (\partial_s Q_+, iQ_+)_{\dot{H}^1(\mathbb{H}^1)} & \|iQ_+\|^2_{\dot{H}^1(\mathbb{H}^1)} & (Q_+ + 2i\partial_s Q_+, iQ_+)_{\dot{H}^1(\mathbb{H}^1)} \\ (\partial_s Q_+, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)} & (iQ_+, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)} & \|Q_+ + 2i\partial_s Q_+\|^2_{\dot{H}^1(\mathbb{H}^1)} \end{pmatrix}.$$

Replacing all the terms by their values, we get

$$\mathrm{d}_{s,\theta,\alpha}G(0, 0, 1, Q_+) = \begin{pmatrix} \frac{\pi^2}{2} & \frac{\pi^2}{2} & 0 \\ 0 & \frac{\pi^2}{2} & 0 \\ 0 & 0 & \pi^2 \end{pmatrix},$$

which is invertible. By the implicit function theorem, we get continuously differentiable functions $S_0(u)$, $\Theta(u)$ and $A(u)$, defined in a neighborhood $\mathcal{V}$ of Q_+ and valued in a neighborhood of $(0, 0, 1)$: if $u \in \mathcal{V}$, then $\|T_{S_0(u),\Theta(u),A(u)}u - Q_+\|_{\dot{H}^1(\mathbb{H}^1)} \le \varepsilon_0$ (where ε_0 is taken from Corollary 4.18). These functions satisfy $(S_0(Q_+), \Theta(Q_+), A(Q_+)) = (0, 0, 1)$ and

$$G(S_0(u), \Theta(u), A(u), u) = 0.$$

Now, since $\|T_{s_n,\theta_0,\alpha_n}u_n - Q_+\|_{\dot{H}^1(\mathbb{H}^1)} \to 0$ as $n \to \infty$, there exists $N \in \mathbb{N}$ such that for all $n \ge N$, $T_{s_n,\theta_0,\alpha_n}u_n \in \mathcal{V}$. Therefore, defining $s_n' = s_n + S_0(T_{s_n,\theta_0,\alpha_n}u_n)$, $\theta_n' = \theta_0 + \Theta(T_{s_n,\theta_0,\alpha_n}u_n)$ and $\alpha_n' = \alpha_n + A(T_{s_n,\theta_0,\alpha_n}u_n)$, we get $\tilde{u}_n := T_{s_n',\theta_n',\alpha_n'}u_n \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+$ such that $\|\tilde{u}_n - Q_+\|_{\dot{H}^1(\mathbb{H}^1)} \le \varepsilon_0$ and

$$(\tilde{u}_n, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)} = (\tilde{u}_n, iQ_+)_{\dot{H}^1(\mathbb{H}^1)} = (\tilde{u}_n, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)} = 0.$$

Moreover, by invariance under symmetries, $\delta(\tilde{u}_n) = \delta(u_n)$, so applying Corollary 4.18 to $\tilde{u}_n = T_{s_n',\theta_n',\alpha_n'}u_n$, we get that for some constant $C > 0$,

$$\|T_{s_n',\theta_n',\alpha_n'}u_n - Q_+\|^2_{\dot{H}^1(\mathbb{H}^1)} \le C\delta(u_n).$$

This is a contradiction with the assumption that

$$\frac{1}{\delta(u_n)} \inf_{(s_0,\theta,\alpha) \in \mathbb{R} \times \mathbb{T} \times \mathbb{R}_+^*} \|T_{s_0,\theta,\alpha}u_n - Q_+\|^2_{\dot{H}^1(\mathbb{H}^1)} \underset{n\to\infty}{\longrightarrow} \infty. \qquad \square$$

5. Uniqueness of traveling waves for the Schrödinger equation

We now show that the study of the limiting profile Q_+, and in particular the linear stability, enables us to prove some uniqueness results about the sequence of traveling waves Q_β with speed β sufficiently close to 1. The argument is similar to that of [Gérard et al. 2018] for the half-wave equation: for β close to 1, Q_β is close to Q_+, so we can make a link between the respective linearized operators.

In order to do so, we first need to show some regularity properties and decay estimates on the profiles Q_β (Section 5A). For the half-wave equation, these estimates came from the Sobolev embedding $H^{\frac{1}{2}}(\mathbb{R}) \hookrightarrow L^p(\mathbb{R})$, $2 \le p < \infty$ and the convergence in $H^{\frac{1}{2}}(\mathbb{R})$.

Recall that from Definition 3.5, $\mathcal{Q}_\beta$ denotes the set of ground states Q_β satisfying (3). One can summarize the convergence of $(Q_\beta)_\beta$ from Section 3B combined with the uniqueness result for Q_+ from Section 3C as follows:

Proposition 5.1. *For all $\beta \in (-1,1)$, fix a ground state $Q_\beta^0 \in \mathcal{Q}_\beta$ of speed β. Then there exist scalings $(\alpha_\beta)_\beta$ in $\mathbb{R}_+^*$, cores $(s_\beta)_\beta$ in $\mathbb{R}$ and an angle θ in $\mathbb{T}$ such that after a change of functions $Q_\beta := e^{i\theta}\alpha_\beta Q_\beta(\alpha_\beta\,\cdot, \alpha_\beta\,\cdot, \alpha_\beta^2(\cdot + s_\beta))$, the sequence $(Q_\beta)_\beta$ of solutions to* (3),

$$-\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} Q_\beta = |Q_\beta|^2 Q_\beta,$$

converges as $\beta \to 1$ in $\dot{H}^1(\mathbb{H}^1)$ to the unique (*up to symmetries*) *ground state solution to* (4), *namely $D_s Q_+ = \Pi_0^+(|Q_+|^2 Q_+)$, which is written*

$$Q_+(x,y,s) = \frac{i\sqrt{2}}{s + i(x^2+y^2) + i}.$$

5A. ***Regularity and decay of the traveling waves Q_β.*** In this section, we collect information on the regularity of the profiles Q_β. We show that after the transformations from Proposition 5.1, they are uniformly bounded in $L^p(\mathbb{H}^1)$ for all $p > 2$ when β is close to 1. We deduce a uniform bound in $L^\infty(\mathbb{H}^1)$, from which we estimate the decay of these profiles when the variable $(x,y,s) \in \mathbb{H}^1$ tends to infinity. Finally, we show that the sequence $(Q_\beta)_\beta$ is bounded in $\dot{H}^k(\mathbb{H}^1)$ for β close to 1 and fixed $k \ge 1$.

The operator $-(\Delta_{\mathbb{H}^1} + \beta D_s)/(1-\beta)$ admits an explicit fundamental solution.

Theorem 5.2 [Stein 1993]. *Let*

$$m_\beta(x,y,s) = -\frac{1-\beta}{2\pi^2}\Gamma\Big(\frac{1-\beta}{2}\Big)\Gamma\Big(\frac{1+\beta}{2}\Big)\frac{1}{(x^2+y^2-is)^{\frac{1-\beta}{2}}(x^2+y^2+is)^{\frac{1+\beta}{2}}}.$$

Then m_β is a fundamental solution for $-\frac{\Delta_{\mathbb{H}^1}+\beta D_s}{1-\beta}$: in the sense of distributions,

$$-\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} m_\beta = \delta_0.$$

The proof of regularity for the Q_β relies on the use of generalized Hölder's and Young's inequalities in weak Lebesgue spaces (see [Vétois 2019] for the strategy). We define the Lorentz spaces as follows:

Definition 5.3 (Lorentz spaces). Fix $p \in [1,\infty)$ and $q \in [1,\infty]$. The Lorentz space $L^{p,q}(\mathbb{H}^1)$ is the set of all functions $f : \mathbb{H}^1 \to \mathbb{C}$ with finite $L^{p,q}(\mathbb{H}^1)$ norm, where

$$\|f\|_{L^{p,q}(\mathbb{H}^1)} := \begin{cases} \left(p \displaystyle\int_0^\infty R^{q-1} \lambda_3\big(\{u \in \mathbb{H}^1 : |f(u)| \geq R\}\big)^{\frac{q}{p}} \, \mathrm{d}R\right)^{\frac{1}{q}} & \text{if } q < \infty, \\ \sup\limits_{R>0} \big(R^p \lambda_3\big(\{u \in \mathbb{H}^1 : |f(u)| \geq R\}\big)\big) & \text{if } q = \infty. \end{cases}$$

The usual $L^p(\mathbb{H}^1)$ spaces coincide with $L^{p,p}(\mathbb{H}^1)$ spaces. In general, $\|\cdot\|_{L^{p,q}(\mathbb{H}^1)}$ is not a norm, since the Minkowski inequality may fail. The following inclusion relations are true [Stein and Weiss 1971]:

Proposition 5.4 (growth of $L^{p,q}$ spaces). *Let $p \in [1,\infty)$ and $q_1, q_2 \in [1,\infty]$ such that $q_1 \leq q_2$. Then $L^{p,q_1}(\mathbb{H}^1) \subset L^{p,q_2}(\mathbb{H}^1)$.*

Note that the functions m_β, $\beta \in [0,1)$, are uniformly bounded in $L^{2,\infty}$. Indeed, let $R > 0$, then

$$\lambda_3(\{(x,y,s) \in \mathbb{H}^1;\ |x|^2 + |y|^2 + |s| \leq R\}) = R^2 \lambda_3(\{(x',y',s') \in \mathbb{H}^1;\ |x'|^2 + |y'|^2 + |s'| \leq 1\}).$$

Moreover, the constants

$$c_\beta := -\frac{1-\beta}{2\pi^2} \Gamma\Big(\frac{1-\beta}{2}\Big) \Gamma\Big(\frac{1+\beta}{2}\Big)$$

are bounded for $\beta \in [0,1)$.

Definition 5.5 (convolution). The convolution product of two functions f and g on $\mathbb{H}^1$ is defined by

$$f \star g(u) = \int_{\mathbb{H}^1} f(v) g(v^{-1}u) \, \mathrm{d}\lambda_3(v) = \int_{\mathbb{H}^1} f(uv^{-1}) g(v) \, \mathrm{d}\lambda_3(v).$$

Note that the convolution in $\mathbb{H}^1$ is not commutative and that the relation

$$P(f \star g) = f \star Pg$$

holds for every left-invariant vector field P in $\mathbb{H}^1$ (for example, $P = -\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta}$), whereas in general $P(f \star g) \neq Pf \star g$.

Let us recall the generalizations of Hölder's and Young's inequalities for Lorentz spaces.

Lemma 5.6 (Hölder). *Let $p_1, p_2, p \in (0,\infty)$ and let $q_1, q_2, q \in (0,\infty]$ such that $\frac{1}{p_1} + \frac{1}{p_2} = \frac{1}{p}$ and $\frac{1}{q_1} + \frac{1}{q_2} \geq \frac{1}{q}$, with the convention $\frac{1}{\infty} = 0$. Then there exists $C = C(p_1, p_2, p, q_1, q_2, q)$ such that for any $f \in L^{p_1,q_1}(\mathbb{H}^1)$ and any $g \in L^{p_2,q_2}(\mathbb{H}^1)$, we have $fg \in L^{p,q}(\mathbb{H}^1)$ and*

$$\|fg\|_{L^{p,q}(\mathbb{H}^1)} \leq C \|f\|_{L^{p_1,q_1}(\mathbb{H}^1)} \|g\|_{L^{p_2,q_2}(\mathbb{H}^1)}.$$

Lemma 5.7 (Young). *Let $p_1, p_2, p \in (1,\infty)$ and let $q_1, q_2, q \in (0,\infty]$ such that $\frac{1}{p_1} + \frac{1}{p_2} = \frac{1}{p} + 1$ and $\frac{1}{q_1} + \frac{1}{q_2} \geq \frac{1}{q}$, with the convention $\frac{1}{\infty} = 0$. Then there exists $C = C(p_1, p_2, p, q_1, q_2, q)$ such that for any $f \in L^{p_1,q_1}(\mathbb{H}^1)$ and any $g \in L^{p_2,q_2}(\mathbb{H}^1)$, we have $f \star g \in L^{p,q}(\mathbb{H}^1)$ and*

$$\|f \star g\|_{L^{p,q}(\mathbb{H}^1)} \leq C \|f\|_{L^{p_1,q_1}(\mathbb{H}^1)} \|g\|_{L^{p_2,q_2}(\mathbb{H}^1)}.$$

Theorem 5.2 implies the following formula for Q_β:

Corollary 5.8. *For all* $\beta \in (-1, 1)$,

$$Q_\beta = (|Q_\beta|^2 Q_\beta) \star m_\beta.$$

Let us now prove the boundedness of Q_β in $L^p(\mathbb{H}^1)$, $p > 2$.

Theorem 5.9. *For all* $p > 2$, *there exist* $C_p > 0$ *and* $\beta_*(p) \in (0, 1)$ *such that for all* $\beta \in (\beta_*(p), 1)$, $\|Q_\beta\|_{L^p(\mathbb{H}^1)} \leq C_p$.

Proof. We proceed by contradiction. Fix $p > 2$. Assume that there exists a sequence $(\beta_n)_{n\in\mathbb{N}}$ in $(0, 1)$ converging to 1 and such that $\|Q_{\beta_n}\|_{L^p(\mathbb{H}^1)} \in [n, \infty]$ for all $n \in \mathbb{N}$. By duality and density of $\mathcal{C}_c^\infty(\mathbb{H}^1)$ in $L^q(\mathbb{H}^1)$, $\frac{1}{p} + \frac{1}{q} = 1$, there exists a sequence $(\varphi_n)_{n\in\mathbb{N}}$ in $L^q(\mathbb{H}^1) \cap L^{\frac{4}{3}}(\mathbb{H}^1)$ such that $\|\varphi_n\|_{L^q(\mathbb{H}^1)} \leq 1$ for all n and

$$\left|\int_{\mathbb{H}^1} Q_{\beta_n} \varphi_n \, \mathrm{d}\lambda_3\right| \underset{n\to\infty}{\longrightarrow} \infty.$$

Let us define

$$K_n := \left\{\varphi \in L^q(\mathbb{H}^1) \cap L^{\frac{4}{3}}(\mathbb{H}^1) : \|\varphi\|_{L^q(\mathbb{H}^1)} \leq \|\varphi_n\|_{L^q(\mathbb{H}^1)} \text{ and } \|\varphi\|_{L^{\frac{4}{3}}(\mathbb{H}^1)} \leq \|\varphi_n\|_{L^{\frac{4}{3}}(\mathbb{H}^1)}\right\}.$$

Since $Q_{\beta_n} \in L^4(\mathbb{H}^1)$, the supremum over functions $\varphi \in K_n$ of $\int_{\mathbb{H}^1} Q_{\beta_n} \varphi \, \mathrm{d}\lambda_3$ is finite. Thus, if we change φ_n to another function φ from K_n, where $\int_{\mathbb{H}^1} Q_{\beta_n} \varphi \, \mathrm{d}\lambda_3$ is closer to this supremum, the K_n corresponding to φ and thus the new supremum will decrease. We can therefore assume up to changing φ_n that

$$2\left|\int_{\mathbb{H}^1} Q_{\beta_n} \varphi_n \, \mathrm{d}\lambda_3\right| \geq \sup_{\varphi \in K_n} \left|\int_{\mathbb{H}^1} Q_{\beta_n} \varphi \, \mathrm{d}\lambda_3\right|.$$

By density, let $(f_k)_{k\in\mathbb{N}}$ be a sequence in $\mathcal{C}_c^\infty(\mathbb{H}^1)$ such that $\||Q_+|^2 - f_k\|_{L^2(\mathbb{H}^1)} \to 0$ as $k \to \infty$. Denote, for $k, n \in \mathbb{N}$, $g_{n,k} := |Q_{\beta_n}|^2 - f_k$. We will use the fact that the functions $g_{n,k}$ have a small norm in $L^2(\mathbb{H}^1)$ when k and n are large enough thanks to Proposition 5.1. Let us cut

$$\begin{aligned}\int_{\mathbb{H}^1} Q_{\beta_n} \varphi_n \, \mathrm{d}\lambda_3 &= \int_{\mathbb{H}^1} \big((|Q_{\beta_n}|^2 Q_{\beta_n}) \star m_{\beta_n}\big) \varphi_n \, \mathrm{d}\lambda_3 \\ &= \int_{\mathbb{H}^1} \big((f_k Q_{\beta_n}) \star m_{\beta_n}\big) \varphi_n \, \mathrm{d}\lambda_3 + \int_{\mathbb{H}^1} \big((g_{n,k} Q_{\beta_n}) \star m_{\beta_n}\big) \varphi_n \, \mathrm{d}\lambda_3\end{aligned}$$

in order to evaluate these terms separately.

Concerning the first term on the right-hand side, using Lemmas 5.6 and 5.7,

$$\begin{aligned}\left|\int_{\mathbb{H}^1} \big((f_k Q_{\beta_n}) \star m_{\beta_n}\big) \varphi_n \, \mathrm{d}\lambda_3\right| &\leq \left\|\big((f_k Q_{\beta_n}) \star m_{\beta_n}\big) \varphi_n\right\|_{L^{1,1}(\mathbb{H}^1)} \\ &\leq C_1(p) \|(f_k Q_{\beta_n}) \star m_{\beta_n}\|_{L^{p,p}(\mathbb{H}^1)} \|\varphi_n\|_{L^{q,q}(\mathbb{H}^1)} \\ &\leq C_2(p) \|f_k Q_{\beta_n}\|_{L^{2p/(2+p),p}(\mathbb{H}^1)} \|m_{\beta_n}\|_{L^{2,\infty}(\mathbb{H}^1)} \|\varphi_n\|_{L^q(\mathbb{H}^1)}\end{aligned}$$

(we used that $2p/(2+p) > 1$ since $p > 2$). Using again Lemma 5.6, choosing any $\tau \in (0, \infty)$ such that $1/\tau \geq (4-p)/(4p)$ and $\sigma = 4p/(4+p) > 1$, we get

$$\left|\int_{\mathbb{H}^1} \big((f_k Q_{\beta_n}) \star m_{\beta_n}\big) \varphi_n \, \mathrm{d}\lambda_3\right| \leq C_3(p) \|f_k\|_{L^{\sigma,\tau}(\mathbb{H}^1)} \|Q_{\beta_n}\|_{L^{4,4}(\mathbb{H}^1)} \|m_{\beta_n}\|_{L^{2,\infty}(\mathbb{H}^1)} \|\varphi_n\|_{L^q(\mathbb{H}^1)}.$$

We know that $\|\varphi_n\|_{L^q(\mathbb{H}^1)} \le 1$ for all n, that $\|m_{\beta_n}\|_{L^{2,\infty}(\mathbb{H}^1)}$ is bounded independently of n and that $(Q_\beta)_{\beta\in[0,1)}$ is bounded in $L^4(\mathbb{H}^1)$, so there exists $C_4(p) > 0$ such that for all $k, n \in \mathbb{N}$,

$$\int_{\mathbb{H}^1} \big((f_k Q_{\beta_n}) \star m_{\beta_n}\big)\varphi_n \,\mathrm{d}\lambda_3 \le C_4(p)\|f_k\|_{L^{\sigma,\tau}(\mathbb{H}^1)}.$$

Applying Fubini's theorem to the second term on the right,

$$\begin{aligned}\int_{\mathbb{H}^1} \big((g_{n,k} Q_{\beta_n}) \star m_{\beta_n}\big)\varphi_n \,\mathrm{d}\lambda_3 &= \int_{\mathbb{H}^1}\int_{\mathbb{H}^1} (g_{n,k}Q_{\beta_n})(v) m_{\beta_n}(v^{-1}u)\varphi_n(u)\,\mathrm{d}\lambda_3(v)\,\mathrm{d}\lambda_3(u)\\ &= \int_{\mathbb{H}^1}\int_{\mathbb{H}^1} (g_{n,k}Q_{\beta_n})(v) m_{\beta_n}(v^{-1}u)\varphi_n(u)\,\mathrm{d}\lambda_3(u)\,\mathrm{d}\lambda_3(v)\\ &= \int_{\mathbb{H}^1}\int_{\mathbb{H}^1} (g_{n,k}Q_{\beta_n})(v) \check{m}_{\beta_n}(u^{-1}v)\varphi_n(u)\,\mathrm{d}\lambda_3(u)\,\mathrm{d}\lambda_3(v)\\ &= \int_{\mathbb{H}^1} (g_{n,k}Q_{\beta_n})(v)(\varphi_n \star \check{m}_{\beta_n})(v)\,\mathrm{d}\lambda_3(v),\end{aligned}$$

where

$$\check{m}_\beta(x,y,s) = m_\beta((x,y,s)^{-1}) = -\frac{1-\beta}{2\pi^2}\Gamma\Big(\frac{1-\beta}{2}\Big)\Gamma\Big(\frac{1+\beta}{2}\Big)\frac{1}{(x^2+y^2+is)^{\frac{1-\beta}{2}}(x^2+y^2-is)^{\frac{1+\beta}{2}}}$$

has the same bounds in $L^{2,\infty}(\mathbb{H}^1)$ as m_β.

But thanks to Lemmas 5.6 and 5.7,

$$\begin{aligned}\|g_{n,k}(\varphi_n \star \check{m}_{\beta_n})\|_{L^q(\mathbb{H}^1)} &\le C_1'(p)\|g_{n,k}\|_{L^{2,\infty}(\mathbb{H}^1)}\|\varphi_n \star \check{m}_{\beta_n}\|_{L^{2p/(p-2),q}(\mathbb{H}^1)}\\ &\le C_2'(p)\|g_{n,k}\|_{L^{2,\infty}(\mathbb{H}^1)}\|\varphi_n\|_{L^{q,q}(\mathbb{H}^1)}\|\check{m}_{\beta_n}\|_{L^{2,\infty}(\mathbb{H}^1)}.\end{aligned}$$

Note that the assumption $p > 2$ ensures that $\frac{2p}{p-2} \in (1,\infty)$.

Moreover, this last inequality still holds with the same reasoning when replacing p by 4 and its conjugate exponent q by $\frac{4}{3}$. Fix

$$C = \max\big(C_2'(p), C_2'(4)\big) \times \sup_{\beta\in[0,1)} \|\check{m}_\beta\|_{L^{2,\infty}(\mathbb{H}^1)}.$$

Then, when $g_{n,k}$ is nonzero in $L^2(\mathbb{H}^1)$, the function

$$\psi_{n,k} := \frac{1}{C\|g_{n,k}\|_{L^{2,\infty}(\mathbb{H}^1)}} g_{n,k}(\varphi_n \star \check{m}_{\beta_n})$$

belongs to K_n. Therefore by definition of φ_n, for all $k, n \in \mathbb{N}$,

$$\left|\int_{\mathbb{H}^1} Q_{\beta_n} g_{n,k}(\varphi_n \star \check{m}_{\beta_n})\,\mathrm{d}\lambda_3\right| \le 2C\|g_{n,k}\|_{L^{2,\infty}(\mathbb{H}^1)}\left|\int_{\mathbb{H}^1} Q_{\beta_n}\varphi_n\,\mathrm{d}\lambda_3\right|.$$

But

$$\|g_{n,k}\|_{L^{2,\infty}(\mathbb{H}^1)} \le \|\,|Q_{\beta_n}|^2 - f_k\|_{L^2(\mathbb{H}^1)} \le \|\,|Q_{\beta_n}|^2 - |Q_+|^2\|_{L^2(\mathbb{H}^1)} + \|\,|Q_+|^2 - f_k\|_{L^2(\mathbb{H}^1)},$$

and this quantity converges to 0 as $\min(n,k)$ goes to ∞ thanks to Proposition 5.1 and the construction of $(f_k)_{k\in\mathbb{N}}$. Therefore, there exists n_0 such that, for all $k \geq n_0$ and $n \geq n_0$, $2C\|g_{n,k}\|_{L^{2,\infty}(\mathbb{H}^1)} \leq \frac{1}{2}$, or in other words,

$$\left|\int_{\mathbb{H}^1} Q_{\beta_n} g_{n,k}(\varphi_n \star \check{m}_{\beta_n})\,\mathrm{d}\lambda_3\right| \leq \frac{1}{2}\left|\int_{\mathbb{H}^1} Q_{\beta_n}\varphi_n\,\mathrm{d}\lambda_3\right|.$$

Since

$$\int_{\mathbb{H}^1} Q_{\beta_n}\varphi_n\,\mathrm{d}\lambda_3 = \int_{\mathbb{H}^1}\big((f_k Q_{\beta_n}) \star m_{\beta_n}\big)\varphi_n\,\mathrm{d}\lambda_3 + \int_{\mathbb{H}^1} Q_{\beta_n} g_{n,k}(\varphi_n \star \check{m}_{\beta_n})\,\mathrm{d}\lambda_3,$$

we get that for all $k \geq n_0$ and $n \geq n_0$,

$$\left|\int_{\mathbb{H}^1} Q_{\beta_n}\varphi_n\,\mathrm{d}\lambda_3\right| \leq 2\left|\int_{\mathbb{H}^1}\big((f_k Q_{\beta_n}) \star m_{\beta_n}\big)\varphi_n\,\mathrm{d}\lambda_3\right|.$$

Fix $k \geq n_0$ and consider this inequality. There is a contradiction when n goes to ∞, since the right-hand side remains bounded by $C_4(p)\|f_k\|_{L^{\sigma,\tau}(\mathbb{H}^1)}$, whereas the left-hand side tends to ∞. □

Corollary 5.10. *For all $p \in (2,\infty)$ and $q \in (1,\infty)$, there exist $C_{p,q} > 0$ and $\beta_*(p,q) \in (0,1)$ such that for all $\beta \in (\beta_*(p,q),1)$, $\|Q_\beta\|_{L^{p,q}(\mathbb{H}^1)} \leq C_{p,q}$.*

We now collect some estimates on the decay of Q_β when β is close to 1.

Theorem 5.11. *There exist $C > 0$ and $\beta_* \in (0,1)$ such that, for all $\beta \in (\beta_*,1)$ and all $(x,y,s) \in \mathbb{H}^1$,*

$$|Q_\beta(x,y,s)| \leq \frac{C}{\rho(x,y,s)^2+1},$$

where $\rho(x,y,s) = ((x^2+y^2)^2+s^2)^{\frac{1}{4}}$ is the distance from $(x,y,s) \in \mathbb{H}^1$ to the origin.

Proof. We first show that the Q_β are uniformly bounded in $L^\infty(\mathbb{H}^1)$ for $\beta \in (\beta_*,1)$ if β_* is large enough. Let $u \in \mathbb{H}^1$. Applying Hölder's inequality (Lemma 5.6) to the right-hand side,

$$|Q_\beta(u)| = \left|\int_{v\in\mathbb{H}^1} |Q_\beta|^2 Q_\beta(v) m_\beta(v^{-1}u)\,\mathrm{d}\lambda_3(v)\right| \leq \||Q_\beta|^2 Q_\beta m_\beta(\cdot^{-1}u)\|_{L^1(\mathbb{H}^1)} \leq \||Q_\beta|^2 Q_\beta\|_{L^{2,1}(\mathbb{H}^1)}\|m_\beta\|_{L^{2,\infty}(\mathbb{H}^1)} \leq \|Q_\beta\|^3_{L^{6,3}(\mathbb{H}^1)}\|m_\beta\|_{L^{2,\infty}(\mathbb{H}^1)}.$$

The conclusion follows from Corollary 5.10.

For every $R > 0$, we set $B_R = \{(x,y,s) \in \mathbb{H}^1;\ \rho(x,y,s) \leq R\}$ and $M(R) = \sup_{(x,y,s)\in B_R^c} |Q_\beta(x,y,s)|$. Let $R > 0$, $u \in B_R^c$. We split the integral:

$$|(|Q_\beta|^2 Q_\beta) \star m(u)| \leq \left|\int_{v\in B_{R/2}} |Q_\beta|^2 Q_\beta(v) m_\beta(v^{-1}u)\,\mathrm{d}\lambda_3(v)\right| + \left|\int_{v\in B_{R/2}^c} |Q_\beta|^2 Q_\beta(v) m_\beta(v^{-1}u)\,\mathrm{d}\lambda_3(v)\right|.$$

For the first summand, $v \in B_{R/2}$ implies $uv^{-1} \in B_{R/2}^c$, so

$$\left|\int_{v\in B_{R/2}} |Q_\beta|^2 Q_\beta(v) m_\beta(v^{-1}u)\,\mathrm{d}\lambda_3(v)\right| \leq \frac{|c_\beta|}{R^2}\|Q_\beta\|^3_{L^3(\mathbb{H}^1)}.$$

Thanks to Theorem 5.9, one knows that up to increasing β_*, there exists some constant C such that $|c_\beta|\|Q_\beta\|^3_{L^3(\mathbb{H}^1)} \le C$ for all $\beta \in (\beta_*, 1)$.

To estimate the second summand we apply Hölder's inequality (Lemma 5.6):

$$\begin{aligned}\left|\int_{v\in B^c_{R/2}} |Q_\beta|^2 Q_\beta(v) m_\beta(v^{-1}u)\,\mathrm{d}\lambda_3(v)\right| &\le \||Q_\beta|^2 m_\beta(\cdot^{-1}u)\|_{L^1(B^c_{R/2})} M\big(\tfrac{R}{2}\big)\\ &\le \||Q_\beta|^2\|_{L^{2,1}(B^c_{R/2})}\|m_\beta(\cdot^{-1}u)\|_{L^{2,\infty}(B^c_{R/2})} M\big(\tfrac{R}{2}\big)\\ &\le \|Q_\beta\|_{L^{4,4}(B^c_{R/2})}\|Q_\beta\|_{L^{4,4/3}(B^c_{R/2})}\|m_\beta\|_{L^{2,\infty}(\mathbb{H}^1)} M\big(\tfrac{R}{2}\big).\end{aligned}$$

Thanks to the convergence of $(Q_\beta)_\beta$ to Q_+ in $\dot H^1(\mathbb{H}^1)$ as β tends to 1 and the Folland–Stein embedding $\dot H^1(\mathbb{H}^1) \hookrightarrow L^4(\mathbb{H}^1)$, the sequence $(Q_\beta)_\beta$ converges to Q_+ in $L^4(\mathbb{H}^1)$ and therefore is tight in $L^4(\mathbb{H}^1)$. Moreover, the norms $\|Q_\beta\|_{L^{4,4/3}(\mathbb{H}^1)}$, for β close to 1, are bounded. Therefore, up to increasing β_* again, one can choose $R_0 > 0$ such that

$$\sup_{\beta\in(\beta_*,1)} \big(\|Q_\beta\|_{L^{4,4/3}(B^c_{R_0/2})}\|m_\beta\|_{L^{2,\infty}(\mathbb{H}^1)}\big) \times \|Q_\beta\|_{L^{4,4}(B^c_{R_0/2})} \le \tfrac{1}{8}.$$

Then, for every $R \ge R_0$,

$$\left|\int_{v\in B^c_{R/2}} |Q_\beta|^2 Q_\beta(v) m_\beta(v^{-1}u)\,\mathrm{d}\lambda_3(v)\right| \le \tfrac{1}{8} M\big(\tfrac{R}{2}\big).$$

Combining the two estimates and applying them to $R = 2^n$, $n \ge n_0$ so that $2^{n_0} \ge R_0$, we get

$$M(2^n) \le \frac{C}{4^n} + \frac{1}{8} M(2^{n-1}).$$

Iterating, one knows that for all $n \ge n_0$,

$$\begin{aligned}M(2^n) &\le C\sum_{k=0}^{n-n_0} \frac{1}{4^{n-k}}\frac{1}{8^k} + \frac{1}{8^{n-n_0+1}} M(2^{n_0-1})\\ &\le C4^{-n}\sum_{k=0}^{n-n_0} 4^{-k} + 8^{n_0+1}M(2^{n_0-1})8^{-n} \le (2C + 8^{n_0+1}M(2^{n_0-1}))4^{-n}.\end{aligned}$$

Since $\rho(u) \sim 2^n$ for $2^n \le \rho(u) \le 2^{n+1}$, this completes the proof of the result. □

Corollary 5.12. *For some $\beta_* \in (0, 1)$, for all $k \ge 1$, there exists $C_k > 0$ such that for all $\beta \in (\beta_*, 1)$,*

$$\|Q_\beta\|_{\dot H^k(\mathbb{H}^1)} \le C_k.$$

Proof. It is enough to prove the first part of the claim for $k \in \mathbb{N}$. We proceed by induction on k. We already know that it is true for $k = 1$, because

$$\|Q_\beta\|^2_{\dot H^1(\mathbb{H}^1)} \le \frac{(-(\Delta_{\mathbb{H}^1} + \beta D_s)Q_\beta, Q_\beta)_{\dot H^{-1}(\mathbb{H}^1)\times \dot H^1(\mathbb{H}^1)}}{1-\beta} = \frac{I_\beta}{(1-\beta)^2},$$

and $\big(\frac{I_\beta}{(1-\beta)^2}\big)_\beta$ is bounded (see 3B).

The following additional assumption will be useful in the induction step: Up to increasing β_*, we can assume that the Q_β are bounded in $L^6(\mathbb{H}^1)$ and in $L^\infty(\mathbb{H}^1)$ for $\beta \in (\beta_*, 1)$.

Suppose now that the Q_β are bounded in $\dot{H}^k(\mathbb{H}^1)$ for an integer $k \geq 1$. Then by Leibniz' rule, since $\Delta_{\mathbb{H}^1} = \frac{1}{4}(X^2 + Y^2)$ for radial functions, with $X = \partial_x + 2y\partial_s$ and $Y = \partial_y - 2x\partial_s$, there exist some coefficients c_λ such that

$$-\Delta_{\mathbb{H}^1}^{k-1}\Big(-\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} Q_\beta\Big) = -\Delta_{\mathbb{H}^1}^{k-1}(|Q_\beta|^2 Q_\beta) = \sum_{|\lambda_1|+|\lambda_2|+|\lambda_3|=2k-2} c_\lambda \partial^{\lambda_1}(Q_\beta)\partial^{\lambda_2}(Q_\beta)\partial^{\lambda_3}(\overline{Q_\beta}).$$

The notation is similar as in $\mathbb{R}^N$, λ_j being a finite sequence of letters X and Y of length $|\lambda_j|$, $\partial^X := X$, $\partial^Y := Y$. The following inequality can be easily proven via the Fourier transform:

$$\begin{aligned}(-\Delta_{\mathbb{H}^1}^{k+1} Q_\beta, Q_\beta)_{\dot{H}^{-1}(\mathbb{H}^1)\times \dot{H}^1(\mathbb{H}^1)} &= (-\Delta_{\mathbb{H}^1}^{k} Q_\beta, -\Delta_{\mathbb{H}^1} Q_\beta)_{\dot{H}^{1}(\mathbb{H}^1)\times \dot{H}^{-1}(\mathbb{H}^1)} \\ &\leq \left(-\Delta_{\mathbb{H}^1}^{k-1}\left(-\frac{\Delta_{\mathbb{H}^1}+\beta D_s}{1-\beta} Q_\beta\right), -\frac{\Delta_{\mathbb{H}^1}+\beta D_s}{1-\beta} Q_\beta\right)_{\dot{H}^{1}(\mathbb{H}^1)\times \dot{H}^{-1}(\mathbb{H}^1)} \\ &\leq \left(-\Delta_{\mathbb{H}^1}^{k-1}\left(-\frac{\Delta_{\mathbb{H}^1}+\beta D_s}{1-\beta} Q_\beta\right), |Q_\beta|^2 Q_\beta\right)_{\dot{H}^{1}(\mathbb{H}^1)\times \dot{H}^{-1}(\mathbb{H}^1)}.\end{aligned}$$

We replace the term on the left by the above sum. By integration by parts and Leibniz' rule again, we can manage so that the following indexes of derivation μ_i all have length less or equal than $(k-1)$:

$$(-\Delta_{\mathbb{H}^1}^{k+1} Q_\beta, Q_\beta)_{\dot{H}^{-1}(\mathbb{H}^1)\times \dot{H}^1(\mathbb{H}^1)} = \sum_{\substack{|\mu_1|+\cdots+|\mu_6|=2k-2 \\ |\mu_1|,\ldots,|\mu_6|\leq k-1}} c'_\mu \int_{\mathbb{H}^1} \partial^{\mu_1}(Q_\beta)\cdots\partial^{\mu_4}(Q_\beta)\partial^{\mu_5}(\overline{Q_\beta})\partial^{\mu_6}(\overline{Q_\beta}).$$

We now apply Hölder's inequality with exponents $p_1, \ldots, p_6 \in (2, \infty)$ satisfying $\frac{1}{p_1} + \cdots + \frac{1}{p_6} = 1$, to be chosen later. Then, denoting $m_j = |\mu_j|$,

$$\left|\int_{\mathbb{H}^1} \partial^{\mu_1}(Q_\beta)\cdots\partial^{\mu_4}(Q_\beta)\partial^{\mu_5}(\overline{Q_\beta})\partial^{\mu_6}(\overline{Q_\beta})\right| \leq \|Q_\beta\|_{\dot{W}^{m_1,p_1}(\mathbb{H}^1)} \cdots \|Q_\beta\|_{\dot{W}^{m_6,p_6}(\mathbb{H}^1)}.$$

Let us choose the p_i appropriately. The aim is to use complex interpolation, and in particular the following relation between homogeneous Sobolev spaces (see, e.g., [Bergh and Löfström 1976], Theorem 6.4.5, assertion (7)):

$$(L^q(\mathbb{H}^1), \dot{H}^k(\mathbb{H}^1))_\theta = \dot{W}^{m,p}(\mathbb{H}^1),$$

where $p, q \in (2, \infty)$, $m = (1-\theta)0 + \theta k$ and $\frac{1}{p} = \frac{1-\theta}{q} + \frac{\theta}{2}$. For example, we choose $\theta_i = \frac{m_i}{k}$ and p_i such that $\frac{1}{p_i} = \frac{1}{6k} + \frac{m_i}{2k}$. Then

$$0 < \frac{1}{p_i} \leq \frac{1}{6k} + \frac{k-1}{2k} = \frac{1+3k-3}{6k} < \frac{1}{2},$$

so $p_i \in (2, \infty)$ and

$$\frac{1}{p_1} + \cdots + \frac{1}{p_6} = \frac{1}{k} + \frac{2k-2}{2k} = 1.$$

This choice leads to the exponents

$$q_i = \frac{6k}{1-m_i/k}.$$

Since $0 \le m_i \le k-1$, $2 < 6k \le q_i \le 6k^2 < \infty$, and we can therefore apply the interpolation result.

Since there is a finite number of terms in the sum, the boundedness of Q_β in $L^6(\mathbb{H}^1)$, in $L^\infty(\mathbb{H}^1)$ and in $\dot{H}^k(\mathbb{H}^1)$ for $\beta > \beta_*$ ensures that there exists $C_{k+1} > 0$ such that for $\beta > \beta_*$,

$$\|(-\Delta_{\mathbb{H}^1})^{\frac{k+1}{2}} Q_\beta\|_{L^2(\mathbb{H}^1)} \le C_{k+1},$$

so the Q_β are bounded in $\dot{H}^{k+1}(\mathbb{H}^1)$. □

5B. *Invertibility of $\mathcal{L}_{Q_\beta}$.* For $\beta \in (-1,1)$ the linearized operator around Q_β for the Schrödinger equation is

$$\mathcal{L}_{Q_\beta} h = -\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} h - 2|Q_\beta|^2 h - Q_\beta^2 \bar{h}, \quad h \in \dot{H}^1(\mathbb{H}^1).$$

We prove the invertibility of this operator on a space of finite codimension.

Proposition 5.13. *There exist a neighborhood $\mathcal{V}$ of Q_+, $\beta_* \in (0,1)$ and some constant $c > 0$ such that for all $\beta \in (\beta_*, 1)$, for all $Q_\beta \in \mathcal{Q}_\beta \cap \mathcal{V}$ and for all $h \in \dot{H}^1(\mathbb{H}^1)$,*

$$\|\mathcal{L}_{Q_\beta} h\|_{\dot{H}^{-1}(\mathbb{H}^1)} + |(h, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(h, iQ_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(h, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}| \ge c\|h\|_{\dot{H}^1(\mathbb{H}^1)}.$$

Proof. Let $\beta \in (0,1)$ and $Q_\beta \in \mathcal{Q}_\beta$. Let $h \in \dot{H}^1(\mathbb{H}^1)$. We decompose $h = h^+ + h_\perp$, where $h^+ \in \dot{H}^1(\mathbb{H}^1) \cap V_0^+$ and $h_\perp = h - h^+ \in \dot{H}^1(\mathbb{H}^1) \cap \bigoplus_{(n,\pm)\neq(0,+)} V_n^\pm$.

We split $\mathcal{L}_{Q_\beta} h$ as

$$\mathcal{L}_{Q_\beta} h = \mathcal{L}h^+ - r_+ - r_- + \mathcal{L}_{Q_\beta}^- h,$$

where

$$\begin{aligned}
\mathcal{L}h^+ &= -\Delta_{\mathbb{H}^1} h^+ - 2\Pi_0^+(|Q_+|^2 h^+) - \Pi_0^+(Q_+^2 \overline{h^+}),\\
r_+ &= 2\Pi_0^+((|Q_\beta|^2 - |Q_+|^2) h^+) + \Pi_0^+((Q_\beta^2 - Q_+^2)\overline{h^+}),\\
r_- &= 2\Pi_0^+(|Q_\beta|^2 h_\perp) + \Pi_0^+(Q_\beta^2 \overline{h_\perp}),\\
\mathcal{L}_{Q_\beta}^- h &= -\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} h_\perp - 2(\mathrm{Id} - \Pi_0^+)(|Q_\beta|^2 h) - (\mathrm{Id} - \Pi_0^+)(Q_\beta^2 \bar{h}).
\end{aligned}$$

We treat each term separately.

- Concerning $\mathcal{L}h^+$, thanks to Corollary 4.17,

$$\|\mathcal{L}h^+\|_{\dot{H}^{-1}(\mathbb{H}^1)} + |(h^+, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(h^+, iQ_+)_{\dot{H}^1(\mathbb{H}^1)}| + |(h^+, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}| \ge c\|h^+\|_{\dot{H}^1(\mathbb{H}^1)}.$$

Since $\partial_s Q_+$, iQ_+ and $(Q_+ + 2i\partial_s Q_+)$ are in V_0^+, we know that $(h^+, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)} = (h, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}$, $(h^+, iQ_+)_{\dot{H}^1(\mathbb{H}^1)} = (h, iQ_+)_{\dot{H}^1(\mathbb{H}^1)}$ and $(h^+, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)} = (h, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)}$.

- Now consider r_+ and r_-. Let K be the constant in the Folland–Stein embedding $\dot{H}^1(\mathbb{H}^1) \hookrightarrow L^4(\mathbb{H}^1)$,

$$\|g\|_{L^4(\mathbb{H}^1)} \le K\|g\|_{\dot{H}^1(\mathbb{H}^1)}, \quad g \in \dot{H}^1(\mathbb{H}^1).$$

Since the sequence $(\|Q_\beta\|_{L^4(\mathbb{H}^1)})_\beta$ is bounded by some constant C_1,

$$\begin{aligned}\|r_-\|_{L^{\frac{4}{3}}(\mathbb{H}^1)} &\le 3C_1^2\|h_\perp\|_{L^4(\mathbb{H}^1)} \le 3KC_1^2\|h_\perp\|_{\dot{H}^1(\mathbb{H}^1)},\\ \|r_+\|_{L^{\frac{4}{3}}(\mathbb{H}^1)} &\le 3\|Q_\beta - Q_+\|_{L^4(\mathbb{H}^1)}(\|Q_\beta\|_{L^4(\mathbb{H}^1)} + \|Q_+\|_{L^4(\mathbb{H}^1)})\|h^+\|_{L^4(\mathbb{H}^1)}\\ &\le 6C_1\|Q_\beta - Q_+\|_{L^4(\mathbb{H}^1)}\|h^+\|_{L^4(\mathbb{H}^1)}\\ &\le 6KC_1\|Q_\beta - Q_+\|_{L^4(\mathbb{H}^1)}\|h^+\|_{\dot{H}^1(\mathbb{H}^1)}.\end{aligned}$$

Fix $\varepsilon > 0$ to be determined later. There exists $\beta_*(\varepsilon)$ such that for $\beta > \beta_*(\varepsilon)$,

$$\|Q_\beta - Q_+\|_{L^4(\mathbb{H}^1)} \le \varepsilon.$$

We conclude by the dual embedding $L^{\frac{4}{3}}(\mathbb{H}^1) \hookrightarrow \dot{H}^{-1}(\mathbb{H}^1)$ that there exists a constant C_2 (independent of ε)) such that for all $\beta \in (\beta_*(\varepsilon), 1)$,

$$\|r_+\|_{\dot{H}^{-1}(\mathbb{H}^1)} + \|r_-\|_{\dot{H}^{-1}(\mathbb{H}^1)} \le C_2\|h_\perp\|_{\dot{H}^1(\mathbb{H}^1)} + C_2\varepsilon\|h^+\|_{\dot{H}^1(\mathbb{H}^1)}.$$

- Finally, we focus on

$$\mathcal{L}^-_{Q_\beta}h = -\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta}h_\perp - 2(\mathrm{Id} - \Pi_0^+)(|Q_\beta|^2 h) - (\mathrm{Id} - \Pi_0^+)(Q_\beta^2\bar{h}).$$

In order to bound the $\dot{H}^{-1}$ norm of this term, we will use the fact that

$$\tfrac{1}{2}\|\mathcal{L}^-_{Q_\beta}h\|^2_{\dot{H}^{-1}(\mathbb{H}^1)} + \tfrac{1}{2}\|h_\perp\|^2_{\dot{H}^1(\mathbb{H}^1)} \ge \|\mathcal{L}^-_{Q_\beta}h\|_{\dot{H}^{-1}(\mathbb{H}^1)}\|h_\perp\|_{\dot{H}^1(\mathbb{H}^1)} \ge (\mathcal{L}^-_{Q_\beta}h, h_\perp)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}.$$

On the one hand, by inequality (8),

$$\left(-\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta}h_\perp, h_\perp\right)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} \ge \frac{1}{2}\frac{1}{1-\beta}\|h_\perp\|^2_{\dot{H}^1(\mathbb{H}^1)}.$$

On the other hand,

$$\begin{aligned}\left|\left(2(\mathrm{Id} - \Pi_0^+)(|Q_\beta|^2 h) + (\mathrm{Id} - \Pi_0^+)(Q_\beta^2\bar{h}), h_\perp\right)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)}\right| &\le 3C_1^2\|h\|_{L^4(\mathbb{H}^1)}\|h_\perp\|_{L^4(\mathbb{H}^1)}\\ &\le \varepsilon^2\|h\|^2_{L^4(\mathbb{H}^1)} + \frac{3C_1^2}{4\varepsilon^2}\|h_\perp\|^2_{L^4(\mathbb{H}^1)}.\end{aligned}$$

To summarize,

$$\frac{1}{2}\|\mathcal{L}^-_{Q_\beta}h\|^2_{\dot{H}^{-1}(\mathbb{H}^1)} + \frac{1}{2}\|h_\perp\|^2_{\dot{H}^1(\mathbb{H}^1)} \ge \frac{1}{2}\frac{1}{1-\beta}\|h_\perp\|^2_{\dot{H}^1(\mathbb{H}^1)} - \varepsilon^2\|h\|^2_{L^4(\mathbb{H}^1)} - \frac{3C_1^2}{4\varepsilon^2}\|h_\perp\|^2_{L^4(\mathbb{H}^1)},$$

and by removing the squares appropriately,

$$\begin{aligned}\|\mathcal{L}^-_{Q_\beta}h\|_{\dot{H}^{-1}(\mathbb{H}^1)} &\ge \sqrt{\frac{\beta}{1-\beta}}\,\|h_\perp\|_{\dot{H}^1(\mathbb{H}^1)} - \sqrt{2}\varepsilon\|h\|_{L^4(\mathbb{H}^1)} - \sqrt{\frac{3C_1^2}{2\varepsilon^2}}\,\|h_\perp\|_{L^4(\mathbb{H}^1)}\\ &\ge \sqrt{\frac{\beta}{1-\beta}}\,\|h_\perp\|_{\dot{H}^1(\mathbb{H}^1)} - \sqrt{2}K\varepsilon\|h\|_{\dot{H}^1(\mathbb{H}^1)} - \sqrt{\frac{3C_1^2}{2\varepsilon^2}}\,K\|h_\perp\|_{\dot{H}^1(\mathbb{H}^1)}.\end{aligned}$$

• We conclude by combining all the estimates. Because of the orthogonality of the decomposition along the spaces $\dot H^{-1}(\mathbb{H}^1)\cap V_n^{\pm}$ in $\dot H^{-1}(\mathbb{H}^1)$,

$$\|\mathcal{L}_{Q_\beta}h\|^2_{\dot H^{-1}(\mathbb{H}^1)} = \|\mathcal{L}h^+ + r_+ + r_-\|^2_{\dot H^{-1}(\mathbb{H}^1)} + \|\mathcal{L}^-_{Q_\beta}h\|^2_{\dot H^{-1}(\mathbb{H}^1)},$$

so we can add up the estimates to get

$$\begin{aligned}\sqrt{2}\,\|\mathcal{L}_{Q_\beta}h\|_{\dot H^{-1}(\mathbb{H}^1)} + |(h,\partial_s Q_+)_{\dot H^1(\mathbb{H}^1)}| + |(h,iQ_+)_{\dot H^1(\mathbb{H}^1)}| + |(h,Q_+ + 2i\partial_s Q_+)_{\dot H^1(\mathbb{H}^1)}| \\ \geq c\|h^+\|_{\dot H^1(\mathbb{H}^1)} - C_2\|h_\perp\|_{\dot H^1(\mathbb{H}^1)} - C_2\varepsilon\|h^+\|_{\dot H^1(\mathbb{H}^1)} + \sqrt{\frac{\beta}{1-\beta}}\,\|h_\perp\|_{\dot H^1(\mathbb{H}^1)} - \sqrt{2}K\varepsilon\|h\|_{\dot H^1(\mathbb{H}^1)} \\ - \sqrt{\frac{3C_1^2}{2\varepsilon^2}}\,K\|h_\perp\|_{\dot H^1(\mathbb{H}^1)}.\end{aligned}$$

The terms compensate as follows: Concerning $\|h^+\|_{\dot H^1(\mathbb{H}^1)}$, fix $\varepsilon>0$ small enough in the sense that

$$(C_2+\sqrt{2}K)\varepsilon < \frac{c}{2}.$$

Then for all $\beta>\beta_*(\varepsilon)$,

$$\begin{aligned}\sqrt{2}\,\|\mathcal{L}_{Q_\beta}h\|_{\dot H^{-1}(\mathbb{H}^1)} + |(h,\partial_s Q_+)_{\dot H^1(\mathbb{H}^1)}| + |(h,iQ_+)_{\dot H^1(\mathbb{H}^1)}| + |(h,Q_+ + 2i\partial_s Q_+)_{\dot H^1(\mathbb{H}^1)}| \\ \geq \frac{c}{2}\|h^+\|_{\dot H^1(\mathbb{H}^1)} + \left(\sqrt{\frac{\beta}{1-\beta}} - \left(C_2+\sqrt{2}K\varepsilon + \sqrt{\frac{3C_1^2}{2\varepsilon^2}}\,K\right)\right)\|h_\perp\|_{\dot H^1(\mathbb{H}^1)}.\end{aligned}$$

Now let $\beta_*\in(0,1)$ such that for all $\beta\in(\beta_*,1)$,

$$\sqrt{\frac{\beta}{1-\beta}} \geq C_2+\sqrt{2}K\varepsilon + \sqrt{\frac{3C_1^2}{2\varepsilon^2}} + \frac{c}{2}.$$

Then for all $\beta\in(\beta_*,1)$,

$$\begin{aligned}\sqrt{2}\|\mathcal{L}_{Q_\beta}h\|_{\dot H^{-1}(\mathbb{H}^1)} + |(h,\partial_s Q_+)_{\dot H^1(\mathbb{H}^1)}| + |(h,iQ_+)_{\dot H^1(\mathbb{H}^1)}| + |(h,Q_+ + 2i\partial_s Q_+)_{\dot H^1(\mathbb{H}^1)}| \\ \geq \frac{c}{2}(\|h^+\|_{\dot H^1(\mathbb{H}^1)} + \|h_\perp\|_{\dot H^1(\mathbb{H}^1)}) \geq \frac{c}{2}\|h\|_{\dot H^1(\mathbb{H}^1)}.\end{aligned}$$ □

5C. *Uniqueness of the traveling waves for β close to 1^-.*

Theorem 5.14. *There exist $\beta_*\in(0,1)$ and a neighborhood $\mathcal{V}$ of Q_+ in $\dot H^1(\mathbb{H}^1)$ such that for all $\beta\in(\beta_*,1)$, there is a unique $Q_\beta\in\mathcal{Q}_\beta\cap\mathcal{V}\cap(\partial_s Q_+, iQ_+, Q_+ + 2i\partial_s Q_+)^{\perp,\dot H^1(\mathbb{H}^1)}$. Moreover*:

(1) *For all $\beta\in(\beta_*,1)$,*

$$\mathcal{Q}_\beta = \{T_{s_0,\theta,\alpha}Q_\beta : (x,y,s)\mapsto e^{i\theta}\alpha Q_\beta(\alpha x,\alpha y,\alpha^2(s+s_0)) \mid (s_0,\theta,\alpha)\in\mathbb{R}\times\mathbb{T}\times\mathbb{R}_+^*\}.$$

(2) *For all $\gamma\in(0,\frac14)$ and all $k\in[1,\infty)$, $\|Q_\beta - Q_+\|_{\dot H^k(\mathbb{H}^1)} = \mathcal{O}((1-\beta)^\gamma)$.*

(3) *The map $\beta\in(\beta_*,1)\mapsto Q_\beta\in\dot H^1(\mathbb{H}^1)$ is smooth, tends to Q_+ as β tends to 1 and its derivative $\dot Q_\beta$ is uniquely determined by*

$$\begin{cases}\mathcal{L}_{Q_\beta}(\dot Q_\beta) = -\dfrac{\Delta_{\mathbb{H}^1}+D_s}{(1-\beta)^2}Q_\beta, \\ \dot Q_\beta\in\dot H^1(\mathbb{H}^1)\cap(\partial_s Q_+, iQ_+, Q_+ + 2i\partial_s Q_+)^{\perp,\dot H^1(\mathbb{H}^1)}.\end{cases} \tag{20}$$

Proof. • Fix any neighborhood $\mathcal{V}$ of Q_+. We first prove the existence of a profile $Q_\beta \in \mathcal{Q}_\beta \cap \mathcal{V} \cap (\partial_s Q_+, iQ_+, Q_+ + 2i\partial_s Q_+)^{\perp, \dot{H}^1(\mathbb{H}^1)}$ for β close enough to 1. For $\beta \in (0,1)$, we choose $Q_\beta \in \mathcal{Q}_\beta$ arbitrarily. By combining Corollary 4.20 with the fact that $\delta(Q_\beta) = \mathcal{O}((1-\beta)^{\frac{1}{2}})$ from Lemma 3.9, we know that

$$\inf_{(s_0,\theta,\alpha)\in\mathbb{R}\times\mathbb{T}\times\mathbb{R}_+^*} \|T_{s_0,\theta,\alpha} Q_\beta - Q_+\|_{\dot{H}^1(\mathbb{H}^1)} = \mathcal{O}((1-\beta)^{\frac{1}{4}}).$$

The same argument as in the proof of Corollary 4.20, based on the implicit function theorem, enables us to state that for β close enough to 1, one can choose $(s_\beta, \theta_\beta, \alpha_\beta) \in \mathbb{R}\times\mathbb{T}\times\mathbb{R}_+^*$ such that $\tilde{Q}_\beta := T_{s_\beta,\theta_\beta,\alpha_\beta} Q_\beta \in \mathcal{V}$ and

$$(\tilde{Q}_\beta, \partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)} = (\tilde{Q}_\beta, iQ_+)_{\dot{H}^1(\mathbb{H}^1)} = (\tilde{Q}_\beta, Q_+ + 2i\partial_s Q_+)_{\dot{H}^1(\mathbb{H}^1)} = 0.$$

This gives the existence part of the result.

• We now prove uniqueness for some small neighborhood $\mathcal{V}$ of Q_+. We first set $\mathcal{V}$ as the neighborhood of Q_+ from Proposition 5.13. Let $\beta \in (\beta_*, 1)$, and fix two profiles Q_β and $\tilde{Q}_\beta$ in $\mathcal{Q}_\beta \cap \mathcal{V} \cap (\partial_s Q_+, iQ_+, Q_+ + 2i\partial_s Q_+)^{\perp, \dot{H}^1(\mathbb{H}^1)}$. We define

$$h := Q_\beta - \tilde{Q}_\beta \in \dot{H}^1(\mathbb{H}^1) \cap (\partial_s Q_+, iQ_+, Q_+ + 2i\partial_s Q_+)^{\perp, \dot{H}^1(\mathbb{H}^1)}.$$

By subtracting the equations solved by Q_β and $\tilde{Q}_\beta$, h satisfies

$$-\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} h = 2\Pi_0^+(|Q_\beta|^2 h) + \Pi_0^+(Q_\beta^2 \bar{h}) + \mathcal{O}(\|h\|^2_{\dot{H}^1(\mathbb{H}^1)}),$$

so that

$$\mathcal{L}_{Q_\beta} h = \mathcal{O}(\|h\|^2_{\dot{H}^1(\mathbb{H}^1)}).$$

Since Q_β belongs to the neighborhood $\mathcal{V}$ from Proposition 5.13, this means that for some constants $c > 0$ and $C > 0$,

$$C\|h\|^2_{\dot{H}^1(\mathbb{H}^1)} \geq \|\mathcal{L}_{Q_\beta} h\|_{\dot{H}^{-1}(\mathbb{H}^1)} \geq c\|h\|_{\dot{H}^1(\mathbb{H}^1)}.$$

Up to reducing the neighborhood $\mathcal{V}$, one can chose it small enough such that h has to be the zero function.

• The description of the set $\mathcal{Q}_\beta$ is then a direct consequence. Indeed, if $\beta \in (\beta_*, 1)$, fix $U_\beta \in \mathcal{Q}_\beta$. We know from the first point that β_* is sufficiently close to 1 to ensure the existence of $(s_\beta, \theta_\beta, \alpha_\beta)$ in $\mathbb{R}\times\mathbb{T}\times\mathbb{R}_+^*$ such that $T_{s_\beta,\theta_\beta,\alpha_\beta} U_\beta \in \mathcal{V} \cap (\partial_s Q_+, iQ_+, Q_+ + 2i\partial_s Q_+)^{\perp, \dot{H}^1(\mathbb{H}^1)}$. By the uniqueness part, $T_{s_\beta,\theta_\beta,\alpha_\beta} U_\beta = Q_\beta$.

• We now show the convergence of $(Q_\beta)_\beta$ to Q_+ in $\dot{H}^k(\mathbb{H}^1)$ for all $k \geq 1$. Applying Corollary 4.18 to $(Q_\beta - Q_+)$, we know that for β close to 1,

$$\delta(Q_\beta) \geq c\|Q_\beta - Q_+\|^2_{\dot{H}^1(\mathbb{H}^1)}.$$

But $\delta(Q_\beta) = \mathcal{O}((1-\beta)^{\frac{1}{2}})$ from Lemma 3.9, therefore $\|Q_\beta - Q_+\|_{\dot{H}^1(\mathbb{H}^1)} = \mathcal{O}((1-\beta)^{\frac{1}{4}})$.

One can now deduce that for all $0 < \gamma < \frac{1}{4}$, as β goes to 1,

$$\|Q_\beta - Q_+\|_{\dot{H}^k(\mathbb{H}^1)} = \mathcal{O}((1-\beta)^\gamma).$$

Indeed, the interpolation formula [Bergh and Löfström 1976], $(\dot{H}^m(\mathbb{H}^1), \dot{H}^1(\mathbb{H}^1))_{4\gamma} = \dot{H}^k(\mathbb{H}^1)$, with $m \in \mathbb{R}$ chosen so that $k = (1-4\gamma)m + 4\gamma$, leads to

$$\|Q_\beta - Q_+\|_{\dot{H}^k(\mathbb{H}^1)} \le \|Q_\beta - Q_+\|_{\dot{H}^m(\mathbb{H}^1)}^{1-4\gamma} \|Q_\beta - Q_+\|_{\dot{H}^1(\mathbb{H}^1)}^{4\gamma},$$

and it only remains to use the fact that $(Q_\beta - Q_+)_\beta$ is bounded in $\dot{H}^m(\mathbb{H}^1)$ for β close to 1 (Corollary 5.12) and that $\|Q_\beta - Q_+\|_{\dot{H}^1(\mathbb{H}^1)}^{4\gamma} = \mathcal{O}((1-\beta)^\gamma)$ as β goes to 1.

• We now prove the last point of the theorem about the smoothness of the map $\beta \mapsto Q_\beta$. We first show that (20) uniquely determines a function $\dot{Q}_\beta$ lying on the appropriate space

$$W_1 := \dot{H}^1(\mathbb{H}^1) \cap (\partial_s Q_+, iQ_+, Q_+ + 2i\partial_s Q_+)^{\perp, \dot{H}^1(\mathbb{H}^1)}.$$

Define

$$W_{-1} := \dot{H}^{-1}(\mathbb{H}^1) \cap (\partial_s Q_+, iQ_+, Q_+ + 2i\partial_s Q_+)^{\perp, L^2(\mathbb{H}^1)},$$

and set

$$F : (\beta, U) \in (\beta_*, 1) \times W_1 \mapsto -\frac{\Delta_{\mathbb{H}^1} + \beta D_s}{1-\beta} U - |U|^2 U \in \dot{H}^{-1}(\mathbb{H}^1).$$

Notice that $\partial_\beta F$ takes values in the space W_{-1}. Indeed, the derivative $\partial_\beta F(\beta, U)$ is equal to

$$\partial_\beta F(\beta, U) = -\frac{\Delta_{\mathbb{H}^1} + D_s}{(1-\beta)^2} U.$$

In particular, since $Q_+, iQ_+, \partial_s Q_+$ and $i\partial_s Q_+$ belong to $\dot{H}^1(\mathbb{H}^1) \cap V_0^+$, and since $-(\Delta_{\mathbb{H}^1} + D_s)$ vanishes on this space,

$$\begin{aligned}(\partial_\beta F(\beta, U), \partial_s Q_+)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} &= (\partial_\beta F(\beta, U), iQ_+)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} \\ &= (\partial_\beta F(\beta, U), Q_+ + 2i\partial_s Q_+)_{\dot{H}^{-1}(\mathbb{H}^1)\times\dot{H}^1(\mathbb{H}^1)} = 0,\end{aligned}$$

or equivalently $\partial_\beta F(\beta, U) \in W_{-1}$.

Consider $\mathcal{L}_{Q_\beta}$ as a self-adjoint operator on $L^2(\mathbb{H}^1)$. Thanks to Proposition 5.13, we get that $\operatorname{Ker}(\mathcal{L}_{Q_\beta}) \subset \operatorname{Vect}_{\mathbb{R}}(\partial_s Q_+, iQ_+, Q_+ 2i\partial_s Q_+)$. Therefore,

$$\operatorname{Im}(\mathcal{L}_{Q_\beta}) = \operatorname{Ker}(\mathcal{L}_{Q_\beta})^{\perp, L^2(\mathbb{H}^1)} = \dot{H}^{-1}(\mathbb{H}^1) \cap \operatorname{Vect}_{\mathbb{R}}(\partial_s Q_+, iQ_+, Q_+ + 2i\partial_s Q_+)^{\perp, L^2(\mathbb{H}^1)},$$

so $\operatorname{Im}(\mathcal{L}_{Q_\beta}) = W_{-1}$. This implies that $\mathcal{L}_{Q_\beta}$ is an isomorphism from W_1 to W_{-1}, with continuous inverse:

$$\|\mathcal{L}_{Q_\beta} h\|_{\dot{H}^{-1}(\mathbb{H}^1)} \ge c\|h\|_{\dot{H}^1(\mathbb{H}^1)}, \quad h \in W_1.$$

In particular, $\partial_\beta F(\beta, Q_\beta) \in W_{-1} = \operatorname{Im}(\mathcal{L}_{Q_\beta})$, and by the invertibility of $\mathcal{L}_{Q_\beta}$ from W_1 to W_{-1}, $\dot{Q}_\beta := (\mathcal{L}_{Q_\beta})^{-1}(\partial_\beta F(\beta, Q_\beta))$ is uniquely determined and satisfies (20).

We now show that $\dot{Q}_\beta$ is a derivative of the map $\beta \in (\beta_*, 1) \mapsto Q_\beta \in \dot{H}^1(\mathbb{H}^1)$. Fix $\beta \in (\beta_*, 1)$. For $\varepsilon > 0$ small enough, $f_\varepsilon := (Q_{\beta+\varepsilon} - Q_\beta)/\varepsilon - \dot{Q}_\beta$ is well-defined. Moreover, since $(\beta + \varepsilon, Q_{\beta+\varepsilon})$ and

(β, Q_β) are both solution to the equation $F(\alpha, U) = 0$, then

$$\begin{aligned} 0 &= F(\beta+\varepsilon, Q_{\beta+\varepsilon}) - F(\beta, Q_\beta) = F(\beta+\varepsilon, Q_{\beta+\varepsilon}) - F(\beta, Q_{\beta+\varepsilon}) + F(\beta, Q_{\beta+\varepsilon}) - F(\beta, Q_\beta) \\ &= \varepsilon\partial_\beta F(\beta+\varepsilon, Q_\beta) + \mathcal{L}_{Q_\beta}(Q_{\beta+\varepsilon} - Q_\beta) + \mathcal{O}(\varepsilon^2 + \|Q_{\beta+\varepsilon} - Q_\beta\|^2_{\dot{H}^1(\mathbb{H}^1)}). \end{aligned}$$

Actually, since F is smooth in the β variable,

$$0 = \varepsilon\partial_\beta F(\beta, Q_\beta) + \mathcal{L}_{Q_\beta}(Q_{\beta+\varepsilon} - Q_\beta) + \mathcal{O}(\varepsilon^2 + \|Q_{\beta+\varepsilon} - Q_\beta\|^2_{\dot{H}^1(\mathbb{H}^1)}).$$

Replacing $\partial_\beta F(\beta, Q_\beta)$ by $\mathcal{L}_{Q_\beta}(\dot{Q}_\beta)$, we get

$$\mathcal{L}_{Q_\beta}(f_\varepsilon) = \mathcal{O}\left(\varepsilon + \frac{\|Q_{\beta+\varepsilon} - Q_\beta\|^2_{\dot{H}^1(\mathbb{H}^1)}}{\varepsilon}\right).$$

Since $f_\varepsilon \in W_1$, we get $\|\mathcal{L}_{Q_\beta}(f_\varepsilon)\|_{\dot{H}^{-1}(\mathbb{H}^1)} \geq c\|f_\varepsilon\|_{\dot{H}^1(\mathbb{H}^1)}$. This implies that for some constant $C > 0$,

$$C\left(\varepsilon + \frac{\|Q_{\beta+\varepsilon} - Q_\beta\|^2_{\dot{H}^1(\mathbb{H}^1)}}{\varepsilon}\right) \geq c\|f_\varepsilon\|_{\dot{H}^1(\mathbb{H}^1)}.$$

But $\|Q_{\beta+\varepsilon} - Q_\beta\|^2_{\dot{H}^1(\mathbb{H}^1)} = \varepsilon^2\|f_\varepsilon + \dot{Q}_\beta\|^2_{\dot{H}^1(\mathbb{H}^1)}$, so

$$C\varepsilon(1 + \|f_\varepsilon + \dot{Q}_\beta\|^2_{\dot{H}^1(\mathbb{H}^1)}) \geq c\|f_\varepsilon\|_{\dot{H}^1(\mathbb{H}^1)}.$$

Letting $\varepsilon \to 0$, we get that $\|f_\varepsilon\|_{\dot{H}^1(\mathbb{H}^1)} \to 0$, so the map $\beta \mapsto Q_\beta$ is indeed $\mathcal{C}^1$ with derivative $\dot{Q}_\beta$. The smoothness follows from an implicit function theorem. Set

$$\Phi : (\beta, U, V) \in (\beta_*, 1) \times W_1 \times W_1 \mapsto \mathcal{L}_{Q_\beta} V - \partial_\beta F(\beta, U) \in W_{-1}.$$

If $\beta \mapsto Q_\beta$ has regularity $\mathcal{C}^n$ for $\beta \in (\beta_*, 1)$, then the function Φ is also $\mathcal{C}^n$. For fixed $\beta \in (\beta_*, 1)$, $\Phi(\beta, Q_\beta, \dot{Q}_\beta) = 0$ and $\partial_V F(\beta, Q_\beta, \cdot) = \mathcal{L}_{Q_\beta}$, which is an isomorphism from W_1 to W_{-1}. Applying the implicit function theorem, there exists a $\mathcal{C}^n$ map V defined on a neighborhood of (β, Q_β) in $(\beta_*, 1) \times W_1$ and valued in W_1 such that $V(\beta, Q_\beta) = \dot{Q}_\beta$ and that

$$F(\beta, U, V(\beta, U)) = 0$$

in this neighborhood. In particular for β' close to β, $F(\beta', Q'_\beta, V(\beta', Q_{\beta'})) = 0$, and since $\dot{Q}_{\beta'}$ is uniquely determined by (20), $\dot{Q}_{\beta'} = V(\beta', Q_{\beta'})$. The function V being $\mathcal{C}^n$, supposing that $\beta \mapsto Q_\beta$ is $\mathcal{C}^n$ for some integer n, then $\beta \mapsto \dot{Q}_\beta$ is $\mathcal{C}^n$ and therefore, $\beta \mapsto Q_\beta$ is $\mathcal{C}^{n+1}$. □

Appendix: Proof of Lemma 4.14

We establish an explicit formula for the orthogonal projections $P_0 F_1$, $P_0 F_2$ and $P_0 F_3$, which are under integral form. Then, we estimate numerically $\langle P_0 F_j, F_j\rangle_{L^2(\mathbb{C}_+)}$, $j = 1, 2, 3$, in order to get Lemma 4.14.

- We know that

$$-\pi P_0(F_1)(s+it) = \int_{v\in\mathbb{R}_+}\int_{u\in\mathbb{R}} \frac{1}{(s-u+i(t+v))^2}\,\frac{1}{(u+i(v+1))}\,\frac{1}{\sqrt{u^2+(v+1)^2}}\,du\,dv.$$

Using the change of variables $u=(v+1)\sinh(y),\ \mathrm{d}u=(v+1)\cosh(y)\,\mathrm{d}y=\sqrt{u^2+(v+1)^2}\,\mathrm{d}y$. Then

$$-\pi P_0(F_1)(s+it)=\int_{v\in\mathbb{R}_+}\int_{y\in\mathbb{R}}\frac{1}{(s-(v+1)\sinh(y)+i(t+v))^2}\frac{1}{(\sinh(y)+i)(v+1)}\,\mathrm{d}y\,\mathrm{d}v.$$

We now apply the change of variables $x=\exp(y),\ \mathrm{d}x=\exp(y)\,\mathrm{d}y$:

$$\begin{aligned}-\pi P_0(F_1)(s+it)&\\ &=\int_{v\in\mathbb{R}_+}\int_{y\in\mathbb{R}}\frac{8\,\mathrm{e}^{3y}}{\big(2(s+i(t+v))\,\mathrm{e}^{y}-(v+1)\,\mathrm{e}^{2y}+(v+1)\big)^2}\frac{1}{(\mathrm{e}^{2y}-1+2i\,\mathrm{e}^{y})(v+1)}\,\mathrm{d}y\,\mathrm{d}v\\ &=\int_{v\in\mathbb{R}_+}\int_{x\in\mathbb{R}_+}\frac{8x^2}{\big(2(s+i(t+v))x-(v+1)x^2+(v+1)\big)^2}\frac{1}{(x^2-1+2ix)(v+1)}\,\mathrm{d}x\,\mathrm{d}v.\end{aligned}$$

Thanks to Fubini's theorem, one can exchange the integral signs so that

$$\begin{aligned}-\pi P_0(F_1)(s+it)&=\int_{x\in\mathbb{R}_+}\frac{8x^2}{(x+i)^2}\int_{v\in\mathbb{R}_+}\frac{1}{\big(2(s+it)x-x^2+1+v(-x^2+2ix+1)\big)^2}\frac{1}{(v+1)}\,\mathrm{d}x\,\mathrm{d}v\\ &=\int_{x\in\mathbb{R}_+}\frac{8x^2}{(x+i)^2(x-i)^4}\int_{v\in\mathbb{R}_+}\frac{1}{\big(\frac{x^2-2(s+it)x-1}{x^2-2ix-1}+v\big)^2}\frac{1}{(v+1)}\,\mathrm{d}v\,\mathrm{d}x.\end{aligned}$$

By the residue formula, for any rational function R such that $\int_{\mathbb{R}_+}R(v)\,\mathrm{d}v$ is convergent, we have

$$\int_{\mathbb{R}_+}R(v)\,\mathrm{d}v=-\sum_{w\in\mathbb{C}}\mathrm{Res}_w(R(w)\log_0(w)),$$

where $\log_0$ is the positive determination of the logarithm. Here, we consider the rational function $R(v)=\big(\frac{x^2-2zx-1}{x^2-2ix-1}+v\big)^{-2}(v+1)^{-1}$, where $z=s+it$. We fix $\lambda=\frac{x^2-2zx-1}{x^2-2ix-1}$.

Assume that $z\neq i$, so $\lambda\neq 1$. The residues at the simple pole -1 and the double pole $-\lambda$ are

$$\mathrm{Res}_{-1}(R(w)\log_0(w))=\Big(\frac{1}{(\lambda+w)^2}\log_0(w)\Big)\Big|_{w=-1}=\frac{1}{(\lambda-1)^2}i\pi,$$

$$\begin{aligned}\mathrm{Res}_{-\lambda}(R(w)\log_0(w))&=\frac{\mathrm{d}}{\mathrm{d}w}\Big(\frac{1}{(w+1)}\log_0(w)\Big)\Big|_{w=-\lambda}\\ &=\Big(\frac{1}{w(w+1)}-\frac{\log_0(w)}{(w+1)^2}\Big)\Big|_{w=-\lambda}=\frac{1}{\lambda(\lambda-1)}-\frac{\log_0(-\lambda)}{(\lambda-1)^2}.\end{aligned}$$

Remark that

$$\lambda=1-2(z-i)\frac{x}{(x-i)^2},\qquad \frac{1}{\lambda-1}=-\frac{1}{2}\frac{(x-i)^2}{x}\frac{1}{z-i}\quad\text{and}\quad\frac{1}{(\lambda-1)^2}=\frac{1}{4}\frac{(x-i)^4}{x^2}\frac{1}{(z-i)^2}.$$

Therefore,

$$\mathrm{Res}_{-1}(R(w)\log_0(w))=i\pi\frac{1}{4}\frac{(x-i)^4}{x^2}\frac{1}{(z-i)^2},$$

$$\mathrm{Res}_{-\lambda}(R(w)\log_0(w))=-\frac{(x-i)^2}{x^2-2zx-1}\frac{(x-i)^2}{2x(z-i)}-\log_0\Big(-1+\frac{2(z-i)x}{(x-i)^2}\Big)\frac{(x-i)^4}{4x^2(z-i)^2}.$$

Consequently,

$$\frac{8x^2}{(x+i)^2(x-i)^2}\int_{\mathbb{R}_+} R(v)\,\mathrm{d}v = \frac{-2i\pi}{(x+i)^2(z-i)^2} + \frac{4x}{(x^2-2zx-1)(x+i)^2(z-i)} + 2\log_0\Big(-1+\frac{2(z-i)x}{(x-i)^2}\Big)\frac{1}{(x+i)^2}\frac{1}{(z-i)^2}.$$

We can integrate every term on the right-hand side. First,

$$\int_{x\in\mathbb{R}_+} \frac{-2i\pi}{(x+i)^2(z-i)^2}\,\mathrm{d}x = \frac{-2\pi}{(z-i)^2}.$$

Then, an integration by parts leads to

$$\int_{x\in\mathbb{R}_+} \log_0\Big(-1+\frac{2(z-i)x}{(x-i)^2}\Big)\frac{1}{(x+i)^2}\,\mathrm{d}x = \pi + 2(z-i)\int_{\mathbb{R}_+}\frac{1}{(x-i)(x^2-2zx-1)}\,\mathrm{d}x.$$

We conclude that

$$\begin{aligned}-\pi P_0(F_1)(z) &= \frac{-2\pi}{(z-i)^2} + \frac{4}{z-i}\int_{x\in\mathbb{R}_+}\frac{1}{x^2-2zx-1}\frac{x}{(x+i)^2}\,\mathrm{d}x \\ &\qquad + \frac{2}{(z-i)^2}\Big(\pi + 2(z-i)\int_{x\in\mathbb{R}_+}\frac{1}{(x-i)(x^2-2zx-1)}\,\mathrm{d}x\Big) \\ &= \frac{4}{z-i}\int_{x\in\mathbb{R}_+}\frac{1}{x^2-2zx-1}\frac{2x^2+ix-1}{(x+i)^2(x-i)}\,\mathrm{d}x.\end{aligned}$$

We apply the residue formula to get an exact expression for $-\pi P_0(F_1)$. We consider

$$R(x) = \frac{1}{x^2-2zx-1}\frac{2x^2+ix-1}{(x+i)^2(x-i)}.$$

Fix $x_\pm := z \pm \sqrt{z^2+1}$. Since $z \neq i$, the rational function R admits three simple poles x_+, x_- and i and one double pole $-i$. We calculate the residue

$$\mathrm{Res}_{x_+}(R(w)\log_0(w)) = \frac{2x_+^2+ix_+-1}{(x_+-x_-)(x_++i)^2(x_+-i)}\log_0(x_+).$$

The identities $x_+^2 = 2zx_+ + 1$, $(x_++i)^2 = 2(z+i)x_+$, $x_+x_- = -1$ and $(x_+-i)(x_--i) = -2i(z-i)$ enable simplification to

$$\mathrm{Res}_{x_+}(R(w)\log_0(w)) = i\,\frac{(z+i)x_- - 2iz}{4(z^2+1)^{\frac{3}{2}}}\log_0(x_+).$$

The same arguments lead to

$$\mathrm{Res}_{x_-}(R(w)\log_0(w)) = \frac{2x_-^2+ix_--1}{(x_--x_+)(x_-+i)^2(x_--i)}\log_0(x_-) = -i\,\frac{(z+i)x_+-2iz}{4(z^2+1)^{\frac{3}{2}}}\log_0(x_-).$$

Moreover, the residue at the pole i is

$$\mathrm{Res}_i(R(w)\log_0(w)) = \frac{1}{-1-2zi-1}\frac{-4}{-4}\frac{i\pi}{2} = -\frac{\pi}{4(z-i)}.$$

Finally, the residue at the double pole $-i$ is

$$\operatorname{Res}_{-i}(R(w)\log_0(w)) = \Big[\frac{1}{x(x^2-2zx-1)}\frac{2x^2+ix-1}{(x-i)} + \frac{4x+i}{(x^2-2zx-1)(x-i)}\log_0(x) \\ - \frac{2x^2+ix-1}{(x^2-2zx-1)(x-i)}\Big(\frac{1}{x-x_+}+\frac{1}{x-x_-}+\frac{1}{x-i}\Big)\log_0(x)\Big]_{x=-i},$$

which simplifies to $\operatorname{Res}_{-i}(R(w)\log_0(w)) = -\frac{i}{2(z+i)}$. We conclude that

$$\int_{x\in\mathbb{R}_+}\frac{1}{x^2-2zx-1}\frac{2x^2+ix-1}{(x+i)^2(x-i)}\,\mathrm{d}x = -i\,\frac{(z+i)x_- - 2iz}{4(z^2+1)^{\frac{3}{2}}}\log_0(x_+) + i\,\frac{(z+i)x_+ - 2iz}{4(z^2+1)^{\frac{3}{2}}}\log_0(x_-) \\ + \frac{\pi}{4(z-i)} + \frac{i}{2(z+i)}.$$

Therefore, as soon as $z \neq i$,

$$-\pi P_0(F_1)(z) = -i\,\frac{(z+i)x_- - 2iz}{(z-i)(z^2+1)^{\frac{3}{2}}}\log_0(x_+) + i\,\frac{(z+i)x_+ - 2iz}{(z-i)(z^2+1)^{\frac{3}{2}}}\log_0(x_-) + \frac{\pi}{(z-i)^2} + \frac{2i}{z^2+1},$$

with $x_\pm = z \pm \sqrt{z^2+1}$. Note that $\log_0(x_\pm)$ is well defined, because if $z \pm \sqrt{z^2+1}$ is real, then z should be real, which we exclude by assumption ($z \in \mathbb{C}_+$).

- We apply the same strategy for $(F_1+F_2)(z) = \frac{2i}{(z+i)^2}\frac{1}{|z+i|}$. We have

$$-\frac{\pi}{2i}P_0(F_1+F_2)(s+it) = \int_{v\in\mathbb{R}_+}\int_{u\in\mathbb{R}}\frac{1}{(s-u+i(t+v))^2}\frac{1}{(u+i(v+1))^2}\frac{1}{\sqrt{u^2+(v+1)^2}}\,\mathrm{d}u\,\mathrm{d}v.$$

With the change of variables $u = (v+1)\sinh(y)$, $\mathrm{d}u = (v+1)\cosh(y)\,\mathrm{d}y = \sqrt{u^2+(v+1)^2}\,\mathrm{d}y$, we get

$$\frac{i\pi}{2}P_0(F_1+F_2(z)) = \int_{v\in\mathbb{R}_+}\int_{y\in\mathbb{R}}\frac{1}{(s-(v+1)\sinh(y)+i(t+v))^2}\frac{1}{(\sinh(y)+i)^2(v+1)^2}\,\mathrm{d}y\,\mathrm{d}v.$$

Now apply the change of variables $x = \exp(y)$, $\mathrm{d}x = \exp(y)\,\mathrm{d}y$:

$$\frac{i\pi}{2}P_0(F_1+F_2(z)) \\ = \int_{v\in\mathbb{R}_+}\int_{y\in\mathbb{R}}\frac{16\,\mathrm{e}^{4y}}{\big(2(s+i(t+v))\,\mathrm{e}^{y}-(v+1)\,\mathrm{e}^{2y}+(v+1)\big)^2}\frac{1}{(\mathrm{e}^{2y}-1+2i\,\mathrm{e}^{y})^2(v+1)^2}\,\mathrm{d}y\,\mathrm{d}v \\ = \int_{v\in\mathbb{R}_+}\int_{x\in\mathbb{R}_+}\frac{16x^3}{\big(2(s+i(t+v))x-(v+1)x^2+(v+1)\big)^2}\frac{1}{(x^2-1+2ix)^2(v+1)^2}\,\mathrm{d}x\,\mathrm{d}v.$$

Thanks to Fubini's theorem, one can exchange the integral signs so that

$$\frac{i\pi}{2}P_0(F_1+F_2(z)) = \int_{x\in\mathbb{R}_+}\frac{16x^3}{(x+i)^4}\int_{v\in\mathbb{R}_+}\frac{1}{\big(2(s+it)x-x^2+1+v(-x^2+2ix+1)\big)^2}\frac{1}{(v+1)^2}\,\mathrm{d}x\,\mathrm{d}v \\ = \int_{x\in\mathbb{R}_+}\frac{16x^3}{(x+i)^4(x-i)^4}\int_{v\in\mathbb{R}_+}\frac{1}{\big(\frac{x^2-2(s+it)x-1}{x^2-2ix-1}+v\big)^2}\frac{1}{(v+1)^2}\,\mathrm{d}v\,\mathrm{d}x.$$

We apply the consequence of the residue formula to $R(v) = \big(\frac{x^2-2zx-1}{x^2-2ix-1}+v\big)^{-2}(v+1)^{-2}$, where $z = s+it$. We fix $\lambda = \frac{x^2-2zx-1}{x^2-2ix-1}$ as in the first point.

Assume that $z \neq i$, therefore $\lambda \neq 1$. The residue at the double pole -1 is equal to

$$\begin{aligned}\operatorname{Res}_{-1}(R(w)\log_0(w)) &= \frac{\mathrm{d}}{\mathrm{d}w}\Big(\frac{1}{(\lambda+w)^2}\log_0(w)\Big)\Big|_{w=-1}\\ &= \Big(\frac{1}{w(w+\lambda)^2} - 2\frac{\log_0(w)}{(w+\lambda)^3}\Big)\Big|_{w=-1}\\ &= \frac{-1}{(-1+\lambda)^2} - 2\frac{1}{(\lambda-1)^3}i\pi\\ &= -\frac{(x-i)^4}{4x^2(z-i)^2} + \frac{i\pi}{4}\frac{(x-i)^6}{x^3(z-i)^3}.\end{aligned}$$

The residue at the double pole $-\lambda$ is

$$\begin{aligned}\operatorname{Res}_{-\lambda}(R(w)\log_0(w)) &= \frac{\mathrm{d}}{\mathrm{d}w}\Big(\frac{1}{(w+1)^2}\log_0(w)\Big)\Big|_{w=-\lambda}\\ &= \Big(\frac{1}{w(w+1)^2} - 2\frac{\log_0(w)}{(w+1)^3}\Big)\Big|_{w=-\lambda}\\ &= \frac{-1}{\lambda(\lambda-1)^2} - 2\frac{-\log_0(-\lambda)}{(\lambda-1)^3}\\ &= -\frac{(x-i)^6}{x^2-2xz-1}\frac{1}{4x^2(z-i)^2} - \frac{(x-i)^6}{4x^3(z-i)^3}\log_0\Big(-1+\frac{2(z-i)x}{(x-i)^2}\Big).\end{aligned}$$

Therefore,

$$\begin{aligned}\frac{16x^3}{(x+i)^4(x-i)^4}\int_{\mathbb{R}_+} R(v)\,\mathrm{d}v = \frac{4x}{(x+i)^4(z-i)^2} - \frac{4i\pi(x-i)^2}{(x+i)^4(z-i)^3} + \frac{4(x-i)^2x}{(x+i)^4(x^2-2xz-1)(z-i)^2}\\ + \frac{4(x-i)^2}{(x+i)^4(z-i)^3}\log_0\Big(-1+\frac{2(z-i)x}{(x-i)^2}\Big).\end{aligned}$$

We now integrate again in x to get that for all $z \neq i$,

$$\frac{i\pi}{2}P_0(F_1+F_2(z)) = \frac{-2(z-2i)}{3(z-i)(z+i)^2} - \frac{(1+2iz)\big(\log_0(z+\sqrt{z^2+1})-\log_0(z-\sqrt{z^2+1})\big)}{3(z-i)(z+i)^2\sqrt{z^2+1}}.$$

- We do the last computation for $(F_1+F_3)(z) = \frac{-2i}{(z+i)(\bar{z}-i)}\frac{1}{|z+i|} = \frac{-2i}{|z+i|^3}$. We have

$$-\frac{\pi}{-2i}P_0(F_1+F_3)(s+it) = \int_{v\in\mathbb{R}_+}\int_{u\in\mathbb{R}}\frac{1}{(s-u+i(t+v))^2}\frac{1}{(u^2+(v+1)^2)^{3/2}}\,\mathrm{d}u\,\mathrm{d}v.$$

Apply the change of variables $u = (v+1)\sinh(y)$, $\mathrm{d}u = (v+1)\cosh(y)\,\mathrm{d}y = \sqrt{u^2+(v+1)^2}\,\mathrm{d}y$. Then

$$-\frac{i\pi}{2}P_0(F_1+F_3)(s+it) = \int_{v\in\mathbb{R}_+}\int_{y\in\mathbb{R}}\frac{1}{(s-(v+1)\sinh(y)+i(t+v))^2}\frac{1}{\cosh(y)^2(v+1)^2}\,\mathrm{d}y\,\mathrm{d}v.$$

We now put $x=\exp(y),\ \mathrm{d}x=\exp(y)\,\mathrm{d}y$:

$$-\frac{i\pi}{2}P_0(F_1+F_3)(s+it)$$
$$=\int_{v\in\mathbb{R}_+}\int_{y\in\mathbb{R}}\frac{16\,\mathrm{e}^{4y}}{\big(2(s+i(t+v))\,\mathrm{e}^{y}-(v+1)\,\mathrm{e}^{2y}+(v+1)\big)^2}\frac{1}{(\mathrm{e}^{2y}+1)^2(v+1)^2}\,\mathrm{d}y\,\mathrm{d}v$$
$$=\int_{v\in\mathbb{R}_+}\int_{x\in\mathbb{R}_+}\frac{16x^3}{\big(2(s+i(t+v))x-(v+1)x^2+(v+1)\big)^2}\frac{1}{(x^2+1)^2(v+1)^2}\,\mathrm{d}x\,\mathrm{d}v.$$

Thanks to Fubini's theorem, one can exchange the integral signs so that

$$-\frac{i\pi}{2}P_0(F_1+F_3)(s+it)$$
$$=\int_{x\in\mathbb{R}_+}\frac{16x^3}{(x+i)^2(x-i)^2}\int_{v\in\mathbb{R}_+}\frac{1}{\big(2(s+it)x-x^2+1+v(-x^2+2ix+1)\big)^2}\frac{1}{(v+1)^2}\,\mathrm{d}x\,\mathrm{d}v$$
$$=\int_{x\in\mathbb{R}_+}\frac{16x^3}{(x+i)^2(x-i)^6}\int_{v\in\mathbb{R}_+}\frac{1}{\big(\frac{x^2-2(s+it)x-1}{x^2-2ix-1}+v\big)^2}\frac{1}{(v+1)^2}\,\mathrm{d}v\,\mathrm{d}x.$$

We have already done the computation of the integral in the v variable in the latter point. We proved that putting $R(v)=\big(\frac{x^2-2(s+it)x-1}{x^2-2ix-1}+v\big)^{-2}(v+1)^{-2}$,

$$\frac{16x^3}{(x+i)^4(x-i)^4}\int_{\mathbb{R}_+}R(v)\,\mathrm{d}v=\frac{4x}{(x+i)^4(z-i)^2}-\frac{4i\pi(x-i)^2}{(x+i)^4(z-i)^3}+\frac{4(x-i)^2x}{(x+i)^4(x^2-2xz-1)(z-i)^2}$$
$$+\frac{4(x-i)^2}{(x+i)^4(z-i)^3}\log_0\Big(-1+\frac{2(z-i)x}{(x-i)^2}\Big).$$

Therefore,

$$\frac{16x^3}{(x+i)^2(x-i)^6}\int_{v\in\mathbb{R}_+}R(v)\,\mathrm{d}v=\frac{4x}{(x+i)^2(x-i)^2(z-i)^2}-\frac{4i\pi}{(x+i)^2(z-i)^3}+\frac{4x}{(x+i)^2(x^2-2xz-1)(z-i)^2}$$
$$+\frac{4}{(x+i)^2(z-i)^3}\log_0\Big(-1+\frac{2(z-i)x}{(x-i)^2}\Big).$$

We now integrate again in x to get that for all $z\neq i$,

$$-\frac{i\pi}{2}P_0(F_1+F_3)(z)=\frac{2(z+2i)}{(z-i)^2(z+i)}+\frac{(1-2iz)\big(\log_0(z+\sqrt{z^2+1})-\log_0(z-\sqrt{z^2+1})\big)}{(z-i)^2(z+i)\sqrt{z^2+1}}$$

• Now we can compute numerically $\langle P_0F_j,F_j\rangle_{L^2(\mathbb{C}_+)}$, $j=1,2,3$, the error estimate, for every term can be chosen almost arbitrarily now that we know P_0F_j.

We set $\varepsilon=10^{-10}$ and we deduce

$$|\langle\pi P_0F_1,F_1\rangle_{L^2(\mathbb{C}_+)}-2|\le\varepsilon,$$
$$\big|\langle\pi P_0F_2,F_2\rangle_{L^2(\mathbb{C}_+)}-\tfrac{10}{9}\big|\le\varepsilon,$$
$$|\langle\pi P_0F_3,F_3\rangle_{L^2(\mathbb{C}_+)}-0.1303955989|\le\varepsilon.$$

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References

[Aubin 1976] T. Aubin, "Problèmes isopérimétriques et espaces de Sobolev", *J. Differential Geom.* **11**:4 (1976), 573–598. MR Zbl

[Bahouri et al. 2000] H. Bahouri, P. Gérard, and C.-J. Xu, "Espaces de Besov et estimations de Strichartz généralisées sur le groupe de Heisenberg", *J. Anal. Math.* **82** (2000), 93–118. MR Zbl

[Bahouri et al. 2016] H. Bahouri, C. Fermanian-Kammerer, and I. Gallagher, "Dispersive estimates for the Schrödinger operator on step-2 stratified Lie groups", *Anal. PDE* **9**:3 (2016), 545–574. MR Zbl

[Békollé et al. 2004] D. Békollé, A. Bonami, G. Garrigós, C. Nana, M. M. Peloso, and F. Ricci, "Lecture notes on Bergman projectors in tube domains over cones: an analytic and geometric viewpoint", *IMHOTEP J. Afr. Math. Pures Appl.* **5** (2004), [exposé] I. MR Zbl

[Benameur 2008] J. Benameur, "Description du défaut de compacité de l'injection de Sobolev sur le groupe de Heisenberg", *Bull. Belg. Math. Soc. Simon Stevin* **15**:4 (2008), 599–624. MR Zbl

[Bergh and Löfström 1976] J. Bergh and J. Löfström, *Interpolation spaces: an introduction*, Grundlehren der Math. Wissenschaften **223**, Springer, 1976. MR Zbl

[Branson et al. 2013] T. P. Branson, L. Fontana, and C. Morpurgo, "Moser–Trudinger and Beckner–Onofri's inequalities on the CR sphere", *Ann. of Math.* (2) **177**:1 (2013), 1–52. MR Zbl

[Burq et al. 2005] N. Burq, P. Gérard, and N. Tzvetkov, "Bilinear eigenfunction estimates and the nonlinear Schrödinger equation on surfaces", *Invent. Math.* **159**:1 (2005), 187–223. MR Zbl

[Cazenave and Lions 1982] T. Cazenave and P.-L. Lions, "Orbital stability of standing waves for some nonlinear Schrödinger equations", *Comm. Math. Phys.* **85**:4 (1982), 549–561. MR Zbl

[Chen et al. 2013] S. Chen, R. L. Frank, and T. Weth, "Remainder terms in the fractional Sobolev inequality", *Indiana Univ. Math. J.* **62**:4 (2013), 1381–1397. MR Zbl

[Dávila et al. 2013] J. Dávila, M. del Pino, and Y. Sire, "Nondegeneracy of the bubble in the critical case for nonlocal equations", *Proc. Amer. Math. Soc.* **141**:11 (2013), 3865–3870. MR Zbl

[Del Hierro 2005] M. Del Hierro, "Dispersive and Strichartz estimates on H-type groups", *Studia Math.* **169**:1 (2005), 1–20. MR Zbl

[Folland and Stein 1974] G. B. Folland and E. M. Stein, "Parametrices and estimates for the $\bar{\partial}_b$ complex on strongly pseudoconvex boundaries", *Bull. Amer. Math. Soc.* **80**:2 (1974), 253–258. MR

[Frank and Lenzmann 2013] R. L. Frank and E. Lenzmann, "Uniqueness of non-linear ground states for fractional Laplacians in $\mathbb{R}$", *Acta Math.* **210**:2 (2013), 261–318. MR Zbl

[Frank and Lieb 2012a] R. L. Frank and E. H. Lieb, "A new, rearrangement-free proof of the sharp Hardy–Littlewood–Sobolev inequality", pp. 55–67 in *Spectral theory, function spaces and inequalities*, edited by B. M. Brown et al., Oper. Theory Adv. Appl. **219**, Birkhäuser, Basel, 2012. MR Zbl

[Frank and Lieb 2012b] R. L. Frank and E. H. Lieb, "Sharp constants in several inequalities on the Heisenberg group", *Ann. of Math.* (2) **176**:1 (2012), 349–381. MR Zbl

[Gérard 1998] P. Gérard, "Description du défaut de compacité de l'injection de Sobolev", *ESAIM Control Optim. Calc. Var.* **3** (1998), 213–233. MR

[Gérard and Grellier 2010a] P. Gérard and S. Grellier, "The cubic Szegő equation", *Ann. Sci. École Norm. Sup.* (4) **43**:5 (2010), 761–810. MR Zbl

[Gérard and Grellier 2010b] P. Gérard and S. Grellier, "L'équation de Szegő cubique", exposé II in *Séminaire: Équations aux Dérivées Partielles* (Palaiseau, France, 2008-2009), École Polytech., Palaiseau, 2010. MR Zbl

[Gérard and Grellier 2012] P. Gérard and S. Grellier, "Effective integrable dynamics for a certain nonlinear wave equation", *Anal. PDE* **5**:5 (2012), 1139–1155. MR Zbl

[Gérard et al. 2018] P. Gérard, E. Lenzmann, O. Pocovnicu, and P. Raphaël, "A two-soliton with transient turbulent regime for the cubic half-wave equation on the real line", *Ann. PDE* **4**:1 (2018), art. id. 7. MR Zbl

[Gidas et al. 1979] B. Gidas, W. M. Ni, and L. Nirenberg, "Symmetry and related properties via the maximum principle", *Comm. Math. Phys.* **68**:3 (1979), 209–243. MR Zbl

[Jerison and Lee 1988] D. Jerison and J. M. Lee, "Extremals for the Sobolev inequality on the Heisenberg group and the CR Yamabe problem", *J. Amer. Math. Soc.* **1**:1 (1988), 1–13. MR Zbl

[Krieger et al. 2013] J. Krieger, E. Lenzmann, and P. Raphaël, "Nondispersive solutions to the L^2-critical half-wave equation", *Arch. Ration. Mech. Anal.* **209**:1 (2013), 61–129. MR Zbl

[Kwong 1989] M. K. Kwong, "Uniqueness of positive solutions of $\Delta u - u + u^p = 0$ in $\mathbb{R}^n$", *Arch. Ration. Mech. Anal.* **105**:3 (1989), 243–266. MR Zbl

[Lieb 1983] E. H. Lieb, "Sharp constants in the Hardy–Littlewood–Sobolev and related inequalities", *Ann. of Math.* (2) **118**:2 (1983), 349–374. MR Zbl

[Liu and Zhang 2015] H. Liu and A. Zhang, "Remainder terms for several inequalities on some groups of Heisenberg-type", *Sci. China Math.* **58**:12 (2015), 2565–2580. MR Zbl

[Pocovnicu 2011] O. Pocovnicu, "Traveling waves for the cubic Szegő equation on the real line", *Anal. PDE* **4**:3 (2011), 379–404. MR Zbl

[Pocovnicu 2012] O. Pocovnicu, "Soliton interaction with small Toeplitz potentials for the Szegő equation on $\mathbb{R}$", *Dyn. Partial Differ. Equ.* **9**:1 (2012), 1–27. MR Zbl

[Rosen 1971] G. Rosen, "Minimum value for c in the Sobolev inequality $\|\phi^3\| \leqq c\|\nabla\phi\|^3$", *SIAM J. Appl. Math.* **21** (1971), 30–32. MR Zbl

[Rudin 1966] W. Rudin, *Real and complex analysis*, McGraw-Hill, New York, 1966. MR Zbl

[Stanton 1989] N. K. Stanton, "Spectral invariants of CR manifolds", *Michigan Math. J.* **36**:2 (1989), 267–288. MR Zbl

[Stein 1993] E. M. Stein, *Harmonic analysis: real-variable methods, orthogonality, and oscillatory integrals*, Princeton Math. Ser. **43**, Princeton Univ. Press, 1993. MR Zbl

[Stein and Weiss 1971] E. M. Stein and G. Weiss, *Introduction to Fourier analysis on Euclidean spaces*, Princeton Math. Ser. **32**, Princeton Univ. Press, 1971. MR Zbl

[Talenti 1976] G. Talenti, "Best constant in Sobolev inequality", *Ann. Mat. Pura Appl.* (4) **110** (1976), 353–372. MR Zbl

[Vétois 2019] J. Vétois, "Decay estimates and symmetry of finite energy solutions to elliptic systems in $\mathbb{R}^n$", *Indiana Univ. Math. J.* **68**:3 (2019), 663–696. MR Zbl

[Weinstein 1982] M. I. Weinstein, "Nonlinear Schrödinger equations and sharp interpolation estimates", *Comm. Math. Phys.* **87**:4 (1982), 567–576. MR Zbl

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RESONANT SPACES FOR VOLUME-PRESERVING ANOSOV FLOWS

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We consider Anosov flows on closed 3-manifolds preserving a volume form Ω. Following Dyatlov and Zworski (*Invent. Math.* **210**:1 (2017), 211–229) we study spaces of invariant distributions with values in the bundle of exterior forms whose wavefront set is contained in the dual of the unstable bundle. Our first result computes the dimension of these spaces in terms of the first Betti number of the manifold, the cohomology class $[\iota_X\Omega]$ (where X is the infinitesimal generator of the flow) and the helicity. These dimensions coincide with the Pollicott–Ruelle resonance multiplicities under the assumption of *semisimplicity*. We prove various results regarding semisimplicity on 1-forms, including an example showing that it may fail for time changes of hyperbolic geodesic flows. We also study non-null-homologous deformations of contact Anosov flows, and we show that there is always a splitting Pollicott–Ruelle resonance on 1-forms and that semisimplicity persists in this instance. These results have consequences for the order of vanishing at zero of the Ruelle zeta function. Finally our analysis also incorporates a flat unitary twist in the resonant spaces and in the Ruelle zeta function.

1. Introduction

We study resonant spaces of invariant distributions with values in the bundle of exterior forms for volume-preserving Anosov flows on 3-manifolds. One of the main motivations for looking at these spaces is that when a natural restriction is placed on the wave front set of the distributions, their dimensions are related to the Pollicott–Ruelle resonance multiplicities, which in turn determine the order of vanishing at zero of the Ruelle zeta function. For the case of contact Anosov flows this analysis was carried out in [Dyatlov and Zworski 2017] and here we show that the transition from "contact" to "volume-preserving" presents some new features, making the overall picture more involved, partially due to the nonsmoothness of the stable plus unstable bundle.

Let (M, Ω) be a closed 3-manifold equipped with a volume form Ω and let φ_t be a volume-preserving Anosov flow with infinitesimal generator X. If we write the Anosov splitting as $TM = \mathbb{R}X \oplus E_s \oplus E_u$, then we define the spaces E_0^*, E_s^* and E_u^* as the duals of $\mathbb{R}X$, E_u and E_s respectively. In particular, this means that for each $x \in M$, $E_u^*(x)$ is the annihilator of $\mathbb{R}X(x) \oplus E_u(x)$ and $E_u^* \subset T^*M$, a closed conic subset. We denote by $\mathcal{D}'_{E_u^*}(M; \Omega^k)$ the space of distributions with values in the bundle of exterior k-forms and with wave front set contained in E_u^* (see Section 2 for background on these notions). The resonant spaces that we are interested in are

$$\mathrm{Res}_k(0) := \{u \in \mathcal{D}'_{E_u^*}(M; \Omega^k) : \iota_X u = 0,\ \iota_X\, du = 0\}.$$

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The dimensions of the spaces can be considered as *geometric multiplicities*. We note that [Dang and Riviere 2017] studies generalised resonant spaces of forms (at zero) for arbitrary Anosov flows and these have a good cohomology theory (see Remark 2.2 for more details and definitions) but in principle these generalised resonant forms are not in the kernel of ι_X and might only be in the kernel of some power of the Lie derivative.

Our first result computes the dimension of these geometric spaces in terms of the first Betti number $b_1(M)$ of the manifold M and two natural characteristics of the flow that we now recall.

Since X preserves the volume form Ω, its Lie derivative $\mathcal{L}_X\Omega$ is equal to 0. Hence the 2-form $\omega := \iota_X\Omega$ must be closed.

Definition 1.1. We say that X is *null-homologous* if the cohomology class $[\omega]$ is equal to 0, i.e., ω is exact. For a null-homologous X, its *helicity* is the number

$$\mathcal{H}(X) := \int_M \tau(X)\,\Omega,$$

where τ is any 1-form such that $d\tau = \omega$.

It is easy to check that this definition is independent of the choice of primitive τ. The helicity (also referred to as the *asymptotic Hopf invariant*) measures how much in average field lines wrap and coil around one another. We refer to [Arnold and Khesin 1998] for a complete account of this concept as well as its interpretation as an average self-linking number.

We can now state our first result:

Theorem 1.2. *Let* (M, Ω) *be a closed* 3*-manifold with volume form* Ω *and let* φ_t *be a volume-preserving Anosov flow. Then*:

(1) $\dim \mathrm{Res}_0(0) = \dim \mathrm{Res}_2(0) = 1$.

(2) *If* $[\omega] \neq 0$, *then* $\dim \mathrm{Res}_1(0) = b_1(M) - 1$.

(3) *If* $[\omega] = 0$, *then*

$$\dim \mathrm{Res}_1(0) = \begin{cases} b_1(M) & \text{if } \mathcal{H}(X) \neq 0, \\ b_1(M) + 1 & \text{if } \mathcal{H}(X) = 0. \end{cases}$$

This result generalises [Dyatlov and Zworski 2017, Proposition 3.1] as a contact Anosov flow fits into $[\omega] = 0$ and $\mathcal{H}(X) \neq 0$, since in that case we can take τ to be the contact 1-form and $\tau(X) = 1$. In Section 5 we give some examples to illustrate the various cases in Theorem 1.2, but we should point out right away that we do not know of any example of a volume-preserving Anosov flow with zero helicity.

We note that all the notions involved in Theorem 1.2 are invariant under time changes. Namely, if f is a positive smooth function, the flow of fX is also Anosov and with the *same* E_u^*. Hence the resonant spaces $\mathrm{Res}_k(0)$ are the same for all such flows. Also the notion of being null-homologous or having nonzero helicity is unaffected by time changes.

As mentioned before, the dimensions of $\mathrm{Res}_k(0)$ are important since they are related to the Pollicott–Ruelle resonance multiplicities $m_k(0)$. In general $m_k(0) \geq \dim \mathrm{Res}_k(0)$, and equality holds under the following condition (see Lemma 2.1):

Definition 1.3. X or φ_t is said to be k-semisimple if given $u \in \mathcal{D}'_{E_u^*}(M; \Omega^k)$ with $\iota_X u = 0$ and $\iota_X du \in \mathrm{Res}_k(0)$, then $u \in \mathrm{Res}_k(0)$, i.e., $\iota_X du = 0$.

Semisimplicity for $k = 0, 2$ will be easy to establish, but 1-semisimplicity does not always hold. In the case of contact Anosov flows, 1-semisimplicity was proved in [Dyatlov and Zworski 2017, Lemma 3.5]. For general volume-preserving Anosov flows the bundle $E_u \oplus E_s$ is only Hölder continuous [Foulon and Hasselblatt 2003] and thus the 1-form adapted to the flow, defined to be zero on $E_u \oplus E_s$ and 1 on the generator X, is only Hölder continuous. As a consequence the computations done in [Dyatlov and Zworski 2017, Lemma 3.5] are no longer viable due to this lack of smoothness.

Our next two results show that the picture for volume-preserving Anosov flow is rather more subtle. Let $\mathcal{X}_\Omega$ denote the set of vector fields that preserve Ω and let $\mathcal{X}_\Omega^0 \subset \mathcal{X}_\Omega$ denote those which are null-homologous.

Theorem 1.4. *Let (M, Ω) be a closed 3-manifold with volume form Ω. Consider a smooth 1-parameter family X_ε of volume-preserving Anosov vector fields with X_0 1-semisimple*:

(1) *If $X_\varepsilon \in \mathcal{X}_\Omega^0$ for every ε and $\mathcal{H}(X_0) \neq 0$, then X_ε is 1-semisimple for all ε sufficiently small.*

(2) *If X_0 is not null-homologous, then X_ε is 1-semisimple for all ε sufficiently small.*

For any hyperbolic surface, there is a time change of the geodesic flow which is not 1-semisimple.

Consider now a contact Anosov flow X with contact form α on a closed 3-manifold M. In particular, by Theorem 1.4 we know that 1-semisimplicity persists in $\mathcal{X}_\Omega^0$ and near X, where $\Omega = -\alpha \wedge d\alpha$. The next theorem gives us a local picture for what happens near X and away from $\mathcal{X}_\Omega^0$.

Theorem 1.5. *Consider $Y \in \mathcal{X}_\Omega \setminus \mathcal{X}_\Omega^0$. Then for sufficiently small ε, the flow $X_\varepsilon = X + \varepsilon Y$ is 1-semisimple. Moreover, there is a splitting Pollicott–Ruelle resonance $-i\lambda_\varepsilon = O(\varepsilon^2)$ of $-i\mathcal{L}_{X_\varepsilon}$ acting on $\Omega^1 \cap \ker \iota_{X_\varepsilon}$ with $\lambda_\varepsilon < 0$ for $\varepsilon \neq 0$, with Pollicott–Ruelle multiplicity 1 (see Figure 1).*

1A. ***Ruelle zeta function.*** We denote the set of primitive closed orbits of X by $\mathcal{G}_0$ (i.e., the ones that are not powers of a closed orbit in M); the period of $\gamma \in \mathcal{G}_0$ is denoted by l_γ. The Ruelle zeta function is defined as

$$\zeta(s) := \prod_{\gamma \in \mathcal{G}_0} (1 - e^{-sl_\gamma}). \tag{1-1}$$

The infinite product converges for $\mathrm{Re}\, s \gg 1$ and its meromorphic continuation to all $\mathbb{C}$ was first established in [Giulietti et al. 2013] in full generality and subsequently in [Dyatlov and Zworski 2016], where a microlocal approach was employed; see [Pollicott 2013] for a survey of dynamical zeta functions. Moreover, it was shown in [Dyatlov and Zworski 2016] that there is a factorisation (assuming that E_s and E_u are orientable)

$$\zeta(s) = \frac{\zeta_1(s)}{\zeta_0(s)\zeta_2(s)}, \tag{1-2}$$

where $\zeta_k(s)$ is an entire function with the order of vanishing at each $s \in \mathbb{C}$ equal to $m_k(is)$ for $k = 0, 1, 2$. Here $m_k(\lambda)$ is the Pollicott–Ruelle resonance multiplicity (see Section 2 for more details). Hence the order of vanishing of ζ at $s = 0$ is determined by $m(0) := m_1(0) - m_0(0) - m_2(0)$. Using this and Theorem 1.2 we derive the following:

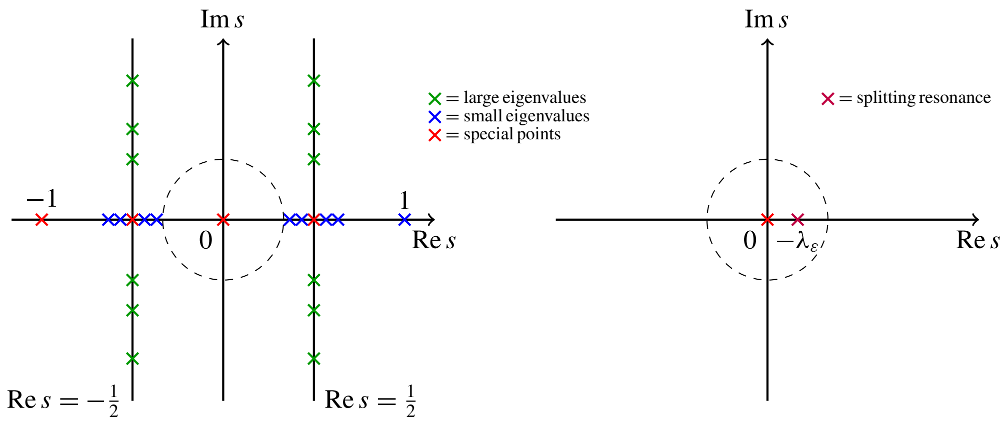

Figure 1. Left: resonance spectrum of $\mathcal{L}_X$ acting on $\Omega^1(S\Sigma)$ for a closed hyperbolic surface Σ. According to [Guillarmou et al. 2018; Dyatlov et al. 2015] and Remark 8.3 below, the green crosses correspond to (large) eigenvalues $\mu \geq \frac{1}{4}$ of $-\Delta_\Sigma$, the blue ones correspond to (small) eigenvalues $\mu \leq \frac{1}{4}$ and the red ones are "special". Right: resonance spectrum of $\mathcal{L}_{X_\varepsilon}$ acting on $\Omega^1(S\Sigma)$ and the splitting resonance, according to Theorem 1.5. We remark that the resonances in the rest of this paper will often be given by $\lambda = is$, i.e., obtained by a rotation of $\frac{\pi}{2}$ from this picture.

Corollary 1.6. *Let* (M, Ω) *be a closed* 3*-manifold with a volume-preserving Anosov flow* φ_t *whose stable and unstable bundles are orientable. Then*

$$s^{n(M,X)}\zeta(s)$$

is holomorphic close to zero, *where*

$$\begin{aligned} n(M, X) &= 3 - b_1(M) && \text{if } [\omega] \neq 0, \\ n(M, X) &= 2 - b_1(M) && \text{if } [\omega] = 0 \text{ and } \mathcal{H}(X) \neq 0, \\ n(M, X) &= 1 - b_1(M) && \text{if } [\omega] = 0 \text{ and } \mathcal{H}(X) = 0. \end{aligned}$$

Moreover, *if* φ_t *is* 1*-semisimple*, *then* $s^{n(M,X)}\zeta(s)|_{s=0} \neq 0$.

The Ruelle zeta function for the suspension of a hyperbolic toral automorphism $A \in \mathrm{SL}(2, \mathbb{Z})$ is equal to

$$\zeta(s) = \frac{(e^{-s} - \lambda)(e^{-s} - 1/\lambda)}{(e^{-s} - 1)^2},$$

where λ and $1/\lambda$ are eigenvalues of A. This has a pole of order 2 at $s = 0$, which of course matches the computation in Corollary 1.6 since $b_1(M) = 1$. However, the corollary asserts that *any* other volume-preserving non-null-homologous Anosov flow on M will have ζ with the same behaviour at $s = 0$ since 1-semisimplicity holds trivially given that $\mathrm{Res}_1(0)$ is zero-dimensional. An interesting class of Anosov flows with $[\omega] \neq 0$ is given in [Bonatti and Langevin 1994]. These examples have a transverse torus, but they are not conjugate to suspensions. We do not know if they are 1-semisimple.

Magnetic flows are also examples to which the previous corollary applies. They are null-homologous (see Section 5), but they are generically *not* contact (see [Dairbekov and Paternain 2005]); hence they were not covered by the main result in [Dyatlov and Zworski 2017]. In this setting, magnetic flows can be described by a vector field of the form $X + (\lambda \circ \pi)V$, where X is the geodesic vector field, V is the vertical vector field of the circle fibration $\pi : S\Sigma \to \Sigma$, and $\lambda \in C^\infty(\Sigma)$ (here M is equal to $S\Sigma$, the unit circle bundle of the orientable surface Σ). They are volume-preserving since X and V preserve the canonical volume form. Suppose the geodesic flow is Anosov. Thanks to item (1) in Theorem 1.4, if λ is small enough, the magnetic flows remain Anosov and 1-semisimple and hence the order of vanishing of the zeta function at zero is the same as for Anosov geodesic flows, namely $-\chi(\Sigma)$.

The last statement in Theorem 1.4 and Theorem 1.5 have consequences for the zeta function. The failure of 1-semisimplicity means that $m_1(0) \geq b_1(M) + 1$, and hence the order of vanishing at zero of the zeta function is *strictly bigger* than that of the geodesic flow case. Hence time changes can a priori produce alterations in the properties of ζ near zero. Similarly the cohomology class $[\omega]$ can also produce alterations. For the particular construction of Theorem 1.4 we do not know the precise order of vanishing at zero.

Corollary 1.7. *The order of vanishing of the zeta function $\zeta_{X_\varepsilon}(s)$ of the flow X_ε from Theorem 1.5 at zero, for $\varepsilon \neq 0$, is equal to $b_1(M) - 3$. Moreover, for the time change fX of the geodesic flow on the hyperbolic surface constructed in Theorem 1.4, the order of vanishing is greater than or equal to $-\chi(\Sigma) + 1$.*

1B. ***Flat unitary twists.*** It is possible (and natural) to introduce a unitary twist in the discussion above. Consider (M, Ω) a closed 3-manifold with volume form Ω and X a volume-preserving Anosov vector field. Let $\mathcal{E}$ be a Hermitian vector bundle over M, equipped with a unitary connection A. We consider $\mathcal{D}'_{E_u^*}(M; \Omega^k \otimes \mathcal{E})$ the space of distributions with values in the bundle of $\mathcal{E}$-valued exterior k-forms and with wave front set contained in E_u^*. We replace the exterior differential d by the covariant derivative d_A (induced by the connection A) acting on $\mathcal{E}$-valued differential forms. Thus we can define resonant spaces

$$\mathrm{Res}_{k,A}(0) := \{u \in \mathcal{D}'_{E_u^*}(M; \Omega^k \otimes \mathcal{E}) : \iota_X u = 0,\ \iota_X\, d_A u = 0\}.$$

We shall compute the dimensions of these spaces in analogy to Theorem 1.2 under the assumption that A is *flat and unitary*, i.e., $d_A^2 = 0$ and d_A is compatible with the Hermitian inner product on $\mathcal{E}$. Recall that flat unitary connections are in 1-1 correspondence with representations of $\pi_1(M)$ into the unitary group. Under this condition, one can define twisted Betti numbers $b_i(M, \mathcal{E})$ in the standard way (we note that these numbers may depend on A). The upshot is a theorem similar to Theorem 1.2 where the Betti numbers $b_i(M)$ are replaced by $b_i(M, \mathcal{E})$; see Theorem 4.1 for the full statement. With this information in hand we can study a *twisted Ruelle zeta function*,

$$\zeta_A(s) := \prod_{\gamma \in \mathcal{G}_0} \det\,(\mathrm{Id} - \alpha_\gamma e^{-s l_\gamma}). \tag{1-3}$$

Here, given a point x_0 on $\gamma \in \mathcal{G}_0$, we denote by α_γ the parallel transport map (i.e., an element of the holonomy group) along the loop determined by γ. It is easy to check that the product is independent of the choice of x_0 on γ, as this amounts to conjugating α_γ by a linear map. Note that if $\mathcal{E} = M \times \mathbb{C}$ and $d_A = d$, the expression in (1-3) reduces to that in (1-1). If the connection A is flat, we recover the definition of the twisted Ruelle zeta function considered in [Fried 1986]; it was also studied in [Adachi 1988; Adachi and Sunada 1987], where functions of this type were called *L-functions* in analogy with number theory. Fried conjectured that the coefficient at zero of ζ_A for an acyclic connection (i.e., one that has vanishing Betti numbers) is related to the analytic torsion, but proved it only for hyperbolic manifolds. For recent progress on this conjecture and more information, see [Dang et al. 2020; Shen 2018; Zworski 2018].

The notion of semisimplicity extends naturally to the twisted case (just replace d by d_A in Definition 1.3). In that case we will say a flow φ_t or X is 1-semisimple with respect to d_A. Putting everything together we shall derive the following corollary:

Corollary 1.8. *Let (M, Ω) be a closed 3-manifold with a volume-preserving Anosov flow φ_t whose stable and unstable bundles are orientable. Let $\mathcal{E}$ be a Hermitian vector bundle equipped with a unitary flat connection A. Then*

$$s^{n(M,X,A)}\zeta_A(s)$$

is holomorphic close to zero, where

$$\begin{aligned} n(M, X, A) &= 3b_0(M, \mathcal{E}) - b_1(M, \mathcal{E}) && \text{if } [\omega] \neq 0, \\ n(M, X, A) &= 2b_0(M, \mathcal{E}) - b_1(M, \mathcal{E}) && \text{if } [\omega] = 0 \text{ and } \mathcal{H}(X) \neq 0, \\ n(M, X, A) &= b_0(M, \mathcal{E}) - b_1(M, \mathcal{E}) && \text{if } [\omega] = 0 \text{ and } \mathcal{H}(X) = 0. \end{aligned}$$

Moreover, if X is 1-semisimple with respect to d_A, then $s^{n(M,X,A)}\zeta_A(s)|_{s=0} \neq 0$.

A particular instance of the corollary arises when we consider A to be the pullback of a flat connection on a surface Σ. In this case it is easy to check that (see Lemma 2.9)

$$2b_0(M, \mathcal{E}) - b_1(M, \mathcal{E}) = \operatorname{rank}(\mathcal{E})\, \chi(\Sigma).$$

Thus:

Corollary 1.9. *Let $\mathcal{E}$ be a Hermitian vector bundle over an oriented closed Riemannian surface (Σ, g), equipped with a unitary flat connection A. We consider $M = S\Sigma$ with footpoint map π and any Anosov flow, 1-semisimple with respect to d_{π^*A}, null-homologous with nonzero helicity, preserving the volume form of $S\Sigma$. We consider the pullback bundle $\pi^*\mathcal{E}$ with the pullback connection π^*A. Then in a neighbourhood of zero we have $s^{\operatorname{rank}(\mathcal{E})\cdot\chi(\Sigma)} \cdot \zeta_{\pi^*A}(s)$ holomorphic such that*

$$s^{\operatorname{rank}(\mathcal{E})\cdot\chi(\Sigma)} \cdot \zeta_{\pi^*A}(s)|_{s=0} \neq 0.$$

We remark that Corollary 1.9 applies in particular to contact flows, since for those 1-semisimplicity holds with respect to any flat and unitary d_A.

This paper is organised as follows. Section 2 gives preliminary information, recalls the Pollicott–Ruelle resonances and proves some necessary lemmas. In Section 3 we recall the factorisation of the twisted zeta function in terms of some traces of operators on $\mathcal{E}$-valued k-forms. In Section 4, we compute the dimension of the resonant spaces $\operatorname{Res}_{k,A}(0)$ and obtain Theorem 1.2 as a particular case. Corollary 1.8 is also proved in this section. Section 5 gives examples and develops material needed for the study of time changes. Section 6 discusses perturbations and proves the main result needed for items (1) and (2) in Theorem 1.4. Theorem 1.5 is proved in Section 7. Finally, Section 8 exhibits a time change of the geodesic flow of a hyperbolic surface for which 1-semisimplicity fails, thus completing the proof of Theorem 1.4.

2. Preliminary results

In this section we review the necessary tools to prove the results stated in the Introduction. In particular, we recall the Pollicott–Ruelle resonances and put forward some preparatory lemmas.

2A. ***Microlocal analysis.*** Here we outline the microlocal tools necessary for our proofs. For more information on distribution spaces and properties of wavefront sets see [Grigis and Sjöstrand 1994, Chapter 7] or [Hörmander 1983, Chapters VI, VIII] and for more about pseudodifferential operators see [Grigis and Sjöstrand 1994, Chapter 3] or [Hörmander 1985, Chapter XVIII].

Let M be a closed manifold and $\mathcal{E}$ a smooth complex vector bundle. We consider the space of infinitely differentiable smooth sections and the space of distributional sections, respectively,

$$C^\infty(M;\mathcal{E}) \quad \text{and} \quad \mathcal{D}'(M;\mathcal{E}).$$

We recall the notion of the *wavefront set* of a distribution, which keeps track of the directional singularities. Given $u \in \mathcal{D}'(\mathbb{R}^n)$, we have $(x,\xi) \notin \mathrm{WF}(u) \subset T^*\mathbb{R}^n \setminus 0 = \mathbb{R}^n \times (\mathbb{R}^n \setminus 0)$ if there exists $\varphi \in C_0^\infty(\mathbb{R}^n)$ with $\varphi(x) \neq 0$ and an open conical neighbourhood U of ξ such that

$$|\widehat{\varphi u}(\eta)| = O(\langle\eta\rangle^{-\infty})$$

for $\eta \in U$. Here we let $\langle\eta\rangle = (1+|\eta|^2)^{1/2}$ and by $O(\langle\eta\rangle^{-\infty})$ we mean an expression bounded by $C_N\langle\eta\rangle^{-N}$ for every N. A vector-valued distribution $u \in \mathcal{D}'(\mathbb{R}^n;\mathbb{R}^m)$ for some $m \in \mathbb{N}$ may be identified with a vector $u = (u_1,\dots,u_m)$ with $u_i \in \mathcal{D}'(\mathbb{R}^n)$. Then

$$\mathrm{WF}(u) := \bigcup_{i=1}^m \mathrm{WF}(u_i).$$

It is standard that these definitions are coordinate invariant, so for $u \in \mathcal{D}'(M;\mathcal{E})$ we have

$$\mathrm{WF}(u) \subset T^*M \setminus 0.$$

It is moreover true that for any pseudodifferential operator A we have

$$\mathrm{WF}(Au) \subset \mathrm{WF}(A) \cap \mathrm{WF}(u) \subset \mathrm{WF}(u),$$

a fact that will be used later on. Then, we introduce for a closed conic set $\Gamma \subset T^*M \setminus 0$ the space

$$\mathcal{D}'_\Gamma(M;\mathcal{E}) = \{u \in \mathcal{D}'(M;\mathcal{E}) \mid \mathrm{WF}(u) \subset \Gamma\}.$$

Note that by the above relation on wavefront sets, the spaces $\mathcal{D}'_\Gamma(M;\mathcal{E})$ are invariant under the action of pseudodifferential operators.

2B. ***Pollicott–Ruelle resonances.*** Let us now quickly recall the microlocal approach to Pollicott–Ruelle resonances, as in [Dyatlov and Zworski 2017]. Let M be a compact smooth manifold without boundary and X be a smooth vector field. We assume that the flow φ_t of X is Anosov, i.e., that there is a splitting of the tangent space

$$T_x M = \mathbb{R}X(x) \oplus E_u(x) \oplus E_s(x)$$

for each $x \in M$, where $E_u(x)$ and $E_s(x)$ depend continuously on x and are invariant under the flow and, moreover, that for some constants $C, \nu > 0$ and a fixed metric on M

$$|d\varphi_t(x) \cdot v| \leq Ce^{-\nu|t|} \cdot |v|, \qquad \begin{cases} t \geq 0, & v \in E_s(x), \\ t \leq 0, & v \in E_u(x). \end{cases}$$

We call $E_s(x)$ the *stable* bundle or direction and $E_u(x)$ the *unstable* bundle or direction. It is a well-known fact that the geodesic flow on the unit tangent bundle $M = SN$ for N with negative sectional curvature is Anosov.

Let us define the spaces $E_0^*(x)$, $E_u^*(x)$, $E_s^*(x)$ as the duals of $E_0(x) := \mathbb{R}X(x)$, $E_s(x)$, $E_u(x)$ respectively. Explicitly, $E_u^*(x)$ is the annihilator of $\mathbb{R}X(x) \oplus E_u(x)$, $E_s^*(x)$ is the annihilator of $\mathbb{R}X(x) \oplus E_s(x)$ and $E_0^*(x)$ is the annihilator of $E_s(x) \oplus E_u(x)$. The continuous vector bundle $E_u^* := \bigcup_{x \in M} E_u^*(x) \subset T^*M$ is a closed conic subset.

Let us consider a complex vector bundle $\mathcal{E}$ over M, equipped with a connection A (which defines the covariant derivative d_A) and a smooth potential Φ (section of the endomorphism bundle of $\mathcal{E}$). This defines a first-order operator

$$P = -i\iota_X d_A + \Phi \tag{2-1}$$

acting on sections of $\mathcal{E}$, denoted by $C^\infty(M; \mathcal{E})$. Later on we will dispense with Φ, but for the moment it can be included without trouble.

For $\lambda \in \mathbb{C}$ with sufficiently large $\operatorname{Im} \lambda > C_0 > 0$, we have the integral

$$R(\lambda) := i \int_0^\infty e^{i\lambda t} e^{-itP}\, dt : L^2(M; \mathcal{E}) \to L^2(M; \mathcal{E}) \tag{2-2}$$

converges and defines a bounded operator, holomorphic in λ and, moreover, $R(\lambda) = (P - \lambda)^{-1}$ on L^2. The propagator e^{itP} is defined by solving the appropriate first-order PDE and the constant C_0 depends on P.

In [Faure and Sjöstrand 2011] (see also [Dyatlov and Zworski 2016]) it is proved that the operator $R(\lambda)$ has a meromorphic extension to the entire complex plane

$$R(\lambda) : C^\infty(M; \mathcal{E}) \to \mathcal{D}'(M; \mathcal{E}) \tag{2-3}$$

for $\lambda \in \mathbb{C}$ and the poles of this continuation are the *Pollicott–Ruelle resonances*.

We proceed to define the multiplicity of a Pollicott–Ruelle resonance λ_0. By definition, there is a Laurent expansion of $R(\lambda)$ at λ_0 (see [Dyatlov and Zworski 2019, Appendix C])

$$R(\lambda) = R_H(\lambda) - \sum_{j=1}^{J(\lambda_0)} \frac{(P - \lambda_0)^{j-1}\Pi}{(\lambda - \lambda_0)^j}, \qquad \Pi,\, R_H(\lambda) : \mathcal{D}'_{E_u^*}(M; \mathcal{E}) \to \mathcal{D}'_{E_u^*}(M; \mathcal{E}) \tag{2-4}$$

where $R_H(\lambda)$ is the holomorphic part at λ_0 and $\Pi = \Pi_{\lambda_0}$ is a finite-rank projector given by

$$\Pi_{\lambda_0} = \frac{1}{2\pi i} \oint_{\lambda_0} (\lambda - P)^{-1}\, d\lambda. \tag{2-5}$$

Here, the integral is along a small closed loop around λ_0 and it can be easily checked that $\Pi_{\lambda_0}^2 = \Pi_{\lambda_0}$, $[\Pi_{\lambda_0}, P] = 0$. The fact that $R_H(\lambda)$ and Π can be extended to continuous operators on $\mathcal{D}'_{E_u^*}$ follows from the restrictions on the wave front sets given in [Dyatlov and Zworski 2016, Proposition 3.3] and [Grigis and Sjöstrand 1994, Theorem 7.8]. The *Pollicott–Ruelle multiplicity* of λ_0, denoted by $m_P(\lambda_0)$, is defined as the dimension of the range of Π_{λ_0}.

By applying $P - \lambda$ to (2-4), we obtain $(P - \lambda_0)^{J(\lambda_0)} \Pi_{\lambda_0} = 0$ and so $\operatorname{ran} \Pi_{\lambda_0} \subset \ker(P - \lambda_0)^{J(\lambda_0)}$. The elements of $\operatorname{ran} \Pi_{\lambda_0}$ are called *generalised resonant states* and we will define, for $j \in \mathbb{N}$,

$$\operatorname{Res}_P^{(j)}(\lambda_0) = \{u \in \mathcal{D}'_{E_u^*}(M; \mathcal{E}) : (P - \lambda_0)^j u = 0\}. \tag{2-6}$$

We also write

$$\operatorname{Res}_P(\lambda_0) = \{u \in \mathcal{D}'_{E_u^*}(M; \mathcal{E}) : (P - \lambda_0)^{J(\lambda_0)} u = 0\}.$$

In fact, we may show that $\operatorname{Res}_P(\lambda_0)$ is equal to the range of Π_{λ_0} and we may think of $J(\lambda_0)$ as the size of the largest Jordan block.

Lemma 2.1. *Let $u \in \mathcal{D}'_{E_u^*}(M; \mathcal{E})$ be such that $(P - \lambda_0)^{j_0} u = 0$ with $j_0 \in \mathbb{N}_0$ the minimal such number. Then $j_0 \le J(\lambda_0)$, $\Pi_{\lambda_0} u = u$ and* $\ker(P - \lambda_0)^{J(\lambda_0)} = \operatorname{ran} \Pi_{\lambda_0}$.

Proof. Assume that $j_0 > J(\lambda_0)$ for the sake of contradiction. Since Sobolev spaces filter out $\mathcal{D}'(M; \mathcal{E})$, there is an $s > 0$ such that $u \in H^{-s}(M; \mathcal{E})$. Recalling the definition of the anisotropic space $\mathcal{H}_{rG}(M; \mathcal{E})$ for $r > 0$ (see (6-1) below), we get

$$\mathcal{D}'_{E_u^*}(M; \mathcal{E}) \cap H^{-r}(M; \mathcal{E}) \subset \mathcal{H}_{rG}(M; \mathcal{E})$$

since $\mathcal{H}_{rG}$ is microlocally equivalent to H^{-r} near E_u^*. Therefore $u \in \mathcal{H}_{rG}(M; \mathcal{E})$ for $r > s$ and by Lemma 6.1 below $(P - \lambda)^{-1} : \mathcal{H}_{rG}(M; \mathcal{E}) \to \mathcal{H}_{rG}(M; \mathcal{E})$ is meromorphic near λ_0 for $r \gg s$.

Let us set $v := (P - \lambda_0)^{j_0 - 1} u$. Then $(P - \lambda)^{-1} v = (\lambda_0 - \lambda)^{-1} v$ and by applying (2-5) to v we get $\Pi_{\lambda_0} v = v$. Note that (2-4) also implies $(P - \lambda_0)^{J(\lambda_0)} \Pi_{\lambda_0} t = 0$ for all $t \in \mathcal{H}_{rG}$. But all this implies

$$(P - \lambda_0)^{j_0 - 1} u = \Pi_{\lambda_0} (P - \lambda_0)^{j_0 - 1} u = (P - \lambda_0)^{j_0 - 1} \Pi_{\lambda_0} u = 0. \tag{2-7}$$

This contradicts the minimality of j_0 and proves the first claim.

For the second claim, take some $u \in \operatorname{Res}_P^{(j_0)}(\lambda_0)$ and use induction on j_0. Note that the first two equalities of (2-7) show $\Pi_{\lambda_0} u = u$ for $j_0 = 1$ and more generally that

$$(P - \lambda_0)^{j_0 - 1} (\Pi_{\lambda_0} u - u) = 0.$$

The fact that Π_{λ_0} is a projector and the induction hypothesis show $\Pi_{\lambda_0} u = u$, proving the claim.

Lastly, if $u \in \operatorname{ran} \Pi_{\lambda_0}$ then $\Pi_{\lambda_0} u = u$ and so $(P - \lambda_0)^{J(\lambda_0)} u = 0$ by (2-4), which together with the previous paragraph shows $\ker(P - \lambda_0)^{J(\lambda_0)} \cap \mathcal{D}'_{E_u^*}(M; \mathcal{E}) = \operatorname{ran} \Pi_{\lambda_0}$. ☐

Remark 2.2. Generalised resonant spaces of forms (at zero) have a good cohomology theory; see [Dang and Riviere 2017, Theorem 2.1]. We emphasise that here we study resonant spaces at zero with $j = 1$ in (2-6) and such that the elements are in the kernel of ι_X, as well as conditions under which there are no Jordan blocks.

2C. *Coresonant states.* Here we study the connection between the semisimplicity and a suitable pairing between resonant and coresonant states. We start off with a lemma relating the adjoint of the spectral projector and the spectral projector of the adjoint.

Lemma 2.3. *Let P be a first-order differential operator acting on sections of $\mathcal{E}$ with principal symbol $-i\sigma(X) \times \mathrm{Id}_{\mathcal{E}}$ and consider the adjoint operator P^*. Denote the spectral projector of P at $\lambda_0 \in \mathbb{C}$ by Π_{λ_0} and of P^* by Π'_{λ_0}. Also, denote the resolvent by $R_P(\lambda) = (P - \lambda)^{-1}$. Then*[1]

$$R_P(\lambda)^* = -R_{-P^*}(-\bar{\lambda}) \quad \text{and} \quad \Pi^*_\lambda = \Pi'_{-\bar{\lambda}}.$$

Proof. Firstly note that for $\operatorname{Im} \lambda \gg 1$ and all $u, v \in L^2(M; \mathcal{E})$, by (2-2) we have the identity

$$\langle R_P(\lambda)u, v\rangle_{L^2} = \langle u, -R_{-P^*}(-\bar{\lambda})v\rangle_{L^2}. \tag{2-8}$$

Then by analytic continuation we have the equality in (2-8) for any $u, v \in C^\infty$ for all $\lambda \in \mathbb{C}$. Moreover, by continuity and the mapping properties of $R_P(\lambda) : \mathcal{D}'_{E_u^*}(M; \mathcal{E}) \to \mathcal{D}'_{E_u^*}(M; \mathcal{E})$ and $R_{-P^*}(-\bar{\lambda}) : \mathcal{D}'_{E_s^*}(M; \mathcal{E}) \to \mathcal{D}'_{E_s^*}(M; \mathcal{E})$ outside the poles, we have (2-8) for all $u \in \mathcal{D}'_{E_u^*}$ and $v \in \mathcal{D}'_{E_s^*}$. This proves the first claim. Now let $u \in \mathcal{D}'_{E_u^*}(M; \mathcal{E})$ and $v \in \mathcal{D}'_{E_s^*}(M; \mathcal{E})$. We may write

$$\langle \Pi_{\lambda_0} u, v\rangle = -\frac{1}{2\pi i}\oint_{\lambda_0} \langle R_P(\lambda)u, v\rangle \, d\lambda = \frac{1}{2\pi i}\oint_{\lambda_0} \langle u, R_{-P^*}(-\bar{\lambda})v\rangle \, d\lambda = \langle u, \Pi'_{-\bar{\lambda}_0} v\rangle.$$

This proves $\Pi^*_{\lambda_0} = \Pi'_{-\bar{\lambda}_0}$. □

We proceed to define the *coresonant states*. Given an operator P as in Lemma 2.3 and a resonance $\lambda_0 \in \mathbb{C}$, the space of coresonant states at λ_0 is $\mathrm{Res}_{-P^*}(-\bar{\lambda}_0) \subset \mathcal{D}'_{E_s^*}(M; \mathcal{E})$. By the wavefront set conditions, notice that we may multiply resonances and coresonances in the scalar case, or form inner products; see, e.g., [Grigis and Sjöstrand 1994, Proposition 7.6]. We are now ready to reinterpret the semisimplicity in terms of the pairing

$$\mathrm{Res}_P(\lambda_0) \times \mathrm{Res}_{-P^*}(-\bar{\lambda}_0) \to \mathbb{C}, \ (u, v) \mapsto \langle u, v\rangle_{L^2}. \tag{2-9}$$

Observe that the pairing (2-9) is nondegenerate: we have $\langle u, v\rangle = 0$ for all $v \in \mathrm{Res}_{-P^*}(-\bar{\lambda}_0)$ if and only if $\langle u, \Pi'_{-\bar{\lambda}_0}\varphi\rangle = 0$ for all $\varphi \in C^\infty(M; \mathcal{E})$. Then by Lemma 2.3 and since $\Pi_{\lambda_0} u = u$, this holds if and only if $u \equiv 0$; by an analogous argument for the other entry, we obtain the nondegeneracy. In particular, $m_P(\lambda_0) = m_{-P^*}(-\bar{\lambda}_0)$ and also $J(\lambda_0) = J'(-\bar{\lambda}_0)$. Here $J'(\mu)$ denotes the size of the largest Jordan block of $-P^*$ at μ.

[1]Here we interpret $-R_{-P^*}(-\bar{\lambda}) : C^\infty(M; \mathcal{E}) \to \mathcal{D}'(M; \mathcal{E})$ as the operator obtained by meromorphic continuation, but with respect to the flow generated by $-X$.

Lemma 2.4. *Assume P satisfies the assumptions of Lemma 2.3. Then we have that the semisimplicity for P at λ_0 holds if and only if the semisimplicity for $-P^*$ at $-\bar{\lambda}_0$ holds. Moreover, P is semisimple at λ_0 if and only if the pairing*

$$\operatorname{Res}_P^{(1)}(\lambda_0) \times \operatorname{Res}_{-P^*}^{(1)}(-\bar{\lambda}_0) \to \mathbb{C}, \quad (u, v) \mapsto \langle u, v\rangle_{L^2}. \tag{2-10}$$

is nondegenerate.

Proof. For the first claim, simply note that by the previous paragraph we have $J(\lambda_0) = J'(-\bar{\lambda}_0)$.

For the second claim, assume first that the pairing (2-10) is nondegenerate. Assume we have $u, u' \in \mathcal{D}'_{E_u^*}(M; \mathcal{E})$, with $(P - \lambda_0)u = u'$ where $u' \in \operatorname{Res}_P^{(1)}(\lambda_0)$. We want to show $u' = 0$. We have, for any $v \in \operatorname{Res}_{-P^*}^{(1)}(-\bar{\lambda}_0)$,

$$\langle u', v\rangle = \langle (P - \lambda_0)u, v\rangle = \langle u, (P^* - \bar{\lambda}_0)v\rangle = 0.$$

Now nondegeneracy implies $u' = 0$.

Assume next the semisimplicity holds for P at λ_0 and let $u \in \operatorname{Res}_P^{(1)}(\lambda_0)$ satisfy $\langle u, v\rangle = 0$ for all $v \in \operatorname{Res}_{-P^*}^{(1)}(-\bar{\lambda}_0)$. Then we have, for all $\varphi \in C^\infty(M; \mathcal{E})$,

$$\langle u, \varphi\rangle = \langle \Pi_{\lambda_0} u, \varphi\rangle = \langle u, \Pi'_{-\bar{\lambda}_0}\varphi\rangle = 0.$$

Here we used Lemma 2.3 and the assumption. Thus $u \equiv 0$. The fact that $-P^*$ is semisimple at $-\bar{\lambda}_0$ and an analogous argument for the other entry proves the nondegeneracy and finishes the proof. □

2D. *Further preparatory results.* We start by quoting an important technical result; see [Dyatlov and Zworski 2017, Lemma 2.3].

Lemma 2.5. *Suppose there exist a smooth volume form on M and a smooth inner product on the fibres of $\mathcal{E}$ for which $P^* = P$ on $L^2(M; \mathcal{E})$. Suppose that $u \in \mathcal{D}'_{E_u^*}(M; \mathcal{E})$ satisfies*[2]

$$Pu \in C^\infty(M; \mathcal{E}), \quad \operatorname{Im}\langle Pu, u\rangle_{L^2} \geq 0.$$

Then $u \in C^\infty(M; \mathcal{E})$. In particular, the conclusion of the lemma holds for u a resonant state with the eigenvalue $\lambda \in \mathbb{R}$—just swap P with $P - \lambda$.

We also need a simple regularity result analogous to [Dyatlov and Zworski 2017, Lemma 2.1]. We give it here for completeness

Lemma 2.6. *Assume d_A is flat and let $\Gamma \subset T^*M \setminus 0$ be a closed conic set. Assume that $u \in \mathcal{D}'_\Gamma(M; \Omega^k \otimes \mathcal{E})$ and $d_A u \in C^\infty(M; \Omega^{k+1} \otimes \mathcal{E})$. Then there exists $v \in C^\infty(M; \Omega^k \otimes \mathcal{E})$ and $w \in \mathcal{D}'_\Gamma(M; \Omega^{k-1} \otimes \mathcal{E})$ such that $u = v + d_A w$.*

Proof. The proof follows formally by replacing d with d_A and δ with d_A^* in the proof [Dyatlov and Zworski 2017, Lemma 2.1]. □

[2]The inner product in this paper is complex conjugate in the second variable.

2E. ***Cohomology in a flat bundle.*** Given a manifold M of dimension n and a Hermitian vector bundle $\mathcal{E}$ with a flat connection A, we may consider the complex given by

$$0 \xrightarrow{d_A} C^\infty(M;\mathcal{E}) \xrightarrow{d_A} C^\infty(M;\Omega^1\otimes\mathcal{E}) \xrightarrow{d_A} \cdots \xrightarrow{d_A} C^\infty(M;\Omega^n\otimes\mathcal{E}) \xrightarrow{d_A} 0. \tag{2-11}$$

Here we extend, as usual, the action of d_A to vector-valued differential forms by asking that the Leibnitz rule holds. The homology of this complex will be denoted by $H^k_A(M;\mathcal{E})$ for $k=0,\dots,n$. Consider now Σ an oriented Riemannian surface and let $\mathcal{E}$ be a Hermitian vector bundle over Σ equipped with a unitary, flat connection A. We can pull back the bundle $\mathcal{E}$ to the unit sphere bundle $\pi: S\Sigma\to\Sigma$ to obtain $\pi^*\mathcal{E}$, equipped with a unitary, flat connection π^*A.

Lemma 2.7. *Assume Σ has genus $g\neq 1$. Then the following map is an isomorphism*:

$$\pi^*: H^1_A(\Sigma;\mathcal{E}) \to H^1_{\pi^*A}(S\Sigma;\pi^*\mathcal{E}). \tag{2-12}$$

Proof. There is a vertical vector field V that generates the rotation in the fibres of $S\Sigma$. We first check π^* is injective, so assume $\pi^*\theta = d_{\pi^*A}F$, where $\theta\in C^\infty(\Sigma;\Omega^1\otimes\mathcal{E})$ is d_A-closed and $F\in C^\infty(S\Sigma;\mathcal{E})$. This implies $\iota_V d_{\pi^*A}F=0$. Note that if $x\in\Sigma$, there is a small ball B with $x\in B$, over which $\mathcal{E}$ is trivial. Thus $\iota_V d_{\pi^*A}F=0$ implies $VF=0$ (since $\iota_V\pi^*A=0$) and so $F=\pi^*f$ locally; this is easily seen to extend to $F=\pi^*f$ globally for some $f\in C^\infty(\Sigma;\mathcal{E})$. This implies $\pi^*(d_Af-\theta)=0$ and so $d_Af=\theta$.

For surjectivity, take $u\in C^\infty(S\Sigma;\Omega^1\otimes\pi^*\mathcal{E})$ with $d_{\pi^*A}u=0$. We want to prove there are v and F such that $u=\pi^*v+d_{\pi^*A}F$, where v is d_A-closed. This implies

$$\iota_V u = \iota_V d_{\pi^*A}F. \tag{2-13}$$

If we solve (2-13), then $w=u-d_{\pi^*A}F$ satisfies $d_{\pi^*A}w=0$ and $\iota_V w=0$. By going to local trivialisations where $A=0$, a computation implies $w=\pi^*v$ for some 1-form v locally. Again, by uniqueness this may be easily extended to some global $v\in C^\infty(\Sigma;\mathcal{E})$ with $d_Av=0$. We now focus on (2-13) and finding such F.

To this end, we introduce the pushforward map $\pi_*: C^\infty(S\Sigma;\Omega^1\otimes\pi^*\mathcal{E})\to C^\infty(\Sigma;\mathcal{E})$ by integrating along the fibres

$$\pi_*: \alpha(x,v)\mapsto \beta(x)=\int_{S_x\Sigma}\alpha. \tag{2-14}$$

One can show that the pushforward is well-defined and that it intertwines d_A and d_{π^*A}; after going to a trivialisation where $A=0$, this reduces to showing commutation with d, which follows from [Bott and Tu 1982, Proposition 6.14.1]. Thus π_* descends to cohomology; i.e., we have $\pi_*: H^1_{\pi^*A}(S\Sigma;\mathcal{E})\to H^0_A(\Sigma;\mathcal{E})$.

Now observe that (2-13) can be solved if and only if $\pi_*u=0$. We introduce the section $s\in C^\infty(\Sigma;\mathcal{E})$ with $s(x)=\pi_*u$. Note that $d_As=0$. Moreover, we have for K the Gaussian curvature of Σ:

$$\int_{S\Sigma}\langle u,\pi^*(sK\,d\,\mathrm{vol}_\Sigma)\rangle = \int_\Sigma\langle \pi_*u, sK\,d\,\mathrm{vol}_\Sigma\rangle = \int_\Sigma \|s\|^2K\,d\,\mathrm{vol}_\Sigma = \|s\|^2 2\pi\chi(\Sigma). \tag{2-15}$$

Here we used that $\|s\|^2$ is constant, since s is parallel and A is unitary, and we applied Gauss–Bonnet theorem. In the first equality we use a generalisation of [Bott and Tu 1982, Proposition 6.15]. We use the convention that $\langle s\alpha, s'\beta\rangle = \langle s,s'\rangle_{\mathcal{E}}\alpha\wedge\bar{\beta}$, where α and β are forms of complementary degree and s, s' are sections.

On the other hand, we have $\pi^*(K\, d\,\mathrm{vol}_\Sigma) = -d\psi$, where ψ is the connection 1-form on $S\Sigma$. Therefore we have the pointwise identity, as $d_{\pi^*A}u = 0$ and $d_A s = 0$,

$$\langle u, \pi^*(sK\, d\,\mathrm{vol}_\Sigma)\rangle = d\langle u, (\pi^* s)\psi\rangle.$$

So by Stokes' theorem we obtain that the first integral in (2-15) is zero. Since $g \neq 1$, we have $\chi(\Sigma) \neq 0$ and so $s = 0$. Therefore $\pi_* u = 0$, which concludes the proof. □

Remark 2.8. Alternatively, we could have proved Lemma 2.7 more abstractly using a version of the Gysin sequence for twisted de Rham complexes; see [Bott and Tu 1982, p. 177] for more details.

We now compute the Euler characteristic of the twisted de Rham complex. This shows that, although the twisted Betti numbers, i.e., dimensions of $H^k_A(M; \mathcal{E})$ can jump by changing A, the Euler characteristic is independent of the choice of flat connection. We could not find an appropriate reference for this result.

Lemma 2.9. *The Euler characteristic of the chain complex* (2-11), *denoted by* $\chi_A(M; \mathcal{E})$, *is equal to*

$$\chi_A(M; \mathcal{E}) = \mathrm{rank}(\mathcal{E})\chi(M).$$

Proof. A way to prove this is given by an application of the Atiyah–Singer index theorem; we sketch the proof here. It starts by noting that, as with the usual nontwisted forms, we have

$$d_A + d_A^* : C^\infty(M; \Omega^{\mathrm{odd}} \otimes \mathcal{E}) \to C^\infty(M; \Omega^{\mathrm{even}} \otimes \mathcal{E}). \tag{2-16}$$

Here $\Omega^{\mathrm{even}} = \bigoplus_i \Omega^{2i}$ and $\Omega^{\mathrm{odd}} = \bigoplus_i \Omega^{2i+1}$ are the bundles of even and odd differential forms, respectively. Let us introduce the twisted Hodge laplacian, $\Delta_A = d_A^* d_A + d_A d_A^*$. By Hodge theory, we have $H^k_A(M; \mathcal{E}) \cong \ker \Delta_A|_{\Omega^k \otimes \mathcal{E}}$. Therefore, we also have $\mathrm{ind}(d_A + d_A^*) = \chi_A(M; \mathcal{E})$, where by ind we denote the index of an operator.

By the Atiyah–Singer index theorem,

$$\begin{aligned} \mathrm{ind}(d_A + d_A^*) &= \int_{T^*M} \mathrm{ch}(\mathrm{d}(d_A + d_A^*))\mathcal{T}(TM) \\ &= \int_{T^*M} \mathrm{ch}(\mathcal{E})\,\mathrm{ch}(\mathrm{d}(d + d^*))\mathcal{T}(TM) \\ &= \mathrm{rank}(\mathcal{E}) \int_{T^*M} \mathrm{ch}(\mathrm{d}(d + d^*))\mathcal{T}(TM) = \mathrm{rank}(\mathcal{E})\chi(M). \end{aligned} \tag{2-17}$$

Here, $\mathcal{T}$ denotes the Todd class and ch denotes the Chern character.[3] The letter d denotes the *difference bundle*. Since $(\mathcal{E}, A)$ is flat by assumption, we have $\mathrm{ch}(\mathcal{E}) = \mathrm{rank}(\mathcal{E})$. The transition to the second line is justified since the principal symbol of $d_A + d_A^*$ is equal to $\sigma(d + d^*) \otimes \mathrm{Id}_{\mathcal{E}}$, so that

$$\mathrm{d}(d_A + d_A^*) = \mathrm{d}(\sigma(d + d^*) \otimes \mathrm{Id}) = [G_1 \otimes \mathcal{E}] - [G_2 \otimes \mathcal{E}] = ([G_1] - [G_2]) \cdot [\mathcal{E}] \in K^{\mathrm{comp}}(T^*M).$$

Here G_1 and G_2 are certain vector bundles over a one-point compactification of T^*M and K^{comp} denotes the suitable K-theory. Since ch is multiplicative over the K-theory, we get the product of characters. The

[3]More explicitly, these are given for a vector bundle V over M with curvature two-form Ω and $w = -\Omega/(2\pi i)$, by $\mathrm{ch}(V) = \mathrm{tr} \exp w$ and $\mathcal{T}(V) = \det(w/(1 - \exp(-w)))$. Here we apply the Taylor series at zero to forms.

last equality follows from the Atiyah–Singer index theorem for the operator $d + d^* : \Omega^{\mathrm{odd}} \to \Omega^{\mathrm{even}}$ and the nontwisted Hodge theory. □

3. Meromorphic continuation of $\zeta_A(s)$

We devote this section to showing meromorphic continuation of $\zeta_A(s)$ given by (1-1) for an arbitrary (possibly nonflat, nonunitary) A. We note that the meromorphic continuation of the Ruelle zeta function was first established in [Giulietti et al. 2013] and later in [Dyatlov and Zworski 2016], and that here we follow the latter microlocal approach. Let (M, g) be a compact Riemannian manifold and $\mathcal{E}$ a Hermitian vector bundle over M equipped with a connection A and an endomorphism-valued function Φ. Also assume M admits an Anosov flow φ_t with generator X. We consider the first-order operator $P = -i\iota_X\, d_A + \Phi$.

Let us denote by $\alpha_{x,t}$ the parallel transport (with respect to P) in the fibres of $\mathcal{E}$ along integral curves of φ_t:

$$\alpha_{x,t} : \mathcal{E}(x) \to \mathcal{E}(\varphi_t(x)). \tag{3-1}$$

Recall now that the propagator e^{-itP} is the one-parameter family of operators, defined by solving the first-order PDE in (t, x) for $u \in C^\infty(M; \mathcal{E})$

$$\Big(\frac{\partial}{\partial t} + iP\Big)(e^{-itP}u) = 0. \tag{3-2}$$

Then the solution $u(t, x) = (e^{-itP}u)(t, x) \in C^\infty(\mathbb{R} \times M; \mathcal{E})$ (we pull back $\mathcal{E}$ to $\mathbb{R} \times M$) and we have

$$(e^{-itP}u)(t, x) = u(t, x) = \alpha_{\varphi_{-t}x,t}\, u(\varphi_{-t}x). \tag{3-3}$$

This follows by a computation in local coordinates. In fact, in a local coordinate system $U \ni x$ over which $\mathcal{E}|_U \cong U \times \mathbb{C}^m$ is trivial and for small t, we have

$$(\partial_t + A(\partial_t) + i\Phi(\varphi_t x))\alpha_{x,t} = 0. \tag{3-4}$$

We write A for the matrix of 1-forms associated to $d_A = d + A$ and identify $\alpha_{x,t}$ with a matrix. Then we may compute, using the chain rule,

$$\begin{aligned}
\partial_t u(t, x) &= -\big(A(X(x)) + i\Phi(x)\big)\alpha_{\varphi_{-t}x,t}u(\varphi_{-t}x) - (X\alpha)_{\varphi_{-t}x,t}u(\varphi_{-t}x) - \alpha_{\varphi_{-t}x,t}Xu(\varphi_{-t}x) \\
&= -iP(\alpha_{\varphi_{-t}x,t}u)(t, x) + X(\alpha_{\varphi_{-t}x,t}u)(t, x) - (X\alpha_{\varphi_{-t}x,t})u(\varphi_{-t}x) - \alpha_{\varphi_{-t}x,t}Xu(\varphi_{-t}x) \\
&= -iPu(t, x).
\end{aligned}$$

Here we used (3-4) in the first equality, the definition of P in the second and the chain rule in the last one. We thus obtain (3-3) for small t and by iteration we obtain it for all t. As a consequence, we obtain for any $f \in C^\infty(M)$ and $u \in C^\infty(M; \mathcal{E})$

$$e^{-itP}(fu) = f \circ \varphi_{-t} \cdot e^{-itP}u. \tag{3-5}$$

Denote by $\mathcal{P}_{x,t}$ the linearised Poincaré map for any time t and point $x \in M$:

$$\mathcal{P}_{x,t} = (d\varphi_t(x))^{-T} : \Omega^1_0(x) \to \Omega^1_0(\varphi_t x),$$

where, for $x \in M$ and $k \in \mathbb{N}$, we define the subbundle of differential forms in the kernel of ι_X by

$$\Omega_0^k = \Omega^k \cap \ker \iota_X.$$

We write $-T$ for the inverse transpose. Note $\mathcal{L}_X$ acts on sections of Ω_0^k for any k. Also, we have that φ_t^* is a one-parameter family of maps acting on Ω_0^k, for any k, such that we may write $(\varphi_t)^* = e^{t\mathcal{L}_X}$. So we obtain that, by the definition of φ_{-t}^* for any η a smooth k-form (see (3-3))

$$\bigwedge^k \mathcal{P}_{x,t}(\eta(x)) = e^{-t\mathcal{L}_X}\eta(\varphi_t x). \tag{3-6}$$

Here $\bigwedge^k \mathcal{P}_{x,t}$ is the exterior product of maps acting on Ω_0^k. Given a closed orbit γ with period T, we consider a point $x_0 \in \gamma$ and define

$$\operatorname{tr}\alpha_\gamma := \operatorname{tr}\alpha_{x_0,T}.$$

Since the maps $\alpha_{\varphi_t x_0,T}$ are conjugate for varying t, the trace is independent of γ. Similarly, we define

$$\det(\mathrm{Id} - \mathcal{P}_\gamma) := \det(\mathrm{Id} - \mathcal{P}_{x_0,T}).$$

In what follows, for technical purposes we assume that we have a constant $\beta \in \mathbb{N}$ such that

$$|\det(\mathrm{Id} - \mathcal{P}_\gamma)| = (-1)^\beta \det(\mathrm{Id} - \mathcal{P}_\gamma). \tag{3-7}$$

This happens in particular if E_s and E_u are orientable, where $\beta = \dim E_s$. This assumption may be removed by using a suitable twist with an orientation bundle; see [Dyatlov and Guillarmou 2016; Dyatlov and Zworski 2016; Giulietti et al. 2013] for details.

We will denote by $\gamma^\#$ a general primitive periodic orbit, and if γ is an arbitrary periodic orbit, then $l_\gamma^\#$ will denote the period of the primitive periodic orbit corresponding to γ.

Theorem 3.1. *Define for* $\operatorname{Re} s \gg 1$

$$F_P(s) := \sum_{\gamma \in \mathcal{G}} \frac{e^{-sl_\gamma} l_\gamma^\# \operatorname{tr}\alpha_\gamma}{|\det(\mathrm{Id} - \mathcal{P}_\gamma)|}, \tag{3-8}$$

where the sum is over all periodic trajectories. Then $F_P(s)$ extends meromorphically to all $s \in \mathbb{C}$. The poles of $F_P(s)$ are precisely $s \in \mathbb{C}$, where is a Pollicott–Ruelle resonance of P. Moreover, the poles are simple with residues equal to the Pollicott–Ruelle multiplicity $m_P(is)$.

Proof. We give only a sketch of the proof here, as it follows from [Dyatlov and Zworski 2016]. The sum (3-8) converges by [loc. cit., Lemma 2.2] and as $\|\alpha_\gamma\| \le Ce^{Cl_\gamma}$ for some $C > 0$. Observe that by (3-3), we have that the Schwartz kernel K of the propagator e^{-itP}, as a distribution $K(t, y, x) \in \mathcal{D}'(\mathbb{R} \times M \times M)$, satisfies $\mathrm{WF}(K) \subset N^*S$, where $S = \{(t, \varphi_t(x), x) : x \in M,\ t \in \mathbb{R}\}$ and N^*S denotes the conormal bundle of S. Therefore, Guillemin's trace formula [loc. cit., Appendix B] applies to give, for $t > 0$,

$$\operatorname{tr}^\flat e^{-itP}|_{C^\infty(M;\mathcal{E})} = \sum_{\gamma \in \mathcal{G}} \frac{l_\gamma^\# \operatorname{tr}\alpha_\gamma \delta(t - l_\gamma)}{|\det(\mathrm{Id} - \mathcal{P}_\gamma)|}.$$

All that is left to do is to note that the remainder of the proof in [loc. cit., Section 4] is not sensitive to changing φ_{-t}^* to a general propagator e^{-itP} for P as above. This completes the proof.

Alternatively, the whole statement follows from more general work [Dyatlov and Guillarmou 2016, Theorem 4] on open systems. □

We now prove the meromorphic extension of the zeta function using the meromorphic continuation of the trace above.

Proposition 3.2. *The zeta function $\zeta_A(s)$ is given by*

$$\zeta_A(s) = \prod_{\gamma^\#} \det\left(\mathrm{Id} - \alpha_{\gamma^\#} e^{-sl_\gamma^\#}\right) \tag{3-9}$$

for large $\operatorname{Re} s$ *and holomorphic in that region. Moreover, it has a meromorphic extension to the whole of* $\mathbb{C}$ *and the poles and zeros of the extension are determined by Pollicott–Ruelle resonances of* $P = -i\iota_X d_A + \Phi$ *acting on differential forms with values in* $\mathcal{E}$.

Proof. We follow the now standard procedure of writing $\log \zeta_A$ as an alternating sum of traces of maps between bundles of differential forms with values in a vector bundle; see [Dyatlov and Zworski 2016, equation (2.5)], originally due to [Ruelle 1976]. We write for large $\operatorname{Re} s$

$$\begin{aligned}
\log \zeta_A(s) &= \sum_{\gamma^\#} \log\det(\mathrm{Id} - \alpha_{\gamma^\#} e^{-sl_\gamma^\#}) = \sum_{\gamma^\#} \operatorname{tr}\log(\mathrm{Id} - \alpha_{\gamma^\#} e^{-sl_\gamma^\#}) \\
&= -\sum_{\gamma^\#, j} \frac{\operatorname{tr}(\alpha_{\gamma^\#}^j) e^{-jsl_\gamma^\#}}{j} = -\sum_{\gamma} \operatorname{tr}(\alpha_\gamma) e^{-sl_\gamma} \frac{l_\gamma^\#}{l_\gamma} \\
&= \sum_{k=0}^{n-1} (-1)^{k+\beta+1} \sum_{\gamma} \frac{\operatorname{tr}\left(\bigwedge^k \mathcal{P}_\gamma\right) \operatorname{tr}(\alpha_\gamma) e^{-sl_\gamma}}{|\det(\mathrm{Id} - \mathcal{P}_\gamma)|} \frac{l_\gamma^\#}{l_\gamma} = \sum_{k=0}^{n-1} (-1)^{k+\beta} g_k(s).
\end{aligned} \tag{3-10}$$

We used the formula $\log\det(\mathrm{Id} + A) = \operatorname{tr}\log(\mathrm{Id} + A)$, which works for $\|A\|$ small enough, the fact that there is a $C > 0$ such that $\|\alpha_\gamma\| \le Ce^{Cl_\gamma}$ and [Dyatlov and Zworski 2016, Lemma 2.2]. The function g_k is defined as

$$g_k(s) = -\sum_{\gamma} \frac{\operatorname{tr}\left(\bigwedge^k \mathcal{P}_\gamma\right) \operatorname{tr}(\alpha_\gamma) e^{-sl_\gamma}}{|\det(\mathrm{Id} - \mathcal{P}_\gamma)|} \frac{l_\gamma^\#}{l_\gamma}.$$

Also, we used the identity

$$\det(\mathrm{Id} - \mathcal{P}_\gamma) = \sum_{k=0}^{n-1} (-1)^k \operatorname{tr}\left(\bigwedge^k \mathcal{P}_\gamma\right),$$

which comes from linear algebra. Introduce then

$$F_k(s) := -g_k'(s) = -\sum_{\gamma} \frac{\operatorname{tr}\left(\bigwedge^k \mathcal{P}_\gamma\right) \operatorname{tr}(\alpha_\gamma) e^{-sl_\gamma} l_\gamma^\#}{|\det(\mathrm{Id} - \mathcal{P}_\gamma)|}. \tag{3-11}$$

This is reminiscent of (3-8). In fact, consider the vector bundle $\mathcal{E}_k := \Omega_0^k \otimes \mathcal{E}$. We extend the action of P on $\mathcal{E}$ to the action on $\mathcal{E}_k$ by the Leibniz rule and denote the associated first-order differential operator by P_k. We have, for $w \in C^\infty(M; \Omega_0^k)$ and $s \in C^\infty(M; \mathcal{E})$,

$$P_k(s \otimes w) = (-i\iota_X d_A + \Phi)(s \otimes w) = Ps \otimes w + s \otimes (-i\mathcal{L}_X w). \tag{3-12}$$

Then we observe that, by using (3-12),

$$(\partial_t + iP_k)(e^{-itP} s \otimes e^{-t\mathcal{L}_X} w) = 0. \tag{3-13}$$

Introduce the parallel transport $\beta_{k,x,t} : \mathcal{E}_k(x) \to \mathcal{E}_k(\varphi_t x)$ along the fibres of $\mathcal{E}_k$. Then by (3-3), (3-6) and (3-13)

$$\begin{aligned}\beta_{k,x,t}(s(x) \otimes w(x)) &= e^{-itP_k}(s \otimes w)(\varphi_t x)\\ &= e^{-itP} s(\varphi_t x) \otimes e^{-t\mathcal{L}_X} w(\varphi_t x) = \alpha_{x,t}(s(x)) \otimes \textstyle\bigwedge^k \mathcal{P}_{x,t}(w(x)).\end{aligned} \tag{3-14}$$

We claim that for $k = 0, 1, \ldots, n-1$

$$F_{P_k}(s) = F_k(s).$$

To see this, observe that along a periodic orbit γ of period l_γ by (3-14) we have

$$\operatorname{tr}(\beta_{k,\gamma}) = \operatorname{tr}\big(\alpha_\gamma \otimes \textstyle\bigwedge^k \mathcal{P}_\gamma\big) = \operatorname{tr}(\alpha_\gamma) \cdot \operatorname{tr}\big(\textstyle\bigwedge^k \mathcal{P}_\gamma\big).$$

Here we write $\beta_{k,\gamma} = \beta_{k,x_0,l_\gamma}$, where x_0 is any point on γ. The trace $\operatorname{tr}\beta_{k,\gamma}$ is independent of x_0. This proves the claim.

By Theorem 3.1 and an elementary argument, for each k there exists a holomorphic function $\zeta_{k,A}(s)$ such that

$$\frac{\zeta_{k,A}'}{\zeta_{k,A}} = -F_k(s) = g_k'(s).$$

Thus by (3-10) we obtain the factorisation

$$\zeta_A(s) = \prod_{k=0}^{n-1} \zeta_{k,A}^{(-1)^{k+\beta}}(s). \tag{3-15}$$

By Theorem 3.1, $s \in \mathbb{C}$ is a zero of $\zeta_{k,A}(s)$ precisely when is is a Pollicott–Ruelle resonance of P_k and the multiplicity of the zero is equal to the Pollicott–Ruelle multiplicity at is. □

For convenience we restate the factorisation above for 3-manifolds.

Corollary 3.3. *Consider a closed* 3*-manifold* (M, g) *with an Anosov flow* X. *Let* $\mathcal{E}$ *be a vector bundle over* M *equipped with a connection* A *and a potential* Φ. *Then, assuming* E_s *is orientable, we have the factorisation, where* $\zeta_{k,A}$ *is entire for* $k = 0, 1, 2$,

$$\zeta_A(s) = \frac{\zeta_{1,A}(s)}{\zeta_{0,A}(s)\zeta_{2,A}(s)}. \tag{3-16}$$

Moreover, the order of zero at a point s *of* $\zeta_A(s)$ *is equal to*

$$m_{P_1}(is) - m_{P_0}(is) - m_{P_2}(is), \tag{3-17}$$

where $m_{P_k}(is)$ *denotes the Pollicott–Ruelle resonance multiplicity at* is *of the operators* $P_k = -i\iota_X d_A + \Phi$ *acting on sections of the vector bundle* $\mathcal{E}_k = \Omega_0^k(M) \otimes \mathcal{E}$ *for* $k = 0, 1, 2$.

4. Resonant spaces

In this section we prove:

Theorem 4.1. *Let* (M, Ω) *be a closed* 3*-manifold with volume form* Ω *and let* φ_t *be a volume-preserving Anosov flow. Let* $\mathcal{E}$ *be a Hermitian vector bundle equipped with a unitary flat connection* A. *Then*:

(1) $\dim \mathrm{Res}_{0,A}(0) = \dim \mathrm{Res}_{2,A}(0) = b_0(M, \mathcal{E})$.

(2) *If* $[\omega] \neq 0$, *then* $\dim \mathrm{Res}_{1,A}(0) = b_1(M, \mathcal{E}) - b_0(M, \mathcal{E})$.

(3) *If* $[\omega] = 0$, *then*

$$\dim \mathrm{Res}_{1,A}(0) = \begin{cases} b_1(M, \mathcal{E}) & \text{if } \mathcal{H}(X) \neq 0, \\ b_1(M, \mathcal{E}) + b_0(M, \mathcal{E}) & \text{if } \mathcal{H}(X) = 0. \end{cases}$$

Moreover, k*-semisimplicity holds for* $k = 0, 2$.

In particular, as a consequence we obtain:

Proof of Theorem 1.2. This is a direct consequence of Theorem 4.1 applied to trivial bundle $\mathcal{E} = M \times \mathbb{C}$ and the trivial connection $d_A = d$. □

We break down the proof of Theorem 4.1 into the following subsections.

4A. ***Smooth invariant 1-forms.*** We first show that smooth resonant 1-forms are zero. The idea is that an invariant 1-form decays along the stable direction in the future and in the unstable direction in the past and so must vanish. This first subsection is quite general and holds in any dimension for any unitary connection A and Hermitian matrix field Φ. Recall that $\Omega_0^k = \Omega^k \cap \ker \iota_X$.

Lemma 4.2. *We have*

$$\mathrm{Res}_{1,A,\Phi}(0) \cap C^\infty(M; \Omega_0^1 \otimes \mathcal{E}) = \{0\}. \tag{4-1}$$

Proof. We start by proving the following formula, which holds for any $u \in C^\infty(M; \Omega^k \otimes \mathcal{E})$:

$$\alpha_{x,t}(u_x(\xi^k)) = e^{-t(\iota_X d_A + i\Phi)} u_{\varphi_t x}\big(\big(\textstyle\bigwedge^k d\varphi_t\big)\xi^k\big). \tag{4-2}$$

Here $\xi^k \in \Lambda_x^k M$ is a k-vector and x is any point in M. The definitions of $\alpha_{x,t}$ are given in (3-1) and (3-3).

Note firstly that it suffices to prove the claim above for $u = s \otimes w$, where w is a k-form and s is a section of $\mathcal{E}$, since we can write u as a sum of such terms near x and a term which is zero close to x. But this follows from (3-14) and by the definition of the map $\mathcal{P}_{x,t}$.

If $u \in \mathrm{Res}_{1,A,\Phi}(0) \cap C^\infty(M; \Omega_0^1 \otimes \mathcal{E})$ we must have $(-i\iota_X d_A + \Phi)u = 0$ and $\iota_X u = 0$. This further implies $e^{-t(\iota_X d_A + i\Phi)} u = u$, since $(\partial_t + \iota_X d_A + i\Phi)u = 0$. Then by (4-2) for $k = 1$ and $\xi \in E_s(x)$

$$|u_x(\xi)| = |\alpha_{x,t} u_x(\xi)| = |u_{\varphi_t x}(d\varphi_t \xi)| \lesssim |d\varphi_t \xi|_g \lesssim e^{-\lambda t}, \quad t > 0. \tag{4-3}$$

Here we used that $\alpha_{x,t}$ is a unitary isomorphism[4] the Anosov property of X and that $t>0$ in the last inequality. By taking the limit $t\to\infty$, we get u is zero in the direction of E_s. Similarly, we get that u is zero in the direction of E_u, so u is zero. □

Remark 4.3. The above method shows that for an arbitrary smooth k-form $u\in \mathrm{Res}_{k,A,\Phi}(0)$, we have $u|_{\bigwedge^k E_u}=0$ and $u|_{\bigwedge^k E_s}=0$, and more generally one could compare rates of contraction and expansion to obtain vanishing on larger subspaces. Other components can be nonzero, as can be seen, e.g., below from the computation for $\mathrm{Res}_{2,A}(0)$ for A flat.

4B. $\mathbf{Res}_{0,A}(0)$ *and* $\mathbf{Res}_{2,A}(0)$.

Recall that $\omega=i_X\Omega$ and assume from now on that A is flat.

Lemma 4.4. *We have*

$$\mathrm{Res}_{0,A}(0)=\{s\in C^\infty(M;\mathcal{E}):d_As=0\}=H^0_A(M,\mathcal{E}),\tag{4-4}$$

$$\mathrm{Res}_{2,A}(0)=\{s\,\omega:s\in C^\infty(M;\mathcal{E}),\ d_As=0\}.\tag{4-5}$$

Moreover, k-semisimplicity holds for $k=0,2$.

Proof. We distinguish the cases $k=0$ or 2.

Case $k=0$: If $s\in\mathrm{Res}_{0,A}(0)$, then $s\in C^\infty(M;\mathcal{E})$ by Lemma 2.5. Since A is flat, $d_A^2s=0$ and therefore $d_As\in\mathrm{Res}_{1,A}(0)\cap C^\infty(M,\Omega^1_0\otimes\mathcal{E})$ and by Lemma 4.2 we have $d_As=0$. So in this case we get a bijection with the parallel sections of $\mathcal{E}$.

For semisimplicity, consider $s\in\mathcal{D}'_{E_u^*}(M;\mathcal{E})$ with $\iota_Xd_As=:v\in\mathrm{Res}_{0,A}(0)$. Then $v\in C^\infty(M;\mathcal{E})$ by Lemma 2.5 and v is parallel by the previous paragraph. For $u\in C^\infty(M;\mathcal{E})$ parallel, since d_A is unitary, we have

$$\int_M\langle\iota_Xd_As,u\rangle_{\mathcal{E}}\,\Omega=\int_M X\langle s,u\rangle_{\mathcal{E}}\,\Omega=0.\tag{4-6}$$

By picking $u=v$, we get $v=0$ and so $s\in\mathrm{Res}_{0,A}(0)$.

Case $k=2$: For $u\in\mathrm{Res}_{2,A}(0)$, we may write $u=s\omega$ for some distributional section $s\in\mathcal{D}'_{E_u^*}(M;\mathcal{E})$. Then $\iota_Xd_Au=0$ implies $\iota_Xd_As=0$, as $\mathcal{L}_X\Omega=d\omega=0$. By the analysis of $\mathrm{Res}_{0,A}(0)$, we immediately get that s is parallel.

For semisimplicity, assume $\iota_Xd_Au=v\in\mathrm{Res}_{2,A}(0)$ with $u\in\mathcal{D}'_{E_u^*}(M;\Omega^2_0\otimes\mathcal{E})$. So $u=s\omega$ for some $s\in\mathcal{D}'_{E_u^*}(M;\mathcal{E})$ and $v=s'\omega$ with s' smooth and parallel. Therefore $s'=\iota_X\,d_As\in\mathrm{Res}_{0,A}(0)$ and by semisimplicity in the $k=0$ case, we obtain $s'=0$. □

Remark 4.5. In the proof of Lemma 4.4, the fact that $J(0)=1$ in the case $k=0$ also holds for A nonflat and unitary. To see this, consider the spectral theoretic inequality, which holds for $\varphi\in C^\infty(M;\mathcal{E})$,

$$\|(P-\lambda)\varphi\|_{L^2}\cdot\|\varphi\|_{L^2}\ge|\operatorname{Im}\langle(P-\lambda)\varphi,\varphi\rangle_{L^2}|=|\operatorname{Im}\lambda|\|\varphi\|^2_{L^2}.\tag{4-7}$$

[4]This can be shown as follows. Fix $x\in M$ and take two parallel sections u_1 and u_2 of $\mathcal{E}$ along the orbit $\{\varphi_tx:t\in\mathbb{R}\}$, solving locally in some trivialisation $(\partial_t+A(\partial_t)+i\Phi)u_j=0$ for $j=1,2$. Then $\partial_t\langle u_1,u_2\rangle_{\mathcal{E}(\varphi_tx)}=\langle(\partial_t+A(\partial_t))u_1,u_2\rangle+\langle u_1,(\partial_t+A(\partial_t))u_2\rangle=-i\langle\Phi u_1,u_2\rangle+i\langle u_1,\Phi u_2\rangle=0$, as d_A is unitary and Φ is Hermitian. Therefore the parallel transport preserves inner products and $\alpha_{x,t}$ is unitary.

Here we used that $P = P^*$ on L^2. Therefore $\|R(\lambda)\|_{L^2\to L^2} \le 1/|\operatorname{Im}\lambda|$ for $\operatorname{Im}\lambda > 0$, which implies $J(0) = 1$.

4C. $\mathrm{Res}_{1,A}(0)$. Recall that $H^0_A(M;\mathcal{E})$ is the space of parallel sections (i.e., smooth sections s of $\mathcal{E}$ such that $d_A s = 0$). We start with a solvability result along the lines of [Dyatlov and Zworski 2017, Proposition 3.3.].

Proposition 4.6. *Assume X preserves a smooth volume form Ω and A is unitary and flat. Let $f \in C^\infty(M;\mathcal{E})$ and assume $\int_M \langle f, s\rangle_{\mathcal{E}}\Omega = 0$ for all $s \in C^\infty(M;\mathcal{E})$ parallel. Then there exists $u \in \mathcal{D}'_{E_u^*}(M;\mathcal{E})$ such that $\iota_X d_A u = f$.*

Proof. Let us set $P = -i\iota_X d_A$. By Lemma 4.4 we have the 0-semisimplicity and so $J(0) = 1$. Thus by (2-4) near zero, where $\Pi = \Pi_0$,

$$R(\lambda) = R_H(\lambda) - \frac{\Pi}{\lambda}.$$

Therefore, by applying $P - \lambda$ to this equation we obtain close to zero

$$(P-\lambda)R_H(\lambda) + \Pi_0 = \mathrm{Id}. \tag{4-8}$$

We introduce $u := -iR_H(0)f$, which lies in $\mathcal{D}'_{E_u^*}(M;\mathcal{E})$ by the mapping properties of $R_H(\lambda)$ in (2-4). Then, assuming $\Pi_0 f = 0$ we have by (4-8), evaluated at $\lambda = 0$,

$$f = f - \Pi_0 f = PR_H(0)f = (iP)(-iR_H(0)f) = \iota_X d_A u.$$

Now we prove that $\Pi_0 f = 0$. By Lemmas 2.1 and 4.4, we get

$$\operatorname{ran}(\Pi_0) = \ker(P|_{\mathcal{D}'_{E_u^*}(M;\mathcal{E})}) = \mathrm{Res}_{0,A}(0) = H^0_A(M;\mathcal{E}).$$

Since X is volume-preserving and A is unitary, we have $P^* = P$. Therefore $\operatorname{ran}\Pi'_0 = H^0_A(M;\mathcal{E})$ analogously, where Π'_0 denotes the spectral projector of $-P$ with respect to the flow $-X$. Now Lemma 2.3 gives $\Pi_0^* = \Pi'_0$ and so for any $g \in C^\infty(M;\mathcal{E})$

$$\langle \Pi_0 f, g\rangle_{L^2} = \langle f, \Pi_0^* g\rangle_{L^2} = 0.$$

Thus $\Pi_0 f = 0$, which concludes the proof. □

We proceed with:

Lemma 4.7. *There is a linear map $T : \mathrm{Res}_{1,A}(0) \to H^0_A(M;\mathcal{E})$ such that $d_A u = T(u)\omega$, where $u \in \mathrm{Res}_{1,A}(0)$. The map T satisfies the following*:

(1) *If $[\omega] \neq 0$ or $\mathcal{H}(X) \neq 0$, then T is trivial.*

(2) *If $\mathcal{H}(X) = 0$, then T is surjective.*

Proof. Let $u \in \mathrm{Res}_{1,A}(0)$. Since A is flat, $d_A^2 = 0$ and hence $d_A u \in \mathrm{Res}_{2,A}(0)$ and so $d_A u = s\omega$ with s parallel and smooth, by Lemma 4.4. If we set $T(u) = s$, this defines a linear map such that $d_A u = T(u)\omega$.

Next note that given parallel sections $p, q \in H^0_A(M; \mathcal{E})$, the inner product $\langle q, p\rangle_{\mathcal{E}}$ is a constant function on M. By Lemma 2.6 there is a smooth v such that $d_A u = d_A v$. We write

$$d\langle T(u), v\rangle_{\mathcal{E}} = \langle T(u), d_A v\rangle_{\mathcal{E}} = \|T(u)\|^2 \omega$$

and observe that the left-hand side is exact. Hence we must have $T \equiv 0$ if $[\omega] \neq 0$.

If $[\omega] = 0$, we set $\omega = d\tau$ and thus

$$d_A(u - T(u)\tau) = 0.$$

Using Lemma 2.6, we can write $u - T(u)\tau = \eta + d_A F$, where η is a smooth 1-form with $d_A \eta = 0$ and $F \in \mathcal{D}'_{E_u^*}(M; \mathcal{E})$. Contracting with X and taking (pointwise) the inner product with $T(u)$ we derive

$$-\|T(u)\|^2 \tau(X) = \varphi(X) + X\langle T(u), F\rangle_{\mathcal{E}}, \tag{4-9}$$

where φ is the smooth, closed 1-form $\varphi := \langle T(u), \eta\rangle$. But note that

$$\int_M \varphi(X)\Omega = \int_M \varphi \wedge d\tau = -\int_M d(\varphi \wedge \tau) = 0.$$

Hence integrating (4-9) yields

$$-\|T(u)\|^2 \mathcal{H}(X) = 0$$

and therefore $T \equiv 0$ if $\mathcal{H}(X) \neq 0$, thus showing item (1) in the lemma.

To show item (2) assume $\mathcal{H}(X) = 0$ and let s be a parallel section. We shall show that there is $u \in \mathrm{Res}_{1,A}(0)$ with $T(u) = s$. Note that for any parallel section p

$$\int_M \langle s\tau(X), p\rangle_{\mathcal{E}}\, \Omega = \langle s, p\rangle_{\mathcal{E}}\, \mathcal{H}(X) = 0.$$

By Proposition 4.6 there is an $F \in \mathcal{D}'_{E_u^*}(M; \mathcal{E})$ such that $\iota_X d_A F = s\tau(X)$ and hence $u := s\tau - d_A F \in \mathrm{Res}_{1,A}(0)$ and $T(u) = s$ as desired. ☐

Lemma 4.8. *There is an injection*

$$\ker T \hookrightarrow H^1_A(M; \mathcal{E}). \tag{4-10}$$

The injection can be described as follows: Let $u \in \ker T$. Then there exists $F \in \mathcal{D}'_{E_u^*}(M; \mathcal{E})$ such that

$$u - d_A F \in C^\infty(M; \mathcal{E} \otimes \Omega^1) \tag{4-11}$$

and also $d_A(u - d_A F) = 0$. The injection map is given by

$$S : u \in \ker T \mapsto [u - d_A F] \in H^1_A(M; \mathcal{E}). \tag{4-12}$$

An element $[\eta] \in H^1_A(M; \mathcal{E})$ is in the image of S if and only if

$$\int_M \langle p, \eta(X)\rangle_{\mathcal{E}}\, \Omega = 0$$

for any parallel section p.

Proof. Let $u \in \ker T$, so that $d_A u = 0$. By Lemma 2.6 there is $F \in \mathcal{D}'_{E_u^*}(M;\mathcal{E})$ such that $u - d_A F \in C^\infty(M;\Omega^1 \otimes \mathcal{E})$. We claim that the class $[u - d_A F] \in H^1_A(M;\mathcal{E})$ is independent of our choice of F. Suppose there is a G such that $u - d_A G$ is smooth and d_A-closed. Then $d_A(F-G) \in C^\infty(M;\Omega^1 \otimes \mathcal{E})$, so by Lemma 2.6 (or ellipticity), $F - G$ is smooth and thus $u - d_A F$ and $u - d_A G$ belong to the same class.

For injectivity, we assume that $u - d_A F$ is exact; so without loss of generality assume $u = d_A F$. Then $\iota_X u = 0$ implies $d_A F(X) = 0$, so by Lemma 4.4 we have F smooth and parallel, so $u = 0$.

If $[\eta]$ is in the image of S, then $\eta = u - d_A F$ for some $F \in \mathcal{D}'_{E_u^*}(M;\mathcal{E})$. Contracting with X, we see that $\eta(X) = -d_A F(X)$ and hence $\langle p, \eta(X)\rangle_{\mathcal{E}} = -X\langle p, F\rangle_{\mathcal{E}}$. Integrating gives

$$\int_M \langle p, \eta(X)\rangle_{\mathcal{E}}\, \Omega = 0.$$

Conversely, if the last integral is zero for all p, Proposition 4.6 gives $F \in \mathcal{D}'_{E_u^*}(M;\mathcal{E})$ such that $-\eta(X) = d_A F(X)$ and $u := \eta + d_A F \in \ker T$ and $Su = [\eta]$. □

And finally we can compute the rank of S in terms of whether X is null-homologous or not.

Lemma 4.9. *We have*:

(1) $\dim S(\ker T) = b_1(M,\mathcal{E})$ *if* $[\omega] = 0$.

(2) $\dim S(\ker T) = b_1(M,\mathcal{E}) - b_0(M,\mathcal{E})$ *if* $[\omega] \neq 0$.

Proof. If X is null-homologous, we write $\omega = d\tau$. We use Lemma 4.8 to show that S is surjective. Consider $\eta \in H^1_A(M;\mathcal{E})$ and $p \in H^0_A(M;\mathcal{E})$. Since the 1-form $\varphi := \langle p, \eta\rangle$ is closed we have

$$\int_M \varphi(X)\,\Omega = \int_M \varphi \wedge d\tau = -\int_M d(\varphi \wedge \tau) = 0$$

and item (1) follows.

Suppose now $[\omega] \neq 0$. We define a map $W : H^1_A(M,\mathcal{E}) \to (H^0_A(M,\mathcal{E}))^*$ by

$$W([\eta])(p) := \int_M \langle p, \eta(X)\rangle_{\mathcal{E}}\, \Omega.$$

By Lemma 4.8 the image of S coincides with the kernel of W. Thus, to prove item (2) it suffices to show that W is surjective. By Poincaré duality there is a closed 1-form φ such that

$$\int_M \varphi \wedge \omega \neq 0.$$

If p and q are parallel sections we compute

$$W([q\varphi])(p) = \langle p, q\rangle_{\mathcal{E}} \int_M \varphi(X)\,\Omega = \langle p, q\rangle_{\mathcal{E}} \int_M \varphi \wedge \omega$$

and hence W is onto. □

We are now in shape to put the ingredients together and prove:

Proof of Theorem 4.1. The theorem follows directly after applying Lemmas 4.7 and 4.9. □

Putting together the material from this section and Section 3 we obtain:

Proof of Corollary 1.8. The order of vanishing of $\zeta(s)$ is equal to $m_1(0)-m_0(0)-m_2(0)$ by Corollary 3.3. By Theorem 4.1 we have that $m_0(0)=m_2(0)=b_0(M,\mathcal{E})$ and $m_1(0)\geq \dim \mathrm{Res}_{1,A}(0)$, which concludes the proof. □

Moreover, we obtain:

Proof of Corollary 1.6. This is a direct consequence of Corollary 1.8 applied to the case $\mathcal{E}=M\times\mathbb{C}$ and the trivial connection $d_A=d$. □

5. Examples

In this section we consider a few noncontact examples of Anosov flows on the unit tangent bundle of a surface. They illustrate the various cases in Theorem 1.2 and give specific deformations for Theorem 1.5.

5A. ***Structural equations.*** As a general reference for structural equations, see [Singer and Thorpe 1967, Chapter 7]. For this section assume (Σ, g) is a compact oriented negatively curved surface. Let X be the geodesic vector field on the unit sphere bundle $S\Sigma$. Denote by $\pi : S\Sigma\to\Sigma$ the footpoint projection. Then, there are 1-forms α, β and ψ on $S\Sigma$ defined by, for $\xi\in T^*_{(x,v)}S\Sigma$,

$$\begin{aligned}\alpha_{(x,v)}(\xi)&=\langle v, d\pi(\xi)\rangle_x,\\ \beta_{(x,v)}(\xi)&=\langle d\pi(\xi), iv\rangle_x,\\ \psi_{(x,v)}(\xi)&=\langle\mathcal{K}(\xi), iv\rangle_x.\end{aligned}\tag{5-1}$$

The 1-form α is called the contact form. From the defining equation one obtains $\iota_X\alpha=0$ and $\iota_X\,d\alpha=0$, and $\Omega=-\alpha\wedge d\alpha$ is a volume form. Also, here $\mathcal{K}:TT\Sigma\to T\Sigma$ is the *connection map*, i.e., the projection along the horizontal subbundle, and ψ is called the *connection* 1*-form*. The expression iv denotes the vector v rotated by an angle of $\frac{\pi}{2}$ (we fix an orientation). Explicitly,

$$\mathcal{K}_{(x,v)}(\xi):=\frac{DZ}{dt}(0)\in T_x\Sigma,\tag{5-2}$$

where $(\gamma(t), Z(t))$ is an arbitrary local curve in $T\Sigma$ with the initial data $(\gamma(0), Z(0))=(x,v)$ and $(\dot\gamma(0),\dot Z(0))=\xi$; $\frac{D}{dt}$ denotes the Levi-Civita derivative along the curve. One can then show that $\{\alpha,\beta,\psi\}$ form a coframe on $S\Sigma$ such that the following *structural equations* (see [Singer and Thorpe 1967, p. 188]) hold:

$$\begin{aligned}d\alpha&=\psi\wedge\beta,\\ d\beta&=-\psi\wedge\alpha,\\ d\psi&=-K\alpha\wedge\beta.\end{aligned}\tag{5-3}$$

From this, we deduce the following properties

$$\iota_X\beta=\iota_X\psi=0,\quad \iota_X\,d\beta=\psi,\quad \iota_X\,d\psi=-K\beta.\tag{5-4}$$

Furthermore, there is a natural choice of metric on $S\Sigma$, called the *Sasaki metric*. It is defined by the splitting

$$T_{(x,v)}S\Sigma=\mathbb{H}(x,v)\oplus\mathbb{V}(x,v)=\ker(\mathcal{K}(x,v)|_{S\Sigma})\oplus\ker(d\pi(x,v))$$

into *horizontal* and *vertical* subspaces, respectively. Then the new metric is defined as

$$\langle\langle \xi, \eta \rangle\rangle := \langle \mathcal{K}(\xi), \mathcal{K}(\eta) \rangle + \langle d\pi(\xi), d\pi(\eta) \rangle. \tag{5-5}$$

It follows after some checking from relations (5-3) and the definitions that $\{\alpha, \beta, \psi\}$ is an orthonormal coframe for $T^*S\Sigma$ with respect to the Sasaki metric. This also yields an orthonormal dual frame $\{X, H, V\}$. We record the structural equations (5-3) for these vector fields:

$$\begin{aligned} [H, V] &= X, \\ [V, X] &= H, \\ [X, H] &= KV. \end{aligned} \tag{5-6}$$

Here V is the generator of rotations in the vertical fibres.

We now use the Hodge star operator $*$ with respect to the Sasaki metric on $S\Sigma$ to write $\mathcal{L}_X^* = - * \mathcal{L}_X *$ on 1-forms. We also have an extra structure given by

$$\alpha \wedge Ju = *u \tag{5-7}$$

for u a section of Ω_0^1. Here $J : \Omega_0^1 \to \Omega_0^1$ is the (dual) almost-complex structure associated to the symplectic form $d\alpha$ on $\ker \alpha = \operatorname{span}\{V, H\}$ and is given by

$$J(u_2\beta + u_3\psi) = u_3\beta - u_2\psi, \quad J^2 = -\mathrm{Id}.$$

Therefore $(\mathcal{L}_X^*)^k u = 0$ for some $k \in \mathbb{N}$ is equivalent to $\mathcal{L}_X^k Ju = 0$ and we obtain

$$\operatorname{Res}_{-i\mathcal{L}_X^*, \Omega_0^1}(0) = J^{-1} \operatorname{Res}_{i\mathcal{L}_X, \Omega_0^1}(0). \tag{5-8}$$

In the next section we use this relation together with time changes to derive an explicit expression for coresonant states at zero.

5B. ***Time-reversal and resonant spaces.*** Here we consider the action under pullback of the time-reversal map $R : S\Sigma \to S\Sigma$, given by $R(x, v) = (x, -v)$. We first collect the information on this action on the orthonormal frames and coframes given in (5-3) and (5-6).

Proposition 5.1. *We have* $R^*\alpha = -\alpha$, $R^*\beta = -\beta$ *and* $R^*\psi = \psi$. *Similarly, we have* $R^*X = -X$, $R^*H = -H$ *and* $R^*V = V$.

Proof. We consider the coframe case first. Simply observe that

$$R^*\alpha_{(x,v)}(\xi) = \langle -v, d\pi\, dR\xi \rangle_x = -\alpha_{(x,v)}(\xi)$$

so $R^*\alpha = -\alpha$. Similarly

$$R^*\beta_{(x,v)}(\xi) = \langle -iv, d\pi\, dR\xi \rangle_x = -\beta_{(x,v)}(\xi)$$

so $R^*\beta = -\beta$. Finally, recall that $\mathcal{K}(\xi) = \frac{DZ}{dt}(0)$, where $c(t) = (\gamma(t), Z(t))$ is any curve in $T\Sigma$ with $\dot{c}(0) = \xi$. Therefore

$$\mathcal{K}(dR\xi) = -\frac{DZ}{dt}(0) = -\mathcal{K}(\xi)$$

since $\tilde{c}(t) = (\gamma(t), -Z(t))$ is the curve adapted to $-dR\xi$. Now we easily see that $R^*\psi = \psi$ from the definition.

The frame case follows from the coframe case, since contractions commute with pullbacks. ☐

Now note that in any unit sphere bundle SN over an Anosov manifold (N, g_1), the pullback by R swaps the stable and unstable bundles. More precisely, we have

$$R^* E^X_{u,s} = E^{R^*X}_{u,s} = E^{-X}_{u,s} = E_{s,u}, \quad R^* E_0 = E_0.$$

The upper index denotes the vector field with respect to which we are taking the stable/unstable bundles. This follows from the fact that R intertwines the flows of X and $-X$. Thus we also have

$$R^* E^*_{u,s} = E^*_{s,u}, \quad R^* E^*_0 = E^*_0.$$

The upshot is of course that R^* is an isomorphism between resonant and coresonant spaces, i.e., the ones with the wavefront set in E^*_u and in E^*_s.

Proposition 5.2. *The pairing* (2-9) *between resonant and coresonant states is equivalent to the pairing on*

$$\operatorname{Res}_{-i\mathcal{L}_X, \Omega^1_0}(0) \times \operatorname{Res}_{-i\mathcal{L}_X, \Omega^1_0}(0), \quad (u, v) := \int_{S\Sigma} u \wedge \alpha \wedge R^* \bar{v}. \tag{5-9}$$

The pairing (5-9) *is Hermitian* (*i.e.*, *conjugate symmetric*).

Proof. We first claim that

$$\operatorname{Res}_{-i\mathcal{L}^*_X, \Omega^1_0}(0) = J^{-1} R^* \operatorname{Res}_{-i\mathcal{L}_X, \Omega^1_0}(0). \tag{5-10}$$

This is obtained from (5-8) and by observing that $v \in \operatorname{Res}_{i\mathcal{L}_X, \Omega^1_0}(0)$ if and only if $R^* v \in \operatorname{Res}_{-i\mathcal{L}_X, \Omega^1_0}(0)$, since R^* commutes with ι_X and d, and as R^* swaps E^*_u and E^*_s by the discussion above. Thus by another application of (5-7), we obtain (5-9). For the symmetry part, observe that R is orientation-preserving and

$$(u, v) = \int_{SM} u \wedge \alpha \wedge R^* \bar{v} = -\int_{SM} R^* u \wedge \alpha \wedge \bar{v} = \overline{(v, u)}.$$ ☐

5C. ***Magnetic flows.*** These flows are determined by a smooth function $\lambda \in C^\infty(\Sigma)$. The relevant vector field is $X_\lambda := X + \lambda V$. A calculation using the structure equations shows

$$\iota_{X_\lambda} \Omega = -d\alpha + \lambda \alpha \wedge \beta = -d\alpha + \lambda \pi^* \sigma,$$

where σ is the area form of g. If Σ has negative Euler characteristic, then $K\sigma$ generates $H^2(\Sigma)$ and thus there is a constant c and a 1-form γ such that

$$\lambda \sigma = cK\sigma + d\gamma.$$

Therefore

$$\iota_{X_\lambda} \Omega = -d\alpha + \lambda \pi^* \sigma = d(-\alpha - c\psi + \pi^* \gamma),$$

and hence $X_\lambda \in \mathcal{X}^0_\Omega$. If X is Anosov and λ is small, X_λ remains Anosov. In general these flows are *not* contact; see [Dairbekov and Paternain 2005].

5D. ***Explicit flows with*** $[\omega] \neq 0$. In this subsection, we construct explicit volume-preserving non-null-homologous Anosov flows that are close to the geodesic flow on a compact oriented negatively curved surface (Σ, g). Let $\theta \neq 0$ be a *harmonic* 1-form on Σ. At the level of $S\Sigma$ this can be seen in terms of two equations

$$\begin{aligned} X(\theta) + HV(\theta) &= 0, \\ H(\theta) - XV(\theta) &= 0. \end{aligned} \tag{5-11}$$

This first is zero divergence, the second is $d\theta = 0$. To check these equations one can argue as follows. We will use that $d\pi_{(x,v)}(X(x,v)) = v$ and $d\pi_{(x,v)}(H(x,v)) = iv$. Given θ, we consider $\pi^*\theta$ and note (using the standard formula for d applied to $\pi^*\theta$)

$$d(\pi^*\theta)(X, H) = X\pi^*\theta(H) - H(\pi^*\theta(X)) - \pi^*\theta([X, H]).$$

By the structural equations, the term $[X, H]$ is purely vertical; hence it is killed by $\pi^*\theta$. Now one can check that $\pi^*\theta(H)(x, v) = \theta(iv) = V(\theta) = -(*\theta)(v)$ and $\pi^*\theta(X) = \theta(v)$. Finally since

$$d(\pi^*\theta)(X, H) = \pi^* d\theta(X, H) = d\theta(d\pi(X), d\pi(H)) = d\theta(v, iv),$$

one obtains that $d\theta = 0$ if and only if $H(\theta) - XV(\theta) = 0$. The form θ has zero divergence if and only if $*\theta$ is closed so the first equation also follows.

We consider the vector field $Y := \theta X + V(\theta)H$. This vector field is dual to the 1-form on $S\Sigma$ given by $\pi^*\theta = \theta\alpha + V(\theta)\beta$. This form is closed as well as $\varphi := -V(\theta)\alpha + \theta\beta$ which is the pullback $\pi^*(*\theta)$. We can easily check that $\varphi(Y) = 0$ and $\pi^*\theta(Y) = [\theta]^2 + [V(\theta)]^2$.

The flows we wish to consider are of the form $X_\varepsilon = X + \varepsilon Y$, where X is the Anosov geodesic vector field and ε is small so that it remains Anosov. Using the above we observe:

- X_ε preserves the volume form $\Omega = \alpha \wedge \beta \wedge \psi$. This is thanks to the fact that θ has zero divergence.
- $[\iota_{X_\varepsilon}\Omega] \neq 0$ for $\varepsilon \neq 0$. This is because $\pi^*\theta(Y) = [\theta]^2 + [V(\theta)]^2 \geq 0$, and hence if θ is not trivial,

$$\int_{S\Sigma} \pi^*\theta(X_\varepsilon)\,\Omega = \varepsilon \int_{S\Sigma} \pi^*\theta(Y)\,\Omega \neq 0. \tag{5-12}$$

What we will prove in the coming sections is that X_ε has a splitting resonance for 1-forms near zero, and the semisimplicity does not break down.

6. Perturbations

In this section we study the behaviour of the Pollicott–Ruelle multiplicities under small deformations and start with the proof of Theorem 1.4.

6A. ***Uniform anisotropic Sobolev spaces.*** We start by laying out the necessary tools to study perturbations of Anosov flows and associated anisotropic Sobolev spaces. We will follow the recent approach of [Guedes Bonthonneau 2020], where a uniform weight function that works in a neighbourhood of the initial vector field is constructed. For brevity, we will only outline the necessary details. We refer the reader to [Faure and Sjöstrand 2011] for more details in the case of a fixed vector field, and to [Dang et al. 2020] for an alternative construction of a weight function that works for perturbed vector fields. The use of anisotropic spaces in hyperbolic dynamics has its origins in the works of many authors; see [Baladi 2005; Baladi and Tsujii 2007; Blank et al. 2002; Butterley and Liverani 2007; Liverani 2004; Gouëzel and Liverani 2006].

Let M be compact and X_0 an Anosov vector field. By [Guedes Bonthonneau 2020, Section 2], there exists a 0-homogeneous weight function $m \in C^\infty(T^*M \setminus 0)$ that applies to all flows with generators $\|X - X_0\|_{C^1} < \eta$, for some $\eta > 0$, in a sense to be explained. It satisfies, for all such X,

$$m = 1 \quad \text{near } E_u^*, \qquad m = -1 \quad \text{near } E_s^*, \qquad X_* m \leq 0.$$

Here X_* is the symplectic lift of X to T^*M. We set $G(x,\xi) \sim m(x,\xi)\log(1+|\xi|)$ for all $|\xi|$ large. The anisotropic Sobolev spaces are defined as, for $r \in \mathbb{R}$,

$$\mathcal{H}_{h,rG} = \mathrm{Op}_h(e^{-rG})L^2(M). \tag{6-1}$$

Here $h > 0$ and Op_h denotes a semiclassical quantisation on M; we write $\mathrm{Op} := \mathrm{Op}_1$. We will write $\mathcal{H}_{rG} = \mathrm{Op}(e^{-rG})L^2(M)$. Frequently we consider a smooth vector bundle $\mathcal{E}$ over M and in that case we consider the corresponding spaces $\mathcal{H}_{h,rG} = \mathrm{Op}_h(e^{-rG\times \mathrm{Id}_{\mathcal{E}}})L^2(M;\mathcal{E})$. We will write

$$\mathcal{H}_{h,rG+k\log\langle\xi\rangle} = \mathrm{Op}_h(e^{-rG})H^k(M;\mathcal{E}).$$

We will use the special notation $\mathcal{H}_{rG,k} := \mathcal{H}_{1,rG+k\log\langle\xi\rangle} = \mathrm{Op}(e^{-rG})H^k(M;\mathcal{E})$. We remark that the spaces $\mathcal{H}_{h,rG}$ for varying h are all the same as sets, equipped with a family of distinct, but equivalent norms.

Let X_ε be a smooth family of Anosov vector fields on M. Consider also a smooth family of differential operators P_ε with principal symbol $\sigma(X_\varepsilon) \times \mathrm{Id}_{\mathcal{E}}$. We will consider any $Q \in \Psi^{-\infty}(M;\mathcal{E})$ compactly microsupported, self-adjoint operator, elliptic in the neighbourhood of the zero section in T^*M. Introduce now the spaces

$$\mathcal{D}^\varepsilon_{h,rG} := \{u \in \mathcal{H}_{h,rG} : P_\varepsilon u \in \mathcal{H}_{h,rG}\}$$

and equip them with the norm $\|u\|^2_{\mathcal{D}^\varepsilon_{h,rG}} = \|u\|^2_{\mathcal{H}_{h,rG}} + \|hP_\varepsilon u\|^2_{\mathcal{H}_{h,rG}}$. Completely analogously with $\mathcal{H}_{rG}$, we introduce $\mathcal{D}^\varepsilon_{rG}$, and also $\mathcal{D}^\varepsilon_{rG,k}$ for an integer k.

Then [Guedes Bonthonneau 2020, Lemma 9] states:

Lemma 6.1. *There exists an $\varepsilon_0 > 0$ such that the following holds. Given any $s_0 > 0$, $k \in \mathbb{Z}$ and $r > r(s_0) + |k|$, there is $h_k > 0$ such that for $0 < h < h_k$, $\operatorname{Im} s > -s_0$, $|\operatorname{Re} s| < h^{-1/2}$ and $|\varepsilon| < \varepsilon_0$,*

$$P_\varepsilon - h^{-1}Q - s : \mathcal{D}^\varepsilon_{h,rG+k\log\langle\xi\rangle} \to \mathcal{H}_{h,rG+k\log\langle\xi\rangle}$$

is invertible and the inverse is bounded as $O(1)$ independently of ε.

Here $r(s)$ is a nonincreasing function of $\operatorname{Im} s$, so that $r(s) > r_{P_\varepsilon}(\operatorname{Im} s)$ for all $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$. Also, here $r_{P_\varepsilon}(s_0)$ represents a certain threshold (see [Guedes Bonthonneau 2020, p. 4]) depending on P_ε such that for r bigger than this quantity the resolvent $(P_\varepsilon - h^{-1}Q - s)^{-1} : \mathcal{H}_{h,rG} \to \mathcal{H}_{h,rG}$ is holomorphic and $(P_\varepsilon - s)^{-1} : \mathcal{H}_{rG} \to \mathcal{H}_{rG}$ admits a meromorphic extension to $\operatorname{Im} s > -s_0$ and $|\operatorname{Re} s| \leq h^{-1/2}$.

6B. ***Pollicott–Ruelle multiplicities are locally constant.*** In this section we prove, using the construction of anisotropic Sobolev spaces in the previous section, that in some fixed bounded region, the sums of multiplicities of resonances are locally constant. Observe that under the assumptions in Lemma 6.1, we have the factorisation property

$$(P_\varepsilon - s)(P_\varepsilon - h^{-1}Q - s)^{-1} = \mathrm{Id} + h^{-1}Q(P_\varepsilon - h^{-1}Q - s)^{-1}. \tag{6-2}$$

This holds for s in $\Omega_{h,s_0} := \{s : \operatorname{Im} s > -s_0,\ |\operatorname{Re} s| < h^{-1/2}\}$. We introduce the notation

$$D(\varepsilon, s) := h^{-1}Q(P_\varepsilon - h^{-1}Q - s)^{-1}.$$

Since Q is smoothing, we have that $D(\varepsilon, s)$ is of trace class, and, moreover, since for any $\varepsilon, \varepsilon'$

$$D(\varepsilon, s) - D(\varepsilon', s) = h^{-1}Q(P_{\varepsilon'} - h^{-1}Q - s)^{-1}(P_{\varepsilon'} - P_\varepsilon)(P_\varepsilon - h^{-1}Q - s)^{-1},$$

we have that $\varepsilon \mapsto D(\varepsilon, s)$ is continuous with values in holomorphic maps from Ω_{h,s_0+1} to $\mathcal{L}(\mathcal{H}_{rG}, \mathcal{H}_{rG})$. Here $\mathcal{L}(A, B)$ denotes the space of bounded operators from A to B, with the operator norm.

Then $P_\varepsilon - s : \mathcal{D}^\varepsilon_{rG} \to \mathcal{H}_{rG}$ are an analytic family of Fredholm operators for $\operatorname{Im} s > -s_0$. Consider now a resonance s_1 of $P = P_0$, and a simple closed curve γ around s_1 containing no resonances on itself or in its interior except s_1, such that $\gamma \subset \Omega_{h,s_0}$. The fact that $D(\varepsilon, s)$ is continuous allows us to say that for ε small, a neighbourhood of γ still contains no resonances of P_ε. Introduce the family of projectors

$$\Pi_\varepsilon := \frac{1}{2\pi i} \oint_\gamma (s - P_\varepsilon)^{-1}\, ds.$$

Our first aim is to prove:

Lemma 6.2. *The ranks of* Π_ε *are locally constant*; *i.e.*, *there is an* $\varepsilon_1 > 0$ *such that* rank Π_ε *is constant for* $\varepsilon \in (-\varepsilon_1, \varepsilon_1)$.

Proof. We first claim that, for ε small enough,

$$\frac{1}{2\pi i} \operatorname{tr} \oint_\gamma \partial_s(\mathrm{Id} + D(\varepsilon, s))^{-1}(\mathrm{Id} + D(\varepsilon, s))\, ds = -\operatorname{rank} \Pi_\varepsilon. \tag{6-3}$$

The left-hand side is well-defined by the generalised argument principle [Dyatlov and Zworski 2019, Theorem C.11], since the contour integral is a finite-rank operator. To prove the equality in (6-3), we apply the residue theorem for meromorphic families of operators. Use (6-2) to obtain the left-hand side of (6-3) is equal to

$$\begin{aligned}&\frac{1}{2\pi i} \operatorname{tr} \oint_\gamma \big((s - P_\varepsilon)^{-1} + (P_\varepsilon - h^{-1}Q - s)(P_\varepsilon - s)^{-2}\big)(P_\varepsilon - s)(P_\varepsilon - h^{-1}Q - s)^{-1}\, ds\\ &\quad= -\frac{1}{2\pi i} \operatorname{tr} \oint_\gamma (P_\varepsilon - h^{-1}Q - s)^{-1}\, ds + \frac{1}{2\pi i} \operatorname{tr} \oint_\gamma (P_\varepsilon - h^{-1}Q - s)(P_\varepsilon - s)^{-1}(P_\varepsilon - h^{-1}Q - s)^{-1}\, ds.\end{aligned}$$

The first integrand in the second line above vanishes, since $(P_\varepsilon - h^{-1}Q - s)^{-1}$ is holomorphic; the second one is equal to $-\operatorname{tr} \Pi_\varepsilon = -\operatorname{rank} \Pi_\varepsilon$, by the cyclicity of traces. This shows (6-3).

Now recall by Jacobi's formula that we have

$$\frac{1}{2\pi i}\operatorname{tr}\oint_\gamma \partial_s(\mathrm{Id}+D(\varepsilon,s))^{-1}(\mathrm{Id}+D(\varepsilon,s))\,ds = -\frac{1}{2\pi i}\oint_\gamma \operatorname{tr}((\mathrm{Id}+D(\varepsilon,s))^{-1}\partial_s D(\varepsilon,s))\,ds$$
$$= -\frac{1}{2\pi i}\oint_\gamma \frac{\partial_s \det(\mathrm{Id}+D(\varepsilon,s))}{\det(\mathrm{Id}+D(\varepsilon,s))}\,ds.$$

Here we used integration by parts, and that $\partial_s D(\varepsilon,s)$ is a smoothing operator to commute trace and integration. In particular, the continuity of $\varepsilon\mapsto D(\varepsilon,s)$ as above and so that of the Fredholm determinant $\varepsilon\mapsto\det(\mathrm{Id}+D(\varepsilon,s))$ and its derivative $\varepsilon\mapsto\partial_s\det(\mathrm{Id}+D(\varepsilon,s))$ imply that for ε small enough the integrand changes by a small margin, and since the integral is integer-valued, we obtain the claim.[5] □

Note that a priori projections Π_ε are continuous only as functions of ε with values in $\mathcal{L}(\mathcal{H}_{rG,1},\mathcal{H}_{rG})$ and $\mathcal{L}(\mathcal{H}_{rG},\mathcal{H}_{rG,-1})$ if the resolvents $(P_\varepsilon-s)^{-1}$ are. The maps $\Pi_\varepsilon:\operatorname{ran}\Pi_0\to\operatorname{ran}\Pi_\varepsilon$ are isomorphisms for small ε by Lemma 6.2. We will show $\varepsilon\mapsto\Pi_\varepsilon\in\mathcal{L}(\mathcal{H}_{rG},\mathcal{H}_{rG})$ is continuous; we follow the argument in [Chaubet and Dang 2019, Appendix A]. Pick a basis $\varphi^j\in\mathcal{H}_{rG,1}$, $j=1,\dots,k=\operatorname{rank}\Pi_0$, of $\operatorname{ran}\Pi_0$, and define $\varphi^j_\varepsilon:=\Pi_\varepsilon\varphi^j$; then $\varepsilon\mapsto\varphi^j_\varepsilon\in\mathcal{H}_{rG}$ is continuous. Define also $\tilde{\varphi}^j_\varepsilon=\Pi_0\Pi_\varepsilon\varphi^j$ and note $\varepsilon\mapsto\tilde{\varphi}^j_\varepsilon\in\mathcal{H}_{rG}$ is also continuous. Let ν^j_ε be the dual basis in $\operatorname{ran}\Pi_0$ of $\tilde{\varphi}^j_\varepsilon$; then $\varepsilon\mapsto\nu^j_\varepsilon\in(\operatorname{ran}\Pi_0)'$ is continuous. Here the prime denotes the dual. Finally, let $l^j_\varepsilon:=\nu^j_\varepsilon\circ\Pi_0\circ\Pi_\varepsilon$, continuous as a map $\varepsilon\mapsto l^j_\varepsilon\in\mathcal{H}'_{rG}$. Then we may write

$$\Pi_\varepsilon=\sum_{j=1}^k\varphi^j_\varepsilon\otimes l^j_\varepsilon.$$

By construction, this map is continuous $\mathcal{H}_{rG}\to\mathcal{H}_{rG}$ for $r>r(s_0)+1$.

One may further bootstrap this argument as in [Chaubet and Dang 2019] to reobtain [Guedes Bonthonneau 2020, Lemma 10]:

Lemma 6.3. *For $r>r(s_0)+k+1$ and ε small enough, $\varepsilon\mapsto\Pi_\varepsilon$ is a C^k family of bounded operators on $\mathcal{H}_{rG}$.*

We are now in good shape to prove some of the basic perturbation statements from the Introduction.

Proof of Theorem 1.4(1) *and* (2). If $X_0\in\mathcal{X}^0_\Omega$ has nonzero helicity, then for ε small enough, $\mathcal{H}(X_\varepsilon)\neq 0$ and we may assume by Lemma 6.2 that $m_{1,X_\varepsilon}(0)\le m_{1,X_0}(0)=b_1(M)$. Thus by Theorem 1.2, we have $\dim\operatorname{Res}_{-i\mathcal{L}_{X_\varepsilon},\Omega^1_0}(0)=b_1(M)=m_{1,X_\varepsilon}(0)$, so that X_ε is 1-semisimple, which proves (1). The proof of (2) is completely analogous to the proof above and we omit it. □

7. Proof of Theorem 1.5

In this section we discuss what happens with semisimplicity if we perturb an arbitrary contact Anosov flow. For this purpose, consider M, a closed orientable 3-manifold, and a contact Anosov flow X on M. This implies there is a contact 1-form α such that $\Omega=-\alpha\wedge d\alpha$ is a volume form, $\alpha(X)=1$ and $\iota_X\,d\alpha=0$.

[5] Alternatively, one may apply the generalised Rouché's theorem [Dyatlov and Zworski 2019, Theorem C.12] to conclude that the sums of *null multiplicities* (in the sense of Gohberg–Sigal theory; see [Dyatlov and Zworski 2019, Appendix C]) over the resonances in the interior of γ of operators $\mathrm{Id}+D(\varepsilon,s)$ for small enough ε are constant. By (6-3), we know that these sums of null multiplicities are equal to $\operatorname{rank}\Pi_\varepsilon$, which proves the claim.

We consider a frame $\{X_1, X_2\}$ of $\ker\alpha$ (such a frame exists since M is parallelizable) such that $d\alpha(X_1, X_2) = -1$. The dual coframe $\{\alpha, \alpha_1, \alpha_2\}$ to $\{X, X_1, X_2\}$ satisfies

$$d\alpha = \alpha_2 \wedge \alpha_1, \quad \Omega = -\alpha \wedge d\alpha = \alpha \wedge \alpha_1 \wedge \alpha_2.$$

Next, consider a Riemannian metric g on M making $\{X, X_1, X_2\}$ an orthonormal frame. Observe that $\Omega^1 = \mathbb{R}\alpha \oplus \Omega_0^1$ and for any $u = u_1\alpha_1 + u_2\alpha_2 \in \mathcal{D}'(M; \Omega_0^1)$, we have for the action of the Hodge star $*$ of g

$$*u = u_1\alpha_2 \wedge \alpha + u_2\alpha \wedge \alpha_1 = \alpha \wedge (u_2\alpha_1 - u_1\alpha_2). \tag{7-1}$$

We introduce the complex structure $J : \Omega_0^1 \to \Omega_0^1$ given by

$$Ju := u_2\alpha_1 - u_1\alpha_2,$$

so that $*u = \alpha \wedge Ju$. In particular, we have $\mathcal{L}_X^* u = - * \mathcal{L}_X * u = 0$ if and only if

$$\mathcal{L}_X Ju = 0. \tag{7-2}$$

Let $Y \in \mathcal{X}_\Omega$. Since Y preserves Ω we may consider the winding cycle map associated to Y:

$$W_Y : H^1(M) \to \mathbb{C}, \quad W_Y(\theta) := \int_M \theta(Y)\,\Omega.$$

Clearly Y is null-homologous if and only if $W_Y \equiv 0$. The next lemma characterises the property of Y being null-homologous in terms of a distinguished resonant state of X. Let Π denote the spectral projector at zero of $-i\mathcal{L}_X$ acting on Ω^1 (see (2-5)). Set

$$u := \Pi\mathcal{L}_Y\alpha \in \operatorname{Res}_{-i\mathcal{L}_X, \Omega^1}(0).$$

Lemma 7.1. *We have $\iota_X u = 0$. Let θ be a (real) smooth closed 1-form and let $\psi \in \mathcal{D}'_{E_s^*}(M)$ be such that $v := (J)^{-1}(\theta + d\psi) \in \operatorname{Res}_{-i\mathcal{L}_X^*, \Omega_0^1}(0)$. Then*

$$\langle u, v\rangle_{L^2} = -W_Y(\theta).$$

In particular, Y is null-homologous if and only if $u = 0$.

Proof. We may write for some $a, a_1, a_2 \in C^\infty(M)$

$$Y = aX + a_1X_1 + a_2X_2$$

and a calculation shows

$$\mathcal{L}_Y\alpha = (\iota_Y d + d\iota_Y)\alpha = a_1\iota_{X_1}\,d\alpha + a_2\iota_{X_2}\,d\alpha + da. \tag{7-3}$$

Therefore, we have

$$\iota_X u = \Pi\iota_X\mathcal{L}_Y\alpha = \Pi Xa = X\Pi a = 0. \tag{7-4}$$

In the previous equation we used that Πa is constant by Theorem 1.2 and that Π commutes with X. Next we compute, using that $*v = \alpha \wedge (\theta + d\psi)$,

$$\begin{aligned}\langle \mathcal{L}_Y \alpha, v\rangle_{L^2} &= \int_M (a_1 \iota_{X_1} d\alpha + a_2 \iota_{X_2}\, d\alpha + da) \wedge \alpha \wedge (\theta + d\psi) \\ &= -\int_M (a_1 \iota_{X_1} + a_2 \iota_{X_2})(\theta + d\psi)\, \Omega \\ &= -\int_M \iota_Y(\theta + d\psi)\, \Omega = -\int_M \iota_Y \theta\, \Omega = -W_Y(\theta). \end{aligned} \tag{7-5}$$

Here we used the graded commutation rule for contractions, integration by parts and the following facts: $\theta + d\psi$ is closed, $\iota_X(\theta + d\psi) = 0$ and Y is volume-preserving. By Lemma 2.3 it follows that $\Pi^* v = v$. By this and the computation in (7-5), it follows that

$$\langle u, v\rangle_{L^2} = \langle \Pi \mathcal{L}_Y \alpha, v\rangle_{L^2} = \langle \mathcal{L}_Y \alpha, v\rangle_{L^2} = -W_Y(\theta)$$

as desired. Clearly, the relation $\langle u, v\rangle = -W_Y(\theta)$ implies that if $u = 0$, then Y is null-homologous. If Y is null-homologous, then $\langle u, v\rangle = 0$ for all v. Since 1-semisimplicity holds for X, Lemma 2.4 implies $u = 0$ and the lemma is proved. □

The next lemma provides important information about the pairing between resonant and coresonant states in the contact case.

Lemma 7.2. *Let θ be a smooth closed 1-form on M. Let $\varphi \in \mathcal{D}'_{E_u^*}(M)$ and $\psi \in \mathcal{D}'_{E_s^*}(M)$ be such that*

$$\begin{aligned} u &= \theta + d\varphi \in \operatorname{Res}_{-i\mathcal{L}_X, \Omega_0^1}(0), \\ v &= (J)^{-1}(\theta + d\psi) \in \operatorname{Res}_{-i\mathcal{L}_X^*, \Omega_0^1}(0). \end{aligned} \tag{7-6}$$

Then

$$\operatorname{Re}\langle u, v\rangle_{L^2} = \operatorname{Re} \int_M (\theta + d\varphi) \wedge \alpha \wedge (\bar\theta + d\bar\psi) \le 0$$

with equality if and only if θ is exact, or in other words $u = v = 0$.

Proof. By (7-6) we have $\iota_X u = 0$ and $\iota_X v = 0$, so $X\varphi = X\psi = -\theta(X)$. We have the chain of equalities

$$\begin{aligned} \operatorname{Re}\langle u, v\rangle_{L^2} &= -\int_M \operatorname{Re}(\theta \wedge \bar\theta) \wedge \alpha - \operatorname{Re}\int_M \varphi\, d\alpha \wedge \bar\theta \\ &= \operatorname{Re}\int_M \varphi \bar\theta(X)\, \Omega = -\operatorname{Re}\langle \varphi, X\varphi\rangle_{L^2} = \operatorname{Im}\langle -iX\varphi, \varphi\rangle_{L^2}. \end{aligned} \tag{7-7}$$

Here we used $X\varphi = -\theta(X)$, $\operatorname{Re}(\theta \wedge \bar\theta) = 0$ and integration by parts.

Assume now $\operatorname{Re}\langle u, v\rangle_{L^2} \ge 0$. By the computation in (7-7), Lemma 2.5 implies $\varphi \in C^\infty(M)$, so $u \in C^\infty(M; \Omega_0^1)$ and Lemma 4.2 implies $u \equiv 0$ and θ exact, so also $v \equiv 0$. □

7A. ***Constructing the splitting resonance.*** Let $Y \in \mathcal{X}_\Omega$ such that Y is *not* null-homologous and consider a perturbation of X

$$X_\varepsilon = X + \varepsilon Y.$$

Consider a simple closed curve γ around zero, so that no resonances of $-i\mathcal{L}_{X_\varepsilon}$ on $\Omega^1(M)$ cross the curve γ for small enough values of the parameter ε. Consider the family of projectors given by

$$\Pi_\varepsilon := \Pi_{\mathcal{L}_{X_\varepsilon}} = \frac{1}{2\pi i}\oint_\gamma (\lambda + i\mathcal{L}_{X_\varepsilon})^{-1}\, d\lambda. \tag{7-8}$$

By Lemma 6.3, the Π_ε are C^k in ε in suitable topologies. More precisely, we have $\varepsilon \mapsto \Pi_\varepsilon \in \mathcal{L}(\mathcal{H}_{rG}, \mathcal{H}_{rG})$ is C^k for $r > r(0) + k + 1$ (i.e., r large enough).

We will construct the splitting resonant state "by hand". For that purpose, consider

$$t_\varepsilon = \mathcal{L}_{X_\varepsilon}\Pi_\varepsilon\alpha = \varepsilon\Pi_\varepsilon\mathcal{L}_Y\alpha.$$

Here we used that Π_ε commutes with ι_{X_ε} and d, which follows since the integral defining Π_ε does so. Our candidate for the splitting resonance is

$$u_\varepsilon := \Pi_\varepsilon\mathcal{L}_Y\alpha.$$

Firstly, we note that $\iota_{X_\varepsilon}u_\varepsilon = 0$, which follows from

$$\iota_{X_\varepsilon}t_\varepsilon = \mathcal{L}_{X_\varepsilon}\Pi_\varepsilon(1 + \varepsilon\alpha(Y)) = 0.$$

This is because

$$\Pi_\varepsilon f = \frac{1}{\mathrm{vol}(M)}\int_M f\,\Omega$$

is constant, which follows from Theorem 1.2. We also understand that Π_ε acts on forms of any degree, and is given by the expression (7-8). This implies directly that $\iota_{X_\varepsilon}u_\varepsilon = 0$ for $\varepsilon \neq 0$, and then by continuity we have $\iota_{X_\varepsilon}u_\varepsilon = 0$ for all ε.

Fix now $\varepsilon \neq 0$. Then either exactly one resonance "splits" by Lemma 6.2 and Theorem 1.2, so we must have $\mathcal{L}_{X_\varepsilon}t_\varepsilon = \mu_\varepsilon t_\varepsilon$ for some $\mu_\varepsilon \neq 0$ and thus $\mathcal{L}_{X_\varepsilon}u_\varepsilon = \mu_\varepsilon u_\varepsilon$, or a resonant state does not split, in which case $\mathcal{L}_{X_\varepsilon}t_\varepsilon = 0$ and so $\mathcal{L}_{X_\varepsilon}u_\varepsilon = 0$. Also, we clearly have $\mathcal{L}_X u_0 = 0$. Therefore, there exists a function λ_ε such that for each small enough ε

$$\mathcal{L}_{X_\varepsilon}u_\varepsilon = \lambda_\varepsilon u_\varepsilon. \tag{7-9}$$

Hence we may write

$$\lambda_\varepsilon = \frac{\langle \mathcal{L}_{X_\varepsilon}u_\varepsilon, u^*\rangle}{\langle u_\varepsilon, u^*\rangle},$$

where u^* is a coresonant 1-form at zero such that $\langle u_0, u^*\rangle \neq 0$. Such a 1-form exists by Lemma 2.4. Therefore, for ε small enough and by continuity the above expression makes sense, so we conclude that λ_ε is in C^2 for ε in an interval around zero. Note that $\lambda_0 = 0$ and that by Lemma 7.1, $u_0 \neq 0$ since Y is not null-homologous.

7B. ***Proving that $\lambda_\varepsilon \neq 0$.*** We dedicate this subsection to proving that $\lambda_\varepsilon \neq 0$ for $\varepsilon \neq 0$ and we achieve this by looking at the second-order derivatives of λ_ε in ε. Recall we have a C^2 family of resonant 1-forms $u_\varepsilon = \Pi_\varepsilon \mathcal{L}_Y \alpha$ corresponding to resonances $-i\lambda_\varepsilon$ for the flow $X + \varepsilon Y$ such that

$$\begin{aligned} \iota_{X+\varepsilon Y}\, du_\varepsilon &= \lambda_\varepsilon u_\varepsilon, \\ \iota_{X+\varepsilon Y} u_\varepsilon &= 0. \end{aligned} \tag{7-10}$$

We will denote u_0 by u and λ_0 by λ, and we apply the same principle to the derivatives of λ and u at zero. We want to linearise (7-10) by taking derivatives in ε.

First linearisation of (7-10): We take the first derivative of (7-10) to get

$$\begin{aligned} \iota_Y\, du_\varepsilon + \iota_{X+\varepsilon Y}\, d\dot{u}_\varepsilon &= \dot{\lambda}_\varepsilon u_\varepsilon + \lambda_\varepsilon \dot{u}_\varepsilon, \\ \iota_Y u_\varepsilon + \iota_{X+\varepsilon Y} \dot{u}_\varepsilon &= 0. \end{aligned} \tag{7-11}$$

Evaluating (7-11) at $\varepsilon = 0$, we get the system

$$\begin{aligned} \iota_Y\, du + \iota_X\, d\dot{u} &= \dot{\lambda} u, \\ \iota_Y u + \iota_X \dot{u} &= 0. \end{aligned} \tag{7-12}$$

This further simplifies, since u is a resonant state at zero, so by Lemma 4.7 we have $du = 0$. By (7-1) we may write $*u^* = \alpha \wedge w$, where $w = Ju^*$ and we have $\mathcal{L}_X w = 0$ and $\iota_X w = 0$. Much as before, since $w \in \mathcal{D}'_{E_s^*}(M; \Omega_0^1)$ we have $dw = 0$. Therefore, by taking the inner product with u^* in (7-12), we get

$$\begin{aligned} \dot{\lambda}\langle u, u^* \rangle = \langle \iota_X\, d\dot{u}, u^* \rangle &= \int_M \iota_X\, d\dot{u} \wedge \alpha \wedge w \\ &= -\int_M d\dot{u} \wedge w = -\int_M \dot{u} \wedge dw = 0. \end{aligned}$$

This implies $\dot{\lambda} = 0$.

Second linearisation of (7-10): By taking the ε derivative of (7-11) we get

$$\begin{aligned} 2\iota_Y\, d\dot{u}_\varepsilon + \iota_{X+\varepsilon Y}\, d\ddot{u}_\varepsilon &= \ddot{\lambda}_\varepsilon u_\varepsilon + 2\dot{\lambda}_\varepsilon \dot{u}_\varepsilon + \lambda_\varepsilon \ddot{u}_\varepsilon, \\ 2\iota_Y \dot{u}_\varepsilon + \iota_{X+\varepsilon Y} \ddot{u}_\varepsilon &= 0. \end{aligned} \tag{7-13}$$

We evaluate (7-13) at $\varepsilon = 0$ to get

$$\begin{aligned} 2\iota_Y\, d\dot{u} + \iota_X\, d\ddot{u} &= \ddot{\lambda} u, \\ 2\iota_Y \dot{u} + \iota_X \ddot{u} &= 0. \end{aligned} \tag{7-14}$$

Consider the same coresonant state u^* as above. Pairing (7-14) with u^* yields

$$\ddot{\lambda}\langle u, u^* \rangle = 2\int_M \iota_Y\, d\dot{u} \wedge \alpha \wedge w + \int_M \iota_X\, d\ddot{u} \wedge \alpha \wedge w. \tag{7-15}$$

Now the second integral above is equal to $-\int_M d\ddot{u} \wedge w = 0$, by integration by parts.

The first integral is a bit trickier and it is equal to

$$\begin{aligned}\int_M \iota_Y \, d\dot{u} \wedge \alpha \wedge w &= \int_M (a_1 \iota_{X_1} + a_2 \iota_{X_2}) \, d\dot{u} \wedge \alpha \wedge w \\ &= \int_M (a_1 \iota_{X_1} + a_2 \iota_{X_2}) w \, d\dot{u} \wedge \alpha = \int_M w(Y) \, d\dot{u} \wedge \alpha. \end{aligned} \tag{7-16}$$

Here we used that $\iota_X \, d\dot{u} = 0$ by the first linearisation analysis and $\iota_X w = 0$. Note that $\iota_X \, d\dot{u} = 0$ also implies that $d\dot{u} \wedge \alpha$ is X-invariant, so the integral $\int_M w(Y) \, d\dot{u} \wedge \alpha$ may be interpreted as "some winding cycle".

Observe that $\mathrm{WF}(d\dot{u}) \subset \mathrm{WF}(\dot{u}) \subset E_u^*$. This follows by differentiating Π_ε at zero to deduce

$$\dot{\Pi}_0 = \frac{1}{2\pi i} \oint_\gamma (\lambda + i\mathcal{L}_X)^{-1} (-i\mathcal{L}_Y)(\lambda + i\mathcal{L}_X)^{-1} \, d\lambda = i(R_H(0)\mathcal{L}_Y \Pi_0 + \Pi_0 \mathcal{L}_Y R_H(0)).$$

At this point, we recall that $(-i\mathcal{L}_X - \lambda)^{-1} = R_H(\lambda) - \Pi_0/\lambda$. Since Π_0 and $R_H(0)$ extend to maps $\mathcal{D}'_{E_u^*}(M; \Omega^1) \to \mathcal{D}'_{E_u^*}(M; \Omega^1)$, we have that $\dot{u} = \dot{\Pi}_0 \mathcal{L}_Y \alpha \in \mathcal{D}'_{E_u^*}(M; \Omega^1)$.

By Theorem 1.2 it follows that $d\dot{u} \wedge \alpha = c\Omega$ for some constant c. In fact, we have

$$\begin{aligned} c \operatorname{vol}(M) &= \int_M d\dot{u} \wedge \alpha = \int_M \dot{u} \wedge d\alpha = -\int_M \dot{u}(X) \, \Omega \\ &= \int_M u(Y) \, \Omega = W_Y(u). \end{aligned} \tag{7-17}$$

In these lines we used the second equation of (7-12) and $\iota_X u = 0$. Combining (7-17), (7-15) and (7-16) we have

$$\ddot{\lambda} \langle u, u^* \rangle = 2c \int_M w(Y) \, \Omega = 2c W_Y(w) = \frac{2 W_Y(u) W_Y(w)}{\operatorname{vol}(M)}. \tag{7-18}$$

Next we choose a special u^*. Namely, if we write $u = \theta + d\varphi$ for some (real) smooth closed 1-form θ and $\varphi \in \mathcal{D}'_{E_u^*}(M)$, then we choose $u^* = v$ as in Lemma 7.2. This ensures that $\langle u, u^* \rangle < 0$ and, moreover, by Lemma 7.1 we have

$$\langle u, u^* \rangle = -W_Y(\theta) < 0.$$

Hence (7-18) simplifies to

$$\ddot{\lambda} = \frac{-2 W_Y(\theta)}{\operatorname{vol}(M)} < 0.$$

By the symmetry of the Pollicott–Ruelle resonance spectrum, we have that λ_ε is real, since otherwise we would contradict Lemma 6.2. We conclude by Taylor's theorem

$$\lambda_\varepsilon = \varepsilon^2 \left(-\frac{W_Y(\theta)}{\operatorname{vol}(M)} + O(\varepsilon) \right).$$

In particular λ_ε is negative (so nonzero) for sufficiently small $\varepsilon \neq 0$. Therefore, the resonance $-i\lambda_\varepsilon$ of $-i\mathcal{L}_{X_\varepsilon}$ splits to the upper half-plane and 0 is a strict local maximum for λ_ε. This completes the proof of Theorem 1.5.

We conclude this section with:

Proof of the first part of Corollary 1.7. By Corollary 3.3, the order of vanishing of the Ruelle zeta function at zero is equal to $m_1(0) - m_0(0) - m_2(0)$. By Theorem 1.2, we know $m_2(0) = m_0(0) = 1$ and by Theorem 1.5 and Lemma 6.2 we have $m_1(0) = b_1(M) - 1$ for small enough nonzero ε. □

8. Time changes

In this section we consider the transformation $X \mapsto \widetilde{X} = fX$, where X is an Anosov vector field and $f > 0$ a positive smooth function and call such a transformation a *time change*. By [de la Llave et al. 1986, Lemma 2.1], we have that $\widetilde{X}$ is also Anosov and, moreover, its stable and unstable bundles $\widetilde{E}^s$ and $\widetilde{E}^u$ are given by

$$\widetilde{E}^s = \{Z + \theta(Z)X : Z \in E^s\}. \tag{8-1}$$

Here the continuous 1-form θ is given by solving $\mathcal{L}_X(f^{-1}\theta) = f^{-2}\,df$. Therefore, we notice that $\widetilde{E}_u^* = (\widetilde{E}^s \oplus \mathbb{R}\widetilde{X})^* = E_u^*$ and $\widetilde{E}_s^* = (\widetilde{E}^u \oplus \mathbb{R}\widetilde{X})^* = E_s^*$, where we used (8-1). This means that the resonant states associated to the flow fX lie in suitable spaces $\mathcal{D}'_{E_u^*}$, which will be very convenient.

We begin by recasting Lemma 2.4 to the case of 1-forms and consider a time change.

Proposition 8.1. *Let X be an Anosov flow on a manifold M and let $f > 0$ be a positive smooth function. Then $\mathcal{L}_{fX}$ acting on Ω_0^1 is semisimple at zero if and only if the pairing*

$$\operatorname{Res}^{(1)}_{-i\mathcal{L}_X,\Omega_0^1}(0) \times \operatorname{Res}^{(1)}_{-i\mathcal{L}_X^*,\Omega_0^1}(0) \to \mathbb{C},\ (u,v) \mapsto \left\langle \frac{u}{f}, v \right\rangle_{L^2(M;\Omega^1)} \tag{8-2}$$

is nondegenerate.

Proof. Let us determine the appropriate resonant spaces of $\mathcal{L}_{fX}$ and $\mathcal{L}_{fX}^*$ at zero. Note first that $\ker \mathcal{L}_{fX} = \ker \mathcal{L}_X$ on $\mathcal{D}'_{E_u^*}(M;\Omega_0^1)$, since time changes preserve the E_u^* set. Next, we compute $\mathcal{L}_{fX}^* = \mathcal{L}_X^*(f\,\cdot)$ on Ω_0^1, with respect to a fixed smooth inner product (e.g., given by a metric). Therefore, we have

$$\operatorname{Res}^{(1)}_{-i\mathcal{L}_{fX}^*,\Omega_0^1}(0) = \frac{1}{f}\operatorname{Res}^{(1)}_{-i\mathcal{L}_X^*,\Omega_0^1}(0).$$

Thus the nondegeneracy of the pairing between resonances and coresonances is equivalent to the nondegeneracy of (8-2) and applying Lemma 2.4 finishes the proof. □

8A. *Time changes of the geodesic flow on a hyperbolic surface.*

The aim of this subsection is to explicitly specify the equations for 1-forms in the kernel of $\mathcal{L}_X$ on the unit sphere bundle $M = S\Sigma$ of a closed hyperbolic surface Σ. We start by considering the case of general variable curvature and use the orthonormal frame $\{\alpha, \beta, \psi\}$ constructed in Section 5A.

Let $u \in \mathcal{D}'(M;\Omega_0^1)$. Then $u = b\beta + f\psi$ for some $b, f \in \mathcal{D}'(M)$ and we have

$$du = \alpha \wedge (X(b) - fK) + \beta \wedge \psi(H(f) - V(b)) + \alpha \wedge \psi(b + X(f)).$$

Therefore, $du = 0$ implies

$$\begin{aligned} X(b) &= Kf, \\ X(f) &= -b, \\ H(f) &= V(b). \end{aligned} \tag{8-3}$$

The first two equations come from $\iota_X\, du = 0$. The third is an additional one, which we know holds if $u \in \mathcal{D}'_{E_u^*}(M; \Omega_0^1)$ and $\iota_X\, du = 0$; it can be explained as an additional horocyclic invariance (see [Guillarmou and Faure 2018] and below).

Now we specialise to $K = -1$, i.e., the case of hyperbolic surfaces. Then in the $\{\beta, \psi\}$ coframe spanning Ω_0^1, the operator $\mathcal{L}_X$ may be written as

$$\mathcal{L}_X = X \times \mathrm{Id} + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and the first two equations in (8-3) then read

$$(X-1)(b-f) = 0,$$
$$(X+1)(b+f) = 0.$$

Thus $f = -b$ as there are no resonances with positive imaginary part, since X is volume-preserving.[6] The third equation in (8-3) now gives $U_- b = 0$, where $U_- = H + V$ is the horocyclic vector field spanning E_u. Now we may also write, where the adjoint is with respect to the Sasaki metric on $S\Sigma$,

$$\mathcal{L}_X^* = -X \times \mathrm{Id} + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Therefore $\mathcal{L}_X^* v = 0$, where $v = b'\beta + f'\psi$ for some $b', f' \in \mathcal{D}'_{E_s^*}(M)$, is the same as

$$(-X+1)(b'+f') = 0,$$
$$(-X-1)(b'-f') = 0.$$

Since we are looking at the vector field $-X$, no resonance with positive imaginary part gives $f' = -b'$ and so $(X+1)b' = 0$. The third equation in (8-3) then reads $U_+ b' = 0$, where $U_+ = H - V$ spans the E_s bundle.

Therefore, we have

$$\begin{aligned} \mathrm{Res}^{(1)}_{-i\mathcal{L}_X}(0) &= \{b(\beta - \psi) \in \mathcal{D}'(M) : (X-1)b = 0,\ (H+V)b = 0\}, \\ \mathrm{Res}^{(1)}_{-i\mathcal{L}_X^*}(0) &= \{b(\beta - \psi) \in \mathcal{D}'(M) : (X+1)b = 0,\ (H-V)b = 0\}. \end{aligned} \tag{8-4}$$

Note that we may drop the wavefront set conditions, since they follow from the equations being satisfied. We remark that since we know $-i\mathcal{L}_X$ at 0 is semisimple by [Dyatlov and Zworski 2017], then so is $-iX$ at $-i$ by the correspondence (8-4) and $\dim \mathrm{Res}_{-iX}(-i) = b_1(M)$. Alternatively, we may use [Guillarmou et al. 2018, Theorem 1] to deduce semisimplicity even at the special point $-i$ for hyperbolic surfaces.

Proposition 8.2. *Let $f \in C^\infty(M)$ and $f > 0$. Semisimplicity for $-i\mathcal{L}_{fX}$ at zero acting on Ω_0^1 is equivalent to the nondegeneracy of the pairing*

$$\mathrm{Res}^{(1)}_{-iX}(-i) \times \mathrm{Res}^{(1)}_{iX}(-i), \quad (b_1, b_2) \mapsto \left\langle \frac{b_1}{f}, b_2 \right\rangle_{L^2(M)}. \tag{8-5}$$

[6] This can be seen from (2-2), since $e^{-itP} = \varphi_{-t}^*$ is an isometric isomorphism on $L^2(M)$ and so the integral defining the resolvent converges for $\mathrm{Im}\,\lambda > 0$.

Proof. The proof is based on the correspondence (8-4) and Proposition 8.1. Then for $b_1(\beta-\psi)\in\mathrm{Res}^{(1)}_{-i\mathcal{L}_{fX}}(0)$ and $(b_2/f)(\beta-\psi)\in\mathrm{Res}^{(1)}_{-i\mathcal{L}^*_{fX}}(0)$, we have

$$\left\langle b_1(\beta-\psi),\, \frac{b_2}{f(\beta-\psi)}\right\rangle_{L^2(M;\Omega^1)} = 2\left\langle b_1,\, \frac{b_2}{f}\right\rangle_{L^2(M)}.$$

This proves that the pairing (8-5) is equivalent to the pairing (8-2), which finishes the proof. □

In the next sections, we would like to find out more about the pairing (8-5), similar to [Dyatlov et al. 2015; Guillarmou et al. 2018], where a pairing formula for generic resonances is proved.

Remark 8.3. Using the decomposition $u=a\alpha+b\beta+f\psi$, by (8-3) it may be seen that $(\mathcal{L}_X+s)u=0$ is equivalent to $(X+1+s)(b+f)=0$, $(X-1+s)(b-f)=0$ and $(X+s)a=0$. This enables us to determine the resonance spectrum of $\mathcal{L}_X$ on 1-forms from the resonance spectrum of X on functions, using the works of [Dyatlov et al. 2015; Guillarmou et al. 2018]. In particular, for $\mathrm{Re}\, s>-1$ we obtain $b+f=0$, which suffices to determine the spectrum on the left in Figure 1. The small and large eigenvalues in this figure are in the sense of [Ballmann et al. 2016].

8B. ***Reduction to distributions on the boundary.*** We follow the notation from [Dyatlov et al. 2015, Section 3]. We consider the hyperboloid model

$$\mathbb{H}^2=\{x=(x_0,x_1,x_2)=(x_0,x')\in\mathbb{R}^3:\langle x,x\rangle_{\mathcal{M}}=x_0^2-x_1^2-x_2^2=1,\ x_0>0\}$$

of hyperbolic geometry, equipped with the Riemannian metric $-\langle\cdot,\cdot\rangle_{\mathcal{M}}$, restricted to $T\mathbb{H}^2$. Here $\langle\cdot,\cdot\rangle_{\mathcal{M}}$ is called the Lorentzian metric. We also consider the action the isometry group $G=\mathrm{PSO}(1,2)$ of $\mathbb{H}^2$, consisting of matrices preserving the Lorentzian metric, orientation and the sign of x_0. This action extends to an action on the unit sphere bundle $S\mathbb{H}^2$, since G consists of isometries and in fact $G\ni\gamma\mapsto\gamma\cdot(1,0,0,0,1,0)\in S\mathbb{H}^2$ is a diffeomorphism. We also have explicitly

$$S\mathbb{H}^2=\{(x,\xi)\in\mathbb{H}^2:x,\xi\in\mathbb{R}^3,\ \langle\xi,\xi\rangle_{\mathcal{M}}=-1,\ \langle x,\xi\rangle_{\mathcal{M}}=0\}. \tag{8-6}$$

We will write φ_t for the geodesic flow on $S\mathbb{H}^2$ and X for the geodesic vector field. In the identification (8-6), we may write

$$X=\xi\cdot\partial_x+x\cdot\partial_\xi.$$

Therefore the geodesic flow on $S\mathbb{H}^2$ may be explicitly written as

$$\varphi_t(x,\xi)=(x\cosh t+\xi\sinh t,\, x\sinh t+\xi\cosh t). \tag{8-7}$$

We may compactify $\mathbb{H}^2$ to the closed unit ball $\bar{B}^2$ by embedding it with the map $\psi_0(x)=x'/(x_0+1)$ and we call S^1 bounding B^2 the *boundary at infinity*. Note that to a point $\nu\in S^1$ we may associate a ray $\{(s,s\nu):s>0\}$, which is asymptotic to the hyperboloid ray $\{(\sqrt{1+s^2},s\nu):s>0\}$. The action of G extends to an action on the boundary at infinity S^1 as follows. Let $\gamma\in G$ and $\nu\in S^1$. Then the matrix action on $\mathbb{R}^3$

$$\gamma\cdot(1,\nu)=N_\gamma(\nu)(1,L_\gamma(\nu)) \tag{8-8}$$

defines an action of $\gamma\in G$ on S^1 via L_γ. It also defines the multiplicative map $N_\gamma:S^1\to\mathbb{R}_+$.

Denote by $\pi : S\mathbb{H}^2 \to \mathbb{H}^2$ the footpoint projection. We will consider the mappings

$$B_\pm(x,\xi) : S\mathbb{H}^2 \to S^1, \quad B_\pm(x,\xi) = \lim_{t\to\pm\infty} \pi(\varphi_t(x,\xi)). \tag{8-9}$$

The limit in (8-9) is interpreted as the point of intersection of the geodesic starting at x and with tangent vector ξ with the boundary at infinity. We introduce also

$$\Phi_\pm : S\mathbb{H}^2 \to \mathbb{R}_+, \quad \Phi_\pm(x,\xi) := x_0 \pm \xi_0 > 0. \tag{8-10}$$

In fact, then we can write for any $(x,\xi) \in S\mathbb{H}^2$

$$x \pm \xi = \Phi_\pm(x,\xi)(1, B_\pm(x,\xi)). \tag{8-11}$$

The maps $B_\pm$ and $\Phi_\pm$ have nice interactions with the geodesic vector field X and the horocyclic vector fields $U_\pm$, defined in Section 8A. By this we mean that

$$dB_\pm \cdot X = 0, \quad U_\pm B_\pm = 0. \tag{8-12}$$

The first equation holds since $B_\pm$ is constant along X and the second one since $B_\pm$ is constant along horospheres. We also have

$$X\Phi_\pm = \pm\Phi_\pm, \quad U_\pm \Phi_\pm = 0. \tag{8-13}$$

Here, the first equation follows from $\Phi_\pm(\varphi_t(x,\xi)) = e^{\pm t}\Phi_\pm(x,\xi)$, which is true by (8-7). The second one also follows from a computation. Finally, since $\langle x+\xi, x-\xi\rangle_{\mathcal{M}} = 2$ and by (8-11), for $(x,\xi) \in S\mathbb{H}^2$, we have

$$\Phi_+(x,\xi)\Phi_-(x,\xi)(1 - B_+(x,\xi)\cdot B_-(x,\xi)) = 2. \tag{8-14}$$

The maps $\Phi_\pm$ and $B_\pm$ are G-equivariant in the following sense. We have

$$B_\pm(\gamma\cdot(x,\xi)) = L_\gamma(B_\pm(x,\xi)), \quad \Phi_\pm(\gamma\cdot(x,\xi)) = N_\gamma(B_\pm(x,\xi))\Phi_\pm(x,\xi). \tag{8-15}$$

Now the Jacobian of the map $L_\gamma : S^1 \to S^1$ may be computed explicitly and is given by

$$\langle dL_\gamma(\nu)\cdot\zeta_1, dL_\gamma(\nu)\cdot\zeta_2\rangle_{\mathbb{R}^2} = N_\gamma(\nu)^{-2}\langle\zeta_1,\zeta_2\rangle_{\mathbb{R}^2}, \quad \zeta_1,\zeta_2 \in T_\nu S^1. \tag{8-16}$$

Consider $\Sigma = \Gamma\backslash\mathbb{H}^2$ a compact hyperbolic surface, where $\Gamma \subset \mathrm{PSO}(1,2)$ is a discrete subgroup. Then we may identify the unit sphere bundle as $S\Sigma = \Gamma\backslash S\mathbb{H}^2$. We introduce the space of boundary distributions as

$$\mathrm{Bd}^0(\lambda) = \{w \in \mathcal{D}'(S^1) \mid L_\gamma^* w(\nu) = N_\gamma^{-\lambda}(\nu)w(\nu),\ \gamma\in\Gamma,\ \nu\in S^1\}. \tag{8-17}$$

The generator X of the geodesic flow descends to $S\Sigma$ and we define the *first band resonant states* by

$$\mathrm{Res}_X^0(\lambda) = \{u \in \mathcal{D}'_{E_u^*}(S\Sigma) \mid (X+\lambda)u = 0,\ U_- u = 0\}.$$

We similarly introduce the first band coresonant states via (see Section 2C)

$$\mathrm{Res}_{X^*}^0(\lambda) = \{u \in \mathcal{D}'_{E_s^*}(S\Sigma) \mid (X-\bar\lambda)u = 0,\ U_+ u = 0\}.$$

Then we have the correspondence, valid for all $\lambda \in \mathbb{C}$ proved in [Dyatlov et al. 2015, Lemma 5.6], which we prove here for completeness. Note that by $\Phi_\pm^\lambda$ for $\lambda \in \mathbb{C}$ we simply mean the exponentiation of the function $\Phi_\pm > 0$ by the exponent λ.

Lemma 8.4. *Let $\pi_\Gamma : S\mathbb{H}^2 \to S\Sigma$ be the natural projection. Then*

$$\pi_\Gamma^* \operatorname{Res}_X^0(\lambda) = \Phi_-^\lambda B_-^* \operatorname{Bd}^0(\lambda). \tag{8-18}$$

Similarly we have, for the space of coresonant states,

$$\pi_\Gamma^* \operatorname{Res}_{X^*}^0(\lambda) = \Phi_+^{\bar\lambda} B_+^* \operatorname{Bd}^0(\bar\lambda). \tag{8-19}$$

We also have $\overline{\operatorname{Bd}^0(\lambda)} = \operatorname{Bd}^0(\bar\lambda)$.

Proof. Let $w \in \operatorname{Bd}^0(\lambda)$ and put $v = \Phi_-^\lambda B_-^* w \in \mathcal{D}'(S\mathbb{H}^2)$ (the pullback of distributions under submersions is well-defined; see [Grigis and Sjöstrand 1994, Corollary 7.9]). We use now the invariance properties $\Phi_\pm$ and $B_\pm$ given by (8-15) to prove v is Γ-invariant. For $\gamma \in \Gamma$ we have

$$\gamma^* v = (\gamma^* \Phi_-)^\lambda \gamma^* B_-^* w = B_-^* (N_\gamma)^\lambda \Phi_-^\lambda B_-^* L_\gamma^* w = \Phi_-^\lambda B_-^* w = v.$$

Thus v is Γ-invariant and descends to $\mathcal{D}'(SM)$.

Now using (8-12) and (8-13), we obtain directly that $(X + \lambda)v = 0$ and $U_- v = 0$. This proves $\Phi_-^\lambda B_-^* \operatorname{Bd}^0(\lambda) \subset \pi_\Gamma^* \operatorname{Res}_X^0(\lambda)$ (the wavefront set condition on v follows from [Grigis and Sjöstrand 1994, Chapter 7]). The other direction follows by reversing the steps above and noting that a function (distribution) invariant by X and U_- is immediately a pullback by B_-. The statement about coresonant states follows similarly. □

We now introduce the set of coordinates $(\nu_-, \nu_+, s) \in (S^1 \times S^1)_\Delta \times \mathbb{R}$ on $S\mathbb{H}^2$, yielding a diffeomorphism $F : (S^1 \times S^1)_\Delta \times \mathbb{R} \to S\mathbb{H}^2$, and given by identification

$$(\nu_-, \nu_+, s) = \left(B_-(x, \xi), B_+(x, \xi), \frac{1}{2} \log \frac{\Phi_+(x, \xi)}{\Phi_-(x, \xi)} \right). \tag{8-20}$$

Here $(S_1 \times S_1)_\Delta$ denotes the torus $S^1 \times S^1$ without the diagonal Δ. The coordinates (8-20) can be interpreted as (ν_-, ν_+) parametrises the geodesic γ starting at ν_- and ending at ν_+ and s is the parameter on this geodesic such that $\gamma(-s)$ is the point on γ closest to $e_0 = (1, 0, 0)$ (or 0 in the disk model). The geodesic flow in these coordinates is simply $\varphi_t : (\nu_-, \nu_+, s) \mapsto (\nu_-, \nu_+, s + t)$.

The coordinates (8-20) enable us to write a product of distributions in resonant and coresonant spaces more explicitly, but we first require an explicit computation of the Jacobian of the change of coordinates $(x, \xi) \to (\nu_-, \nu_+, s)$.

Lemma 8.5. *For the coordinate system introduced in* (8-20), *we have the equality*

$$F^*(dx d\xi) = \frac{2 d\nu_- d\nu_+ ds}{|\nu_- - \nu_+|^2}. \tag{8-21}$$

Proof. This is the content of [Nicholls 1989, Theorem 8.1.1]. □

Remark 8.6. The Jacobian popping up in Lemma 8.5 is well known and the current in (8-21) is called the *Liouville current*.

We now prove that the invariant distributions formed as products of resonant and coresonant states have a very nice form in the coordinates (8-20).

Proposition 8.7. *Let* $w_1 \in \mathrm{Bd}^0(\lambda)$ *and* $w_2 \in \mathrm{Bd}^0(\bar{\lambda})$, *and consider the invariant distributions* $v_1 = \Phi_-^{\lambda} B_-^* w_1$ *and* $v_2 = \Phi_+^{\bar{\lambda}} B_+^* w_2$ *constructed in Lemma 8.4. Then the product distribution in* (ν_-, ν_+, s) *coordinates takes the form*[7]

$$F^*((v_1\bar{v}_2)(x,\xi)\,dx\,d\xi) = 2^{2\lambda+1}\frac{w_1(\nu_-)\bar{w}_2(\nu_+)}{|\nu_- - \nu_+|^{2(\lambda+1)}}\,d\nu_-\,d\nu_+\,ds. \tag{8-22}$$

In particular, for $\lambda = -1$ *the product* $F^*(v_1\bar{v}_2)$ *extends to a distribution on* $S^1 \times S^1 \times \mathbb{R}$.

Proof. By definition, we have the following expression for the product $v_1\bar{v}_2$:

$$(v_1\bar{v}_2)(x,\xi) = (\Phi_-(x,\xi)\Phi_+(x,\xi))^{\lambda} B_-^* w_1(x,\xi) B_+^* \bar{w}_2(x,\xi). \tag{8-23}$$

Now changing the coordinates to (ν_-, ν_+, s) given in (8-20) and by using the identity (8-14) we get

$$F^*(v_1\bar{v}_2)(\nu_-,\nu_+,s) = 2^{\lambda}(1-\nu_-\cdot\nu_+)^{-\lambda} w_1(\nu_-)\bar{w}_2(\nu_+) = 2^{2\lambda}\frac{w_1(\nu_-)\bar{w}_2(\nu_+)}{|\nu_- - \nu_+|^{2\lambda}}. \tag{8-24}$$

Using the Jacobian computation in Lemma 8.5, we establish (8-22).

In the special case $\lambda = -1$, using (8-22) we may write

$$F^*(v_1\bar{v}_2(x,\xi)\,dx\,d\xi) = \tfrac{1}{2} w_1(\nu_-)\bar{w}_2(\nu_+)\,ds\,d\nu_-\,d\nu_+. \tag{8-25}$$

In particular, for $\lambda = -1$ the distribution $F^*(v_1\bar{v}_2)$ extends to a distribution on the space $S^1 \times S^1 \times \mathbb{R}$. □

Remark 8.8. The distributions in (8-14) are called distributions of Patterson–Sullivan type. See [Anantharaman and Zelditch 2007] for more details, where the particular case of $\lambda = -\frac{1}{2} + ir_j$ is studied, in connection to eigenvalues of Δ on Σ with eigenvalue $\frac{1}{4} + r_j^2$. Note however there is an extra factor of $|\nu_- - \nu_+|^2$ compared to (8-24), obtained by changing coordinates according to (8-20).

8C. ***Construction of a time change that is not semisimple on 1-forms.*** Here we construct a smooth, positive function on the unit sphere bundle $S\Sigma$ of a compact hyperbolic surface $\Sigma = \Gamma\backslash\mathbb{H}^2$ such that under a time change of the geodesic flow, the action of the Lie derivative on resonant 1-forms at zero is not semisimple. We establish a few auxiliary lemmas first. We denote by $\pi_\Gamma : \mathbb{H}^2 \to \Gamma\backslash\mathbb{H}^2$ the associated projection.

Lemma 8.9. *Let* $w \in \mathrm{Bd}^0(-1)$. *Then* $w(\nu)\,d\nu$ *is* Γ*-invariant and we have*

$$\int_{S^1} w(\nu)\,d\nu = 0.$$

[7] Formally, by (8-22) we mean an equality in the sense of 0-currents. More explicitly, we mean an equality in the sense of distributions $\langle 2^{2\lambda+1} w_1(\nu_-)\bar{w}_2(\nu_+)/|\nu_- - \nu_+|^{2(\lambda+1)}, f\rangle_{(S^1\times S^1)_\Delta\times\mathbb{R}} = \langle v_1\bar{v}_2, f\circ F^{-1}\rangle_{S\mathbb{H}^2}$.

Proof. For the first claim, recall that by (8-16) we have $L_\gamma^* \, d\nu = N_\gamma^{-1}(\nu)\, d\nu$ for any $\gamma \in G$. Therefore, by (8-17) we have also $L_\gamma^*(w\, d\nu) = w\, d\nu$ for any $\gamma \in \Gamma$, which gives the required property.

The second property is a direct consequence of the works [Dyatlov et al. 2015; Guillarmou et al. 2018] on pairings. Note that [Dyatlov et al. 2015, Lemma 5.11] proves a pairing formula, which for $\lambda = -1$ gives

$$\langle \pi_* v_1, \pi_* v_2 \rangle_\Sigma = 0 \tag{8-26}$$

for all v_1 resonance states at -1 and v_2 coresonant states at -1. Here π_* maps first band resonant and coresonant states at -1 to eigenfunctions of Δ on Σ at zero by [Dyatlov et al. 2015, Lemma 5.8], so $\pi_* v_1$ and $\pi_* v_2$ are constants. Using the time-reversal map R from Section 5B we may identify resonant and coresonant states; i.e., we have $R^* : \mathrm{Res}_X^0(-1) \to \mathrm{Res}_{X^*}^0(-1)$ is an isomorphism. Moreover, we claim that $\pi_* R^* v = \pi_* v$ for any $v \in \mathrm{Res}_X^0(-1)$. For this recall the connection 1-form ψ on $S\Sigma$ (dual to the vertical fibre), and observe that $\pi_* v = \pi_*(v\psi)$. Then for any 2-form θ on Σ

$$\langle \pi_*(R^* v\psi), \theta \rangle_\Sigma = \int_{S\Sigma} R^* v\psi \wedge \pi^*\theta = \langle \pi_*(v\psi), \theta \rangle_\Sigma.$$

Here we used $R^*\psi = \psi$ and $\pi \circ R = \pi$. By applying (8-26) to $v_2 = R^* v_1$, we obtain that π_* is zero on both resonant and coresonant states.

Alternatively, this follows directly from the proof of [Guillarmou et al. 2018, Theorem 1] (more precisely, see p. 19 of that work and the start of discussion of the $\lambda_0 = -n$ case). □

Next we prove an auxiliary lemma that relies on the dynamics of the action of Γ on S^1.

Lemma 8.10. *Let $w \in \mathrm{Bd}^0(-1)$ and let $(\nu_-, \nu_+) \in S^1 \times S^1$ with $\nu_- \neq \nu_+$. Then there exists a $\varphi \in C^\infty(S^1)$, such that*:

(1) $\varphi \geq 0$.

(2) $\varphi(\nu_+) \neq 0$.

(3) *φ vanishes in a neighbourhood of ν_-.*

(4) $\langle w, \varphi \rangle_{S^1} = 0$.

Proof. We denote by $B_\varepsilon(A)$ the ε-neighbourhood of a set A. Let $\varphi_\varepsilon \in C^\infty(S^1)$ be a nonnegative function with $\varphi_\varepsilon = 1$ outside $B_\varepsilon(\nu_-)$ and $\varphi_\varepsilon = 0$ in $B_{\varepsilon/2}(\nu_-)$; assume also $0 \leq \varphi_\varepsilon \leq 1$. Here $\varepsilon > 0$ is a small enough positive number. If $\langle w, \varphi_\varepsilon \rangle = 0$ for some ε, we are done by setting $\varphi = \varphi_\varepsilon$. If not, then we may assume $\langle w, \varphi_\varepsilon \rangle > 0$ for every $\varepsilon > 0$. Assume $\langle w, \varphi_\varepsilon \rangle > 0$ and $\langle w, \varphi_\delta \rangle < 0$ for some $\varepsilon, \delta > 0$. Then if we take $s = -\langle w, \varphi_\varepsilon \rangle / \langle w, \varphi_\delta \rangle > 0$, we have $\langle w, \varphi_\varepsilon + s\varphi_\delta \rangle = 0$ and so we are done by setting $\varphi = \varphi_\varepsilon + s\varphi_\delta$.

Next, we may without loss of generality assume $\langle w, \varphi_\varepsilon \rangle > 0$ for all $\varepsilon > 0$ small enough. By Lemma 8.9 we have $\langle w, 1 \rangle = 0$, which implies $\langle w, 1 - \varphi_\varepsilon \rangle < 0$. The invariance of $w(\nu)\, d\nu$ under the action of Γ following from Lemma 8.9 then yields that for any $\psi \in C^\infty(S^1)$

$$\langle w, \psi \rangle = \int_{S^1} L_\gamma^*(w(\nu)\, d\nu)\psi = \int_{S^1} w(\nu)\psi \circ L_{\gamma^{-1}}(\nu)\, d\nu = \langle w, \psi \circ L_{\gamma^{-1}} \rangle. \tag{8-27}$$

Now use that since $\Gamma \cong \pi_1(M)$ has $2g \geq 4$ generators, it is not elementary by [Katok 1992, Theorem 2.4.3]. Therefore, by Exercise 2.13 of that work we have that Γ contains infinitely many hyperbolic elements (fixing exactly two elements of S^1), no two of which have a common fixed points.

So take $\gamma \in \Gamma$ hyperbolic such that ν_-, ν_+ are not in the set of fixed points of γ, which we denote by $\{p_1, p_2\}$. Assume without loss of generality p_1 is an attractor and p_2 is a repeller.

By (8-27) for $\psi = 1-\varphi_\varepsilon$, we get $\langle w, 1-\varphi_\varepsilon\rangle = \langle w, (1-\varphi_\varepsilon)\circ L_{\gamma^{-1}}\rangle < 0$. Since $\operatorname{supp}((1-\varphi_\varepsilon)\circ L_{\gamma^{-1}}) = L_\gamma(B_\varepsilon(\nu_-))$, we have that for $n \geq N_0$ large enough, $\varphi_{\varepsilon,n} := (1-\varphi_\varepsilon)\circ L_{\gamma^{-n}}$ has support arbitrarily close to p_1, so disjoint from ν_- and ν_+. Therefore, for $s = -\langle w, \varphi_\varepsilon\rangle / \langle w, \varphi_{\varepsilon,n}\rangle > 0$, we have

$$\langle w, \varphi_\varepsilon + s\varphi_{\varepsilon,n}\rangle = 0.$$

Then $\varphi = \varphi_\varepsilon + s\varphi_{\varepsilon,n}$ does the job. □

With this in hand, we can prove the following claim:

Theorem 8.11. *Let $\Sigma = \Gamma\backslash\mathbb{H}^2$ be a closed hyperbolic surface. Fix $w_2 \in \mathrm{Bd}^0(-1)$ and let $v_2 \in \mathrm{Res}^0_{X^*}(-1)$ be the corresponding coresonant state, according to Lemma 8.4. Then there exists an $f \in C^\infty(S\Sigma)$ with $f > 0$ such that*

$$\int_{S\Sigma} f v_1 \bar{v}_2 \, dx\, d\xi = 0 \tag{8-28}$$

for all $v_1 \in \mathrm{Res}^0_X(-1)$. In other words, semisimplicity of the Lie derivative $\mathcal{L}_{-iX/f}$ acting on resonant 1-forms at zero fails.

Proof. We divide the construction of f into several steps.

<u>Step 1</u>: First, fix $(x_0, \xi_0) \in S\mathbb{H}^2$. Denote the corresponding coordinates of (x_0, ξ_0) by $(\nu_{0-}, \nu_{0+}, s_0)$, according to (8-20). By Lemma 8.10, there is a nonnegative $\varphi_+ \in C^\infty(S^1)$, nonvanishing at ν_{0+}, vanishing near ν_{0-} and in the kernel of w_2. Now let $\varphi_- \in C^\infty(S^1)$ be such that $\varphi_- \geq 0$, $\varphi_-(\nu_{0-}) \neq 0$ and $\operatorname{supp}(\varphi_+) \cap \operatorname{supp}(\varphi_-) = \varnothing$. Also, let $\psi \in C_0^\infty(\mathbb{R})$ be such that $\psi(s_0) \neq 0$ and $\psi \geq 0$. Set $\chi(\nu_-, \nu_+, s) := \varphi_+(\nu_+)\varphi_-(\nu_-)\psi(s)$. Take any $w_1 \in \mathrm{Bd}^0(-1)$ and denote the corresponding element of $\mathrm{Res}^0_X(-1)$ by v_1. Then by the computation in Proposition 8.7 for $\lambda = -1$, we have $F^*\pi_\Gamma^*(v_1\bar{v}_2\, dx\, d\xi) = \frac{1}{2} w_1(\nu_-)\bar{w}_2(\nu_+)\, d\nu_-\, d\nu_+\, ds$ and

$$\begin{aligned}\langle \pi_\Gamma^*(v_1\bar{v}_2\, dx\, d\xi), F_*\chi\rangle_{S\mathbb{H}^2} &= \tfrac{1}{2}\langle w_1(\nu_-)\bar{w}_2(\nu_+)\, d\nu_-\, d\nu_+\, ds, \chi\rangle_{(S^1\times S^1)_\Delta\times\mathbb{R}} \\ &= \tfrac{1}{2}\langle w_1, \varphi_-\rangle\langle \bar{w}_2, \varphi_+\rangle\langle ds, \psi\rangle = 0\end{aligned} \tag{8-29}$$

since $\langle w_2, \varphi_+\rangle = 0$ by the construction. We will denote the χ above by $\chi_{(x_0,\xi_0)}$ and by $U_{(x_0,\xi_0)}$ a neighbourhood of (x_0, ξ_0) where $F_*\chi_{(x_0,\xi_0)} > 0$. Note that χ is a function in $C_0^\infty((S^1\times S^1)_\Delta \times \mathbb{R})$, by the condition on disjoint supports of φ_- and φ_+ in the construction, and as $\psi \in C_0^\infty(\mathbb{R})$. Therefore we have $F_*\chi$ a function in $C_0^\infty(S\mathbb{H}^2)$.

<u>Step 2</u>: Denote by $\mathcal{D} \subset \mathbb{H}^2$ a compact fundamental domain for Σ. Then $S\mathcal{D}$ is a fundamental domain for $S\Sigma$. By compactness, we have an $N > 0$ and $(x_i, \xi_i) \in S\mathbb{H}^2$ for $i = 1, 2, \dots, N$ such that

$$S\mathcal{D} \subset \bigcup_{(x_i,\xi_i)} U_{(x_i,\xi_i)}.$$

Define then

$$F_*\chi(x,\xi) := \sum_{i=1}^{N} F_*\chi_{(x_i,\xi_i)}(x,\xi) \in C_0^\infty(S\mathbb{H}^2).$$

By the construction, we have

$$\langle \pi_\Gamma^*(v_1\bar{v}_2\,dx\,d\xi),\, F_*\chi\rangle_{S\mathbb{H}^2} = \frac{1}{2}\sum_{i=1}^{N}\langle w_1(\nu_-)\bar{w}_2(\nu_+)\,d\nu_-\,d\nu_+\,ds,\, \chi_{(x_i,\xi_i)}\rangle_{(S^1\times S^1)_\Delta\times\mathbb{R}} = 0. \tag{8-30}$$

Step 3: We introduce the pushforward map $\pi_* : C_0^\infty(S\mathbb{H}^2) \to C^\infty(S\Sigma)$ by defining for any $\eta \in C_0^\infty(S\mathbb{H}^2)$

$$\pi_*\eta(x,\xi) := \sum_{\gamma\in\Gamma} \eta(\gamma\cdot(x_0,\xi_0)) \in C^\infty(S\Sigma). \tag{8-31}$$

Here $(x_0,\xi_0) \in \pi_\Gamma^{-1}(x,\xi) \subset S\mathbb{H}^2$ is an arbitrary point in the fibre and the definition of π_* is independent of any choices. Note that the only accumulation points of orbits of Γ are on the boundary at infinity S^1, so the pushforward is well-defined and sequentially continuous. Note also that π_* is dual to π_Γ^* in the sense of distributions.

Then we observe that $f(x,\xi) := \pi_* F_*\chi(x,\xi) \in C^\infty(S\Sigma)$ satisfies the required properties. Firstly,

$$\langle v_1\bar{v}_2\,dx\,d\xi,\, f\rangle_{S\Sigma} = \langle \pi_\Gamma^*(v_1\bar{v}_2\,dx\,d\xi),\, F_*\chi\rangle_{S\mathbb{H}^2} = 0 \tag{8-32}$$

by (8-30) from Step 2 and duality of π_* with π_Γ^*. Secondly, we have $f > 0$. To see this, let $(x,\xi) \in S\Sigma$ and denote a lift to $S\mathbb{H}^2$ by (x_0,ξ_0). Then there exists $\gamma' \in \Gamma$ with $\gamma'\cdot(x_0,\xi_0) \in \mathcal{D}$. Therefore, there is an $i \in \{1,2,\dots,N\}$ with $\gamma'\cdot(x_0,\xi_0) \in U_{(x_i,\xi_i)}$ and so $F_*\chi_{(x_i,\xi_i)}(\gamma'\cdot(x_0,\xi_0)) > 0$. Hence

$$f(x,\xi) = \sum_{\gamma\in\Gamma} F_*\chi(\gamma\cdot(x_0,\xi_0)) \geq \sum_{i=1}^{N} F_*\chi_{(x_i,\xi_i)}(\gamma'\cdot(x_0,\xi_0)) \geq F_*\chi_{(x_i,\chi_i)}(\gamma'\cdot(x_0,\xi_0)) > 0.$$

This proves the first claim. The final claim now follows directly from the correspondence in (8-4) and Proposition 8.1. □

Remark 8.12. One may see the element in the kernel of $\mathcal{L}_{X/f}^2$ and not in the kernel of $\mathcal{L}_{X/f}$ constructed in Theorem 8.11 more explicitly. Namely, one such element is given by the formula

$$u' = -iR_H(0)(fu).$$

Here $u \in \mathrm{Res}_X^0(-1)$ is an element such that $\int_{S\Sigma} fuv\,dx\,d\xi = 0$ for all $v \in \mathrm{Res}_{X^*}^0(-1)$ and $R_H(\lambda)$ is the holomorphic part at zero of $(-i\mathcal{L}_X - \lambda)^{-1}$ on 1-forms. The conclusion follows as $\Pi_0(fu) = 0$ and $-iR_H(0)$ is an inverse to $\mathcal{L}_X$ on $\ker \Pi_0 \cap \mathcal{D}'_{E_u^*}(M;\Omega^1)$.

Theorem 8.11 completes the proof of Theorem 1.4. We conclude this section with the following:

Proof of the second part of Corollary 1.7. By Theorem 1.4 there is a time change fX on the unit sphere bundle $S\Sigma$ of a closed hyperbolic surface Σ with $\ker \mathcal{L}_{fX}^2 \neq \ker \mathcal{L}_{fX}$ on $\Omega_0^1(S\Sigma)$. By Theorem 1.2, for the flow fX we have $m_0(0) = m_2(0) = 1$ and $\dim \mathrm{Res}_1(0) = b_1(\Sigma)$, so that $m_1(0) \geq b_1(\Sigma) + 1$. The claim then follows by applying Corollary 3.3. □

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References

[Adachi 1988] T. Adachi, "Meromorphic extension of L-functions of Anosov flows and profinite graphs", *Kumamoto J. Math.* **1** (1988), 9–24. MR Zbl

[Adachi and Sunada 1987] T. Adachi and T. Sunada, "Twisted Perron–Frobenius theorem and L-functions", *J. Funct. Anal.* **71**:1 (1987), 1–46. MR Zbl

[Anantharaman and Zelditch 2007] N. Anantharaman and S. Zelditch, "Patterson–Sullivan distributions and quantum ergodicity", *Ann. Henri Poincaré* **8**:2 (2007), 361–426. MR Zbl

[Arnold and Khesin 1998] V. I. Arnold and B. A. Khesin, *Topological methods in hydrodynamics*, Applied Mathematical Sciences **125**, Springer, 1998. MR Zbl

[Baladi 2005] V. Baladi, "Anisotropic Sobolev spaces and dynamical transfer operators: C^∞ foliations", pp. 123–135 in *Algebraic and topological dynamics*, edited by S. Kolyada et al., Contemp. Math. **385**, Amer. Math. Soc., Providence, RI, 2005. MR Zbl

[Baladi and Tsujii 2007] V. Baladi and M. Tsujii, "Anisotropic Hölder and Sobolev spaces for hyperbolic diffeomorphisms", *Ann. Inst. Fourier* (*Grenoble*) **57**:1 (2007), 127–154. MR Zbl

[Ballmann et al. 2016] W. Ballmann, H. Matthiesen, and S. Mondal, "Small eigenvalues of closed surfaces", *J. Differential Geom.* **103**:1 (2016), 1–13. MR Zbl

[Blank et al. 2002] M. Blank, G. Keller, and C. Liverani, "Ruelle–Perron–Frobenius spectrum for Anosov maps", *Nonlinearity* **15**:6 (2002), 1905–1973. MR Zbl

[Bonatti and Langevin 1994] C. Bonatti and R. Langevin, "Un exemple de flot d'Anosov transitif transverse à un tore et non conjugué à une suspension", *Ergodic Theory Dynam. Systems* **14**:4 (1994), 633–643. MR Zbl

[Bott and Tu 1982] R. Bott and L. W. Tu, *Differential forms in algebraic topology*, Graduate Texts in Mathematics **82**, Springer, 1982. MR Zbl

[Butterley and Liverani 2007] O. Butterley and C. Liverani, "Smooth Anosov flows: correlation spectra and stability", *J. Mod. Dyn.* **1**:2 (2007), 301–322. MR Zbl

[Chaubet and Dang 2019] Y. Chaubet and N. V. Dang, "Dynamical torsion for contact Anosov flows", preprint, 2019. arXiv

[Dairbekov and Paternain 2005] N. S. Dairbekov and G. P. Paternain, "Longitudinal KAM-cocycles and action spectra of magnetic flows", *Math. Res. Lett.* **12**:5-6 (2005), 719–729. MR Zbl

[Dang and Riviere 2017] N. V. Dang and G. Riviere, "Topology of Pollicott–Ruelle resonant states", preprint, 2017. To appear in *Ann. Sc. Norm. Sup. di Pisa*. arXiv

[Dang et al. 2020] N. V. Dang, C. Guillarmou, G. Rivière, and S. Shen, "The Fried conjecture in small dimensions", *Invent. Math.* **220**:2 (2020), 525–579. MR Zbl

[Dyatlov and Guillarmou 2016] S. Dyatlov and C. Guillarmou, "Pollicott–Ruelle resonances for open systems", *Ann. Henri Poincaré* **17**:11 (2016), 3089–3146. MR Zbl

[Dyatlov and Zworski 2016] S. Dyatlov and M. Zworski, "Dynamical zeta functions for Anosov flows via microlocal analysis", *Ann. Sci. Éc. Norm. Supér.* (4) **49**:3 (2016), 543–577. MR Zbl

[Dyatlov and Zworski 2017] S. Dyatlov and M. Zworski, "Ruelle zeta function at zero for surfaces", *Invent. Math.* **210**:1 (2017), 211–229. MR Zbl

[Dyatlov and Zworski 2019] S. Dyatlov and M. Zworski, *Mathematical theory of scattering resonances*, Graduate Studies in Mathematics **200**, Amer. Math. Soc., Providence, RI, 2019. MR Zbl

[Dyatlov et al. 2015] S. Dyatlov, F. Faure, and C. Guillarmou, "Power spectrum of the geodesic flow on hyperbolic manifolds", *Anal. PDE* **8**:4 (2015), 923–1000. MR Zbl

[Faure and Sjöstrand 2011] F. Faure and J. Sjöstrand, "Upper bound on the density of Ruelle resonances for Anosov flows", *Comm. Math. Phys.* **308**:2 (2011), 325–364. MR Zbl

[Foulon and Hasselblatt 2003] P. Foulon and B. Hasselblatt, "Zygmund strong foliations", *Israel J. Math.* **138** (2003), 157–169. MR Zbl

[Fried 1986] D. Fried, "Analytic torsion and closed geodesics on hyperbolic manifolds", *Invent. Math.* **84**:3 (1986), 523–540. MR Zbl

[Giulietti et al. 2013] P. Giulietti, C. Liverani, and M. Pollicott, "Anosov flows and dynamical zeta functions", *Ann. of Math.* (2) **178**:2 (2013), 687–773. MR Zbl

[Gouëzel and Liverani 2006] S. Gouëzel and C. Liverani, "Banach spaces adapted to Anosov systems", *Ergodic Theory Dynam. Systems* **26**:1 (2006), 189–217. MR Zbl

[Grigis and Sjöstrand 1994] A. Grigis and J. Sjöstrand, *Microlocal analysis for differential operators*: *an introduction*, London Mathematical Society Lecture Note Series **196**, Cambridge University Press, 1994. MR Zbl

[Guedes Bonthonneau 2020] Y. Guedes Bonthonneau, "Perturbation of Ruelle resonances and Faure–Sjöstrand anisotropic space", *Rev. Un. Mat. Argentina* **61**:1 (2020), 63–72. MR Zbl

[Guillarmou and Faure 2018] C. Guillarmou and F. Faure, "Horocyclic invariance of Ruelle resonant states for contact Anosov flows in dimension 3", *Math. Res. Lett.* **25**:5 (2018), 1405–1427. MR Zbl

[Guillarmou et al. 2018] C. Guillarmou, J. Hilgert, and T. Weich, "Classical and quantum resonances for hyperbolic surfaces", *Math. Ann.* **370**:3-4 (2018), 1231–1275. MR Zbl

[Hörmander 1983] L. Hörmander, *The analysis of linear partial differential operators, I*: *Distribution theory and Fourier analysis*, Grundlehren der Mathematischen Wissenschaften **256**, Springer, 1983. MR Zbl

[Hörmander 1985] L. Hörmander, *The analysis of linear partial differential operators, III*: *Pseudodifferential operators*, Grundlehren der Mathematischen Wissenschaften **274**, Springer, 1985. MR Zbl

[Katok 1992] S. Katok, *Fuchsian groups*, University of Chicago Press, 1992. MR Zbl

[Liverani 2004] C. Liverani, "On contact Anosov flows", *Ann. of Math.* (2) **159**:3 (2004), 1275–1312. MR Zbl

[de la Llave et al. 1986] R. de la Llave, J. M. Marco, and R. Moriyón, "Canonical perturbation theory of Anosov systems and regularity results for the Livšic cohomology equation", *Ann. of Math.* (2) **123**:3 (1986), 537–611. MR Zbl

[Nicholls 1989] P. J. Nicholls, *The ergodic theory of discrete groups*, London Mathematical Society Lecture Note Series **143**, Cambridge University Press, 1989. MR Zbl

[Pollicott 2013] M. Pollicott, "Dynamical zeta functions", lecture notes, 2013, available at https://homepages.warwick.ac.uk/~masdbl/grenoble-16july.pdf.

[Ruelle 1976] D. Ruelle, "Zeta-functions for expanding maps and Anosov flows", *Invent. Math.* **34**:3 (1976), 231–242. MR Zbl

[Shen 2018] S. Shen, "Analytic torsion, dynamical zeta functions, and the Fried conjecture", *Anal. PDE* **11**:1 (2018), 1–74. MR Zbl

[Singer and Thorpe 1967] I. M. Singer and J. A. Thorpe, *Lecture notes on elementary topology and geometry*, Scott, Foresman and Co., Glenview, IL, 1967. MR Zbl

[Zworski 2018] M. Zworski, "Commentary on "Differentiable dynamical systems" by Stephen Smale", *Bull. Amer. Math. Soc.* (*N.S.*) **55**:3 (2018), 331–336. MR Zbl

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SEMICLASSICAL RESOLVENT ESTIMATES FOR HÖLDER POTENTIALS

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We first prove semiclassical resolvent estimates for the Schrödinger operator in $\mathbb{R}^d$, $d \geq 3$, with real-valued potentials which are Hölder with respect to the radial variable. Then we extend these resolvent estimates to exterior domains in $\mathbb{R}^d$, $d \geq 2$, and real-valued potentials which are Hölder with respect to the space variable. As an application, we obtain the rate of the decay of the local energy of the solutions to the wave equation with a refraction index which may be Hölder, Lipschitz or just L^∞.

1. Introduction and statement of results

In this paper we are going to study the resolvent of the Schrödinger operator

$$P(h) = -h^2\Delta + V(x),$$

where $0 < h \leq 1$ is a semiclassical parameter, Δ is the negative Laplacian in $\mathbb{R}^d$, $d \geq 2$, and $V \in L^\infty(\mathbb{R}^d)$ is a real-valued potential satisfying the condition

$$V(x) \leq p(|x|), \tag{1.1}$$

where $p(r) > 0$, $r \geq 0$, is a decreasing function such that $p(r) \to 0$ as $r \to \infty$. More precisely, we are interested in bounding the quantity

$$g_s^{\pm}(h,\varepsilon) := \log\left\| (|x|+1)^{-s}(P(h) - E \pm i\varepsilon)^{-1}(|x|+1)^{-s} \right\|_{L^2 \to L^2}$$

from above by an explicit function of h, independent of ε, without imposing extra assumptions on the function p. Here $L^2 := L^2(\mathbb{R}^d)$, $0 < \varepsilon < 1$, $s > \frac{1}{2}$ is independent of h and $E > 0$ is a fixed energy level independent of h. Instead, we impose some regularity on the potential with respect to the radial variable $r = |x|$. Note that throughout this paper, the space C^1 will denote the Lipschitz functions, that is, the ones with first derivatives belonging to L^∞ (and not necessarily continuous).

We will first extend the result of [Datchev 2014] to a larger class of potentials. Recall that in [Datchev 2014] the bound

$$g_s^{\pm}(h,\varepsilon) \leq Ch^{-1} \tag{1.2}$$

is proved when $d \geq 3$, with some constant $C > 0$ independent of h and ε, for potentials $V \in C^1(\overline{\mathbb{R}^+})$ with respect to the radial variable r and satisfying (1.1) with $p(|x|) = C_1(|x|+1)^{-\delta}$, as well as the condition

$$\partial_r V(x) \leq C_2(|x|+1)^{-\beta}, \tag{1.3}$$

where $C_1, C_2, \delta > 0$ and $\beta > 1$ are some constants. We will prove the following:

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Keywords: Schrödinger operator, resolvent estimates, Hölder potentials.

Theorem 1.1. *Let $d \geq 3$ and suppose that the potential V satisfies the conditions* (1.1) *and* (1.3). *Then there exists a constant $C > 0$ independent of h and ε but depending on s, E and the function p, such that the bound* (1.2) *holds for all $0 < h \leq 1$.*

Note that the bound (1.2) was first proved for smooth potentials in [Burq 2002]. A high-frequency analog of (1.2) on Riemannian manifolds was also proved in [Burq 1998] and [Cardoso and Vodev 2002]. When $d = 2$, the bound (1.2) is proved in [Shapiro 2019] for potentials $V \in C^1(\mathbb{R}^2)$ satisfying (1.1) with $p(|x|) = C_1(|x|+1)^{-\delta}$ as well as the condition

$$|\nabla V(x)| \leq C_2(|x|+1)^{-\beta}, \tag{1.4}$$

where $C_1, C_2, \delta > 0$ and $\beta > 1$ are some constants.

On the other hand, for compactly supported L^∞ potentials without any regularity, the weaker bound

$$g_s^{\pm}(h, \varepsilon) \leq C h^{-4/3} \log(h^{-1}) \tag{1.5}$$

was proved for $0 < h \ll 1$ in [Klopp and Vogel 2019] and [Shapiro 2020] when $d \geq 2$. When $d \geq 3$, the bound (1.5) has been extended in [Vodev 2019] to potentials satisfying the condition

$$|V(x)| \leq C_3(|x|+1)^{-\delta}, \tag{1.6}$$

where $C_3 > 0$ and $\delta > 3$ are some constants. Note that (1.5) has been recently proved in [Galkowski and Shapiro 2020] for potentials satisfying (1.6) with $\delta > 2$. For potentials satisfying (1.6) with $1 < \delta \leq 3$, the much weaker bound

$$g_s^{\pm}(h, \varepsilon) \leq C h^{-(2\delta+5)/(3(\delta-1))} \big(\log(h^{-1})\big)^{1/(\delta-1)} \tag{1.7}$$

was proved in [Vodev 2020c].

In the present paper we show that the bound (1.5) can be improved if some small regularity of the potential is assumed. To be more precise, given $0 < \alpha < 1$ and $\beta > 0$, we introduce the space $C_\beta^\alpha(\overline{\mathbb{R}^+})$ of all Hölder functions a such that

$$\sup_{r' \geq 0:\, 0 < |r - r'| \leq 1} \frac{|a(r) - a(r')|}{|r - r'|^\alpha} \leq C(r+1)^{-\beta}, \quad \forall r \in \overline{\mathbb{R}^+},$$

for some constant $C > 0$. We now suppose that the function $V(r, w) := V(rw)$ satisfies the condition

$$V(\cdot, w) \in C_4^\alpha(\overline{\mathbb{R}^+}), \quad 0 < \alpha < 1, \tag{1.8}$$

uniformly in $w \in \mathbb{S}^{d-1}$.

Theorem 1.2. *Let $d \geq 3$, and suppose that the potential V satisfies the conditions* (1.1) *and* (1.8). *Then there exists a constant $C > 0$ independent of h and ε but depending on s, E and the function p, such that the bound*

$$g_s^{\pm}(h, \varepsilon) \leq C h^{-4/(\alpha+3)} \log(h^{-1}) + C \tag{1.9}$$

holds for all $0 < h \leq 1$.

The proofs of the above theorems are based on the global Carleman estimates proved in [Vodev 2020c], but with different phase and weight functions (see Theorem 4.1). In fact, in the case of Hölder or Lipschitz potentials, we need to construct better phase functions, and hence get better Carleman estimates. Such functions are constructed in Section 2, modifying the construction in [Vodev 2020c] in a suitable way. In order for the Carleman estimates (see (4.1) and (4.6) below) to hold, the phase and weight functions must satisfy some inequalities (see (2.5), (2.9) and (2.21) below), so most of the proofs of the above theorems consist of verifying these inequalities. Note also that the above theorems have been recently proved in [Galkowski and Shapiro 2020] by using similar Carleman estimates, but with a better choice of the phase function. Consequently, the bound (1.9) is proved in [Galkowski and Shapiro 2020] for a larger class of α-Hölder potentials. On the other hand, it is shown in [Vodev 2020a] that the logarithmic term in the right-hand side of (1.9) can be removed for radial potentials.

We next extend the above results to arbitrary obstacles and all dimensions $d \geq 2$. To do so, we need to replace the conditions (1.3) and (1.8) by stronger ones. To be more precise, we let $\Omega \subset \mathbb{R}^d$, $d \geq 2$, be a connected domain with smooth boundary $\partial\Omega$ such that $\mathbb{R}^d \setminus \Omega$ is compact. Let $r_0 > 0$ be such that $\mathbb{R}^d \setminus \Omega \subset \{x \in \mathbb{R}^d : |x| \leq r_0\}$. Given a real-valued potential $V \in L^\infty(\Omega)$ satisfying (1.1) for $|x| \geq r_0$, we denote by $P(h)$ the Dirichlet self-adjoint realization of the operator $-h^2\Delta + V(x)$ on the Hilbert space $L^2(\Omega)$. We define the quantity $g_s^\pm$ in the same way as above with $L^2 = L^2(\Omega)$. Given $0 < \alpha \leq 1$ and $\beta > 0$, we introduce the space $C^\alpha_\beta(\overline{\Omega})$ of all Hölder functions a such that

$$\sup_{x' \in \overline{\Omega}:\, 0<|x-x'|\leq 1} \frac{|a(x) - a(x')|}{|x - x'|^\alpha} \leq C(|x| + 1)^{-\beta}, \quad \forall x \in \overline{\Omega},$$

for some constant $C > 0$. Note that the case $\alpha = 1$ corresponds to the Lipschitz functions. We suppose that

$$V \in C^\alpha_\beta(\overline{\Omega}), \quad 0 < \alpha \leq 1, \beta > 1. \tag{1.10}$$

Theorem 1.3. *Let* $d \geq 2$, *and suppose that the potential* $V \in L^\infty(\Omega)$ *satisfies* (1.1) *for* $|x| \geq r_0$. *If* V *satisfies* (1.10) *with* $\alpha = 1$ *and* $\beta > 1$, *then the bound* (1.2) *holds for all* $0 < h \leq 1$. *If* V *satisfies* (1.10) *with* $0 < \alpha < 1$ *and* $\beta = 4$, *then the bound* (1.9) *holds for all* $0 < h \leq 1$.

To prove this theorem we follow the same strategy as in [Vodev 2020b], where the bound (1.5) is proved in all dimensions $d \geq 2$ for potentials $V \in L^\infty(\Omega)$ satisfying (1.6). It consists of gluing up two different types of estimates — one in a compact set coming from the local Carleman estimates proved in [Lebeau and Robbiano 1995] (see Theorem 3.1) with a global Carleman estimate outside a sufficiently big compact (see Theorem 4.2). This is carried out in Section 4.

Theorem 1.3 together with Theorem 1.1 of [Vodev 2020b] allow us to get uniform bounds for the resolvent of the Dirichlet self-adjoint realization, G, of the operator $-n(x)^{-1}\Delta$ in the Hilbert space $H = L^2(\Omega, n(x)dx)$, where $n \in L^\infty(\Omega)$ is a real-valued function called the refraction index, satisfying the conditions

$$n_1 \leq n(x) \leq n_2 \quad \text{in } \Omega, \tag{1.11}$$

with some constants $n_1, n_2 > 0$, and

$$|n(x) - 1| \le C(|x| + 1)^{-\delta} \quad \text{in } \Omega, \tag{1.12}$$

with some constants $C, \delta > 0$. More precisely, we have the following:

Corollary 1.4. *Suppose that the function n satisfies the conditions* (1.11) *and* (1.12). *Then, given any $s > \frac{1}{2}$ and $\lambda_0 > 0$, there is a constant $C > 0$ depending on s and λ_0 such that the estimate*

$$\left\| (|x| + 1)^{-s} (G - \lambda^2 \pm i\varepsilon)^{-1} (|x| + 1)^{-s} \right\|_{H \to H} \le e^{C\psi(\lambda)} \tag{1.13}$$

holds for all $\lambda \ge \lambda_0$ uniformly in ε, where $\psi(\lambda) = \lambda^{4/3} \log(\lambda + 1)$ if $n \in L^\infty(\Omega)$ satisfies (1.12) *with $\delta > 3$, $\psi(\lambda) = \lambda^{4/(\alpha+3)} \log(\lambda + 1)$ if $n \in C_4^\alpha(\overline{\Omega})$ with $0 < \alpha < 1$ and $\psi(\lambda) = \lambda$ if $n \in C_\beta^1(\overline{\Omega})$ with $\beta > 1$.*

To get (1.13) we apply the theorems mentioned above with $h = \lambda_0/\lambda$, $V = \lambda_0^2(1 - n)$, $E = \lambda_0^2$ and ε replaced by $\varepsilon h^2 n$.

Using Corollary 1.4 one can extend the result of [Shapiro 2018] on the local energy decay of the solutions of the wave equation

$$\begin{cases} (n(x)\partial_t^2 - \Delta)u(t, x) = 0 & \text{in } \mathbb{R} \times \Omega, \\ u(t, x) = 0 & \text{on } \mathbb{R} \times \partial\Omega, \\ u(0, x) = f_1(x),\ \partial_t u(0, x) = f_2(x) & \text{in } \Omega. \end{cases} \tag{1.14}$$

Given any $r_0 \gg 1$, denote $\Omega_{r_0} = \{x \in \Omega : |x| \le r_0\}$.

Corollary 1.5. *Suppose that the function n satisfies* (1.11) *and that $n = 1$ outside some compact subset of Ω. Then, the solution $u(t, x)$ to* (1.14) *with compactly supported initial data $(f_1, f_2) \in H_0^2(\Omega) \times H_0^1(\Omega)$ satisfies the estimate*

$$\|\nabla u(t, \cdot)\|_{L^2(\Omega_{r_0})} + \|\partial_t u(t, \cdot)\|_{L^2(\Omega_{r_0})} \le C\omega(t)\big(\|f_1\|_{H^2(\Omega)} + \|f_2\|_{H^1(\Omega)}\big) \tag{1.15}$$

for $t \gg 1$, where

$$\omega(t) = \left(\frac{\log\log t}{\log t} \right)^{3/4}.$$

Suppose, in addition, that $n \in C^\alpha(\overline{\Omega})$ with $0 < \alpha \le 1$. Then, the estimate (1.15) *holds with*

$$\omega(t) = \left(\frac{\log\log t}{\log t} \right)^{(\alpha+3)/4}$$

if $0 < \alpha < 1$ and with $\omega(t) = (\log t)^{-1}$ if $\alpha = 1$. The estimate (1.15) *remains valid when $\Omega = \mathbb{R}^d$.*

Remark 1.6. In view of the recent results in [Vodev 2020a], when $\Omega = \mathbb{R}^d$, $d \ge 3$ and the function n depends only on the radial variable r, the estimate (1.15) holds with $\omega(t) = (\log t)^{-3/4}$ if $n \in L^\infty$ and with $\omega(t) = (\log t)^{-(\alpha+3)/4}$ if n is α-Hölder in r.

Note that estimates similar to (1.15) were first proved by [Burq 1998] in the case $n \equiv 1$. Note also that an analog of the above theorem is proved by [Shapiro 2018] in the case $\Omega = \mathbb{R}^d$. Then, an estimate similar to (1.15) is proved with $\omega(t)$ replaced by $(\log t)^{-3/4+\varepsilon}$, $\varepsilon > 0$ being arbitrary. Moreover, if in addition the function n is supposed Lipschitz, then the decay rate is improved to $\omega(t) = (\log t)^{-1}$. The proof in [Shapiro 2018] is based on the resolvent estimates obtained in [Datchev 2014], [Shapiro 2019] and [Shapiro 2020].

The assumption that $n = 1$ outside some compact set is only necessary to study the low-frequency behavior of the cut-off resolvent of G. Indeed, under this assumption one can easily see that this behavior is exactly the same as in the case when $n \equiv 1$, which in turn is well known (see Appendix B.2 of [Burq 1998]). Therefore, in this case the low-frequency analysis can be carried out in precisely the same way as in [Shapiro 2018]. Most probably, the condition (1.12) with $\delta > 2$ would be enough. The high-frequency analysis, in our case, is also very similar to the one in [Shapiro 2018], with some slight modifications allowing to deduce from (1.13) the sharp decay rate $\omega(t)$ (instead of $(\log t)^{-3/4+\varepsilon}$).

2. Construction of the phase and weight functions

Let $\rho \in C_0^\infty([0, 1])$, $\rho \geq 0$, be a real-valued function independent of h such that $\int_0^\infty \rho(\sigma)\, d\sigma = 1$. If V satisfies (1.8), we approximate it by the function

$$V_\theta(r, w) = \theta^{-1} \int_0^\infty \rho\Big(\frac{r'-r}{\theta}\Big) V(r', w)\, dr' = \int_0^\infty \rho(\sigma) V(r + \theta\sigma, w)\, d\sigma,$$

where $\theta = h^{2/(\alpha+3)}$. Indeed, we have

$$\begin{aligned} |V(r, w) - V_\theta(r, w)| &\leq \int_0^\infty \rho(\sigma) |V(r + \theta\sigma, w) - V(r, w)|\, d\sigma \\ &\lesssim \theta^\alpha (r+1)^{-4} \int_0^\infty \sigma^\alpha \rho(\sigma)\, d\sigma \lesssim \theta^\alpha (r+1)^{-4}. \end{aligned} \tag{2.1}$$

This bound together with (1.1) implies

$$V_\theta(r, w) \leq p(r) + \mathcal{O}\big((r+1)^{-4}\big). \tag{2.2}$$

Clearly, V_θ is C^1 with respect to the variable r, and its first derivative V_θ' is given by

$$\begin{aligned} V_\theta'(r, w) &= \theta^{-2} \int_0^\infty \rho'\Big(\frac{r'-r}{\theta}\Big) V(r', w)\, dr' \\ &= \theta^{-1} \int_0^\infty \rho'(\sigma) V(r + \theta\sigma, w)\, d\sigma = \theta^{-1} \int_0^\infty \rho'(\sigma)(V(r + \theta\sigma, w) - V(r, w))\, d\sigma, \end{aligned}$$

where we have used that $\int_0^\infty \rho'(\sigma)\, d\sigma = 0$. Hence,

$$|V_\theta'(r, w)| \lesssim \theta^{-1+\alpha} (r+1)^{-4} \int_0^\infty \sigma^\alpha |\rho'(\sigma)|\, d\sigma \lesssim \theta^{-1+\alpha} (r+1)^{-4}. \tag{2.3}$$

We now construct the weight function μ as follows:

$$\mu(r) = \begin{cases} (r+1)^{2k} - (r+1)^{2k_0} & \text{for } 0 \leq r \leq a, \\ (a+1)^{2k} - (a+1)^{2k_0} + (a+1)^{-2s+1} - (r+1)^{-2s+1} & \text{for } r \geq a, \end{cases}$$

where $a = a_0 h^{-m}$ with $a_0 \gg 1$ independent of h, $m = 0$ if V satisfies (1.3) and $m = 2$ if V satisfies (1.8). We choose $k = \frac{1}{4}\min\{1, \beta - 1\}$, $k_0 = 0$ if V satisfies (1.3) and $k = 1$, $k_0 = \frac{1}{2}$ if V satisfies (1.8). Furthermore,

s is independent of h such that

$$\frac{1}{2} < s < \begin{cases} \frac{1}{4}\min\{3, \beta+1\} & \text{if } V \text{ satisfies (1.3)}, \\ \frac{3}{4} & \text{if } V \text{ satisfies (1.8)}. \end{cases} \tag{2.4}$$

Clearly, the first derivative of μ is given by

$$\mu'(r) = \begin{cases} 2k(r+1)^{2k-1} - 2k_0(r+1)^{2k_0-1} & \text{for } 0 \le r < a, \\ (2s-1)(r+1)^{-2s} & \text{for } r > a. \end{cases}$$

Lemma 2.1. *For all $r > 0$, $r \neq a$, we have the inequalities*

$$2r^{-1}\mu(r) - \mu'(r) \ge 0, \tag{2.5}$$

$$\frac{\mu(r)^j}{\mu'(r)} \lesssim a^{2kj}(r+1)^{2s}, \tag{2.6}$$

for every $j \ge 0$.

Proof. It is shown in Section 2 of [Vodev 2020c] that when $k_0 = 0$ the inequality (2.5) holds for all $0 < k \le 1$. Here, we will prove it when $\nu := 2k - 2k_0 \ge 1$ and $0 < k \le 1$. For $r < a$ we have

$$\begin{aligned} 2\mu(r) - r\mu'(r) &= 2(1-k)(r+1)^{2k} - 2(1-k_0)(r+1)^{2k_0} + 2k(r+1)^{2k-1} - 2k_0(r+1)^{2k_0-1} \\ &= 2(r+1)^{2k_0-1}\big((1-k)(r+1)^{\nu+1} - (1-k_0)(r+1) + k(r+1)^{\nu} - k_0\big) \\ &= 2(r+1)^{2k_0-1}\big((1-k)r((r+1)^{\nu} - 1) + (r+1)^{\nu} - \nu r/2 - 1\big) \\ &\ge 2(r+1)^{2k_0-1}\big((r+1)^{\nu} - \nu r/2 - 1\big) \ge \nu r(r+1)^{2k_0-1} > 0, \end{aligned}$$

where we have used the well-known inequality $(r+1)^{\nu} \ge \nu r + 1$, as long as $\nu \ge 1$. For $r > a$ the left-hand side of (2.5) is bounded from below by

$$2r^{-1}\big((a+1)^{2k} - (a+1)^{2k_0} - s\big) > 0,$$

provided a is taken large enough. To prove (2.6) observe that for $r < a$ we have

$$\mu'(r) \ge 2(k-k_0)(r+1)^{2k-1} \ge 2(k-k_0)(r+1)^{-1} \ge 2(k-k_0)(r+1)^{-2s},$$

which clearly implies the bound (2.6) with $j = 0$. This together with the fact that $\mu = \mathcal{O}(a^{2k})$ implies the bound (2.6) with any $j > 0$. □

We will now construct a phase function $\varphi \in C^1([0, +\infty))$ such that $\varphi(0) = 0$ and $\varphi(r) > 0$ for $r > 0$. We define the first derivative of φ by

$$\varphi'(r) = \begin{cases} \tau(r+1)^{-k} - \tau(a+1)^{-k} & \text{for } 0 \le r \le a, \\ 0 & \text{for } r \ge a, \end{cases}$$

where

$$\tau = \begin{cases} \tau_0 & \text{if } V \text{ satisfies (1.3)}, \\ \tau_0\theta^{2\alpha/3}h^{-1/3} & \text{if } V \text{ satisfies (1.8)}, \end{cases} \tag{2.7}$$

with some parameter $\tau_0 \gg 1$ independent of h to be fixed later on. We choose now the parameter a_0 of the form $a_0 = \tau_0^{\ell}$, where $\ell > 0$ is a constant such that $k\ell > 2$ and $(\beta - 2k - 2s)\ell > 2$. Note that the choice of the parameters k and s guarantees that $\beta - 2k - 2s > 0$.

Clearly, the first derivative of φ' satisfies

$$\varphi''(r) = \begin{cases} -k\tau(r+1)^{-k-1} & \text{for } 0 \le r < a, \\ 0 & \text{for } r > a. \end{cases}$$

Lemma 2.2. *For all $r \ge 0$ we have the bounds*

$$h^{-1}\varphi(r) \lesssim \begin{cases} h^{-1} & \text{if } V \text{ satisfies (1.3)}, \\ h^{-4/(\alpha+3)}\log(h^{-1})+1 & \text{if } V \text{ satisfies (1.8)}. \end{cases} \tag{2.8}$$

Proof. The lemma follows from the bounds

$$\max\varphi = \int_0^a \varphi'(r)\,dr \le \tau\int_0^a (r+1)^{-k}\,dr \lesssim \begin{cases} \tau a^{1-k} & \text{if } k<1, \\ \tau\log a & \text{if } k=1. \end{cases} \qquad \square$$

For $r > 0$, $r \ne a$, set

$$A(r) = \big(\mu\varphi'^2\big)'(r),$$
$$B(r) = B_1(r) + B_2(r),$$

where

$$B_1(r) = (r+1)^{-\beta}\mu(r) + p(r)\mu'(r),$$
$$B_2(r) = \frac{(\mu(r)\varphi''(r))^2}{h^{-1}\varphi'(r)\mu(r)+\mu'(r)},$$

with $\beta > 1$ if V satisfies (1.3) and

$$B_1(r) = \theta^{-1+\alpha}(r+1)^{-\beta}\mu(r) + (p(r)+(r+1)^{-\beta})\mu'(r),$$
$$B_2(r) = \frac{\big(\mu(r)(h^{-1}\theta^{\alpha}(r+1)^{-\beta}+|\varphi''(r)|)\big)^2}{h^{-1}\varphi'(r)\mu(r)+\mu'(r)},$$

with $\beta = 4$ if V satisfies (1.8). The following lemma will play a crucial role in the proof of the Carleman estimates (4.1) and (4.6) in the case $d \ge 3$:

Lemma 2.3. *Given any constant $C > 0$, there exists a positive constant $\tau_1 = \tau_1(C, E)$ such that for τ satisfying* (2.7) *with $\tau_0 \ge \tau_1$ and for all $0 < h \le 1$, we have the inequality*

$$A(r) - CB(r) \ge -\frac{E}{2}\mu'(r) \tag{2.9}$$

for all $r > 0$, $r \ne a$.

Proof. For $r < a$ we have

$$\begin{aligned} A(r) &= -\big((r+1)^{2k_0}\varphi'^2\big)' + \tau^2\partial_r\big(1-(r+1)^k(a+1)^{-k}\big)^2 \\ &= -2(r+1)^{2k_0}\varphi'(r)\varphi''(r) - 2k_0(r+1)^{2k_0-1}\varphi'(r)^2 - 2k\tau^2(r+1)^{k-1}(a+1)^{-k}\big(1-(r+1)^k(a+1)^{-k}\big) \\ &\ge 2\tau(k-k_0)(r+1)^{2k_0-k-1}\varphi'(r) - 2k\tau^2(r+1)^{k-1}(a+1)^{-k} \\ &\ge 2\tau(k-k_0)(r+1)^{2k_0-k-1}\varphi'(r) - \mathcal{O}\big(\tau^2a^{-k}\big)\mu'(r) \\ &\ge 2\tau(k-k_0)(r+1)^{2k_0-k-1}\varphi'(r) - \mathcal{O}\big(\tau_0^2a_0^{-k}\big)\mu'(r) \\ &\ge 2\tau(k-k_0)(r+1)^{2k_0-k-1}\varphi'(r) - \mathcal{O}\big(\tau_0^{-k\ell+2}\big)\mu'(r). \end{aligned}$$

Hence, taking τ_0 large enough, we can arrange the inequality

$$A(r) \geq 2\tau(k-k_0)(r+1)^{2k_0-k-1}\varphi'(r) - \frac{E}{4}\mu'(r) \tag{2.10}$$

for all $r < a$. Observe now that if $0 < r \leq a/2$, then

$$\varphi'(r) \geq \gamma\tau(r+1)^{-k} \tag{2.11}$$

with some constant $\gamma > 0$. By (2.10) and (2.11) we conclude

$$A(r) \geq \tilde{\gamma}\tau^2(r+1)^{-2(k-k_0)-1} - \frac{E}{4}\mu'(r) \tag{2.12}$$

for all $r \leq a/2$ with some constant $\tilde{\gamma} > 0$, and

$$A(r) \geq -\frac{E}{4}\mu'(r) \quad \text{for all } r \neq a. \tag{2.13}$$

We will now bound the function B_1 from above. Since the function p is decreasing, tending to zero, there is $b > 0$ such that

$$p(r) + (r+1)^{-\beta} \leq \frac{E}{9C} \quad \text{for } r \geq b.$$

Hence, for every $N > 0$, there is a constant $C_N > 0$ such that we have

$$\big(p(r) + (r+1)^{-\beta}\big)\mu'(r) \leq C_N(r+1)^{-N} + \frac{E}{9C}\mu'(r) \quad \text{for all } r \neq a. \tag{2.14}$$

Let $0 < r < a$. Then $\mu(r) < (r+1)^{2k}$, and in view of (2.14) with N big enough, we have

$$B_1(r) \leq \widetilde{C}(r+1)^{2k-\beta} + \frac{E}{9C}\mu'(r)$$

if V satisfies (1.3), and

$$B_1(r) \leq \widetilde{C}\theta^{-1+\alpha}(r+1)^{2k-\beta} + \frac{E}{9C}\mu'(r)$$

with $\beta = 4$ if V satisfies (1.8). Observe now that the choice of the parameters k, k_0 and θ guarantees that $\beta - 2k \geq 2(k-k_0)+1$ and $\theta^{-1+\alpha} = \theta^{4\alpha/3}h^{-2/3}$. Therefore, the above inequalities imply

$$B_1(r) \leq \mathcal{O}\big(\tau_0^{-2}\big)\tau^2(r+1)^{-2(k-k_0)-1} + \frac{E}{9C}\mu'(r) \quad \text{for } r \leq \frac{a}{2} \tag{2.15}$$

in both cases. Similarly, we get

$$B_1(r) \leq \mathcal{O}\big(\tau^2 a^{-\beta+1}\big)\mu'(r) + \frac{E}{9C}\mu'(r) \quad \text{for } \frac{a}{2} < r < a \tag{2.16}$$

and

$$B_1(r) \leq \mathcal{O}\big(\tau^2 a^{-\beta+2k+2s}\big)\mu'(r) + \frac{E}{9C}\mu'(r) \quad \text{for } r > a. \tag{2.17}$$

Since

$$\tau^2 a^{-\beta+1} < \tau^2 a^{-\beta+2k+2s} \leq \tau_0^2 a_0^{-\beta+2k+2s} = \tau_0^{-(\beta-2k-2s)\ell+2},$$

we obtain from (2.16) and (2.17),

$$B_1(r) \le \frac{E}{8C}\mu'(r) \quad \text{for } r > \frac{a}{2}, r \neq a, \tag{2.18}$$

provided τ_0 is taken large enough.

We will now bound the function B_2 from above. We will first consider the case when V satisfies (1.8). Let $0 < r \le a/2$. In view of (2.11), we have

$$\begin{aligned} B_2(r) &\lesssim \frac{\mu(r)\big(h^{-2}\theta^{2\alpha}(r+1)^{-2\beta}+\varphi''(r)^2\big)}{h^{-1}\varphi'(r)} \\ &\lesssim h^{-1}\theta^{2\alpha}\frac{\mu(r)(r+1)^{-2\beta}}{\varphi'(r)} + h\frac{\mu(r)\varphi''(r)^2}{\varphi'(r)} \\ &\lesssim \tau^{-1}\theta^{2\alpha}h^{-1}(r+1)^{3k-2\beta} + h\tau(r+1)^{k-2} \\ &\lesssim \tau_0^{-3}\tau^2(r+1)^{-2(k-k_0)-1} + \tau(r+1)^{k-2}, \end{aligned}$$

where we have used that $5k-2k_0 < 2\beta-1$. Since $3k-2k_0-1>0$, we have the inequality

$$(r+1)^{k-2} \le b^{3k-2k_0-1}(r+1)^{-2(k-k_0)-1} + b^{-k-1}(r+1)^{2k-1}$$

for every $b>1$. We take b such that $b^{3k-2k_0-1} = b_0\tau$, where $b_0>0$ is a small parameter independent of τ and h to be fixed below. Then the above inequality takes the form

$$\tau(r+1)^{k-2} \lesssim b_0\tau^2(r+1)^{-2(k-k_0)-1} + \tau^{-2(1-k+k_0)/(3k-2k_0-1)}\mu'(r) \lesssim b_0\tau^2(r+1)^{-2(k-k_0)-1} + \tau_0^{-1}\mu'(r).$$

Thus, taking τ_0 big enough depending on b_0, E and C, we get the bound

$$B_2(r) \le \mathcal{O}\big(\tau_0^{-1}+b_0\big)\tau^2(r+1)^{-2(k-k_0)-1} + \frac{E}{8C}\mu'(r) \quad \text{for } 0<r\le\frac{a}{2}. \tag{2.19}$$

When V satisfies (1.3), we have $3k-2k_0-1 \le 0$, and hence

$$\tau(r+1)^{k-2} \le \tau(r+1)^{-2(k-k_0)-1} \le \tau_0^{-1}\tau^2(r+1)^{-2(k-k_0)-1}.$$

Therefore, the inequality (2.19) still holds in this case.

Let us now see that

$$B_2(r) \le \frac{E}{8C}\mu'(r) \quad \text{for } r > \frac{a}{2}, r \neq a. \tag{2.20}$$

Let $a/2 < r < a$. Since in this case $\mu(r)/\mu'(r) = \mathcal{O}(r)$, we get the bound

$$\begin{aligned} B_2(r) &\lesssim \Big(\frac{\mu(r)}{\mu'(r)}\Big)^2\big(h^{-1}\theta^{\alpha}(r+1)^{-\beta}+|\varphi''(r)|\big)^2\mu'(r) \\ &\lesssim \big(h^{-2}\theta^{2\alpha}(r+1)^{2-2\beta}+\tau^2(r+1)^{-2k}\big)\mu'(r) \\ &\lesssim \big(h^{-2}a^{2-2\beta}+\tau^2a^{-2k}\big)\mu'(r) \\ &\lesssim \big(h^{2m(\beta-1)-2}a_0^{2-2\beta}+h^{2m-2/3}\tau_0^2a_0^{-2k}\big)\mu'(r) \\ &\lesssim \big(a_0^{2-2\beta}+\tau_0^2a_0^{-2k}\big)\mu'(r) \lesssim \big(\tau_0^{-2\ell(\beta-1)}+\tau_0^{-2k\ell+2}\big)\mu'(r), \end{aligned}$$

which clearly implies (2.20) in this case, provided τ_0 is taken big enough. Let $r > a$. Using (2.6) with $j = 1$, we get

$$\begin{aligned} B_2(r) &\lesssim \Big(\frac{\mu(r)}{\mu'(r)}\Big)^2 \big(h^{-1}\theta^\alpha (r+1)^{-\beta}\big)^2 \mu'(r) \\ &\lesssim h^{-2} a^{4k} (r+1)^{4s-2\beta} \mu'(r) \\ &\lesssim h^{-2} a^{4k+4s-2\beta} \mu'(r) \\ &\lesssim h^{2m(\beta-2k-2s)-2} a_0^{4k+4s-2\beta} \mu'(r) \\ &\lesssim a_0^{4k+4s-2\beta} \mu'(r) \lesssim \tau_0^{-2\ell(\beta-2k-2s)} \mu'(r), \end{aligned}$$

which again implies (2.20), provided τ_0 is taken big enough. Similarly, in the case when V satisfies (1.3), one concludes that the inequality (2.20) holds for all $r > 0$, $r \neq a$.

It is easy to see that for $r \le a/2$, the estimate (2.9) follows from (2.12), (2.15) and (2.19) by taking b_0 and τ_0^{-1} small enough, while for $r \ge a/2$, $r \ne a$, it follows from (2.13), (2.18) and (2.20). □

Remark 2.4. It is easy to see from the proof that when V satisfies (1.8), the inequality (2.9) holds as long as $\frac{1}{2} \le k \le 1$, $k_0 = k - \frac{1}{2}$. The choice $k = 1$, however, provides the best resolvent bound in the semiclassical regime, that is, for $0 < h \le h_0$ with some constant $0 < h_0 \ll 1$. When $h_0 < h \le 1$, the choice of k does not really matter, because in this case $g_s^{\pm}(h, \varepsilon)$ is bounded from above by a constant. For example, we may take $k = \frac{1}{2}$ and $k_0 = 0$.

The following lemmas will play a crucial role in the proof of the Carleman estimate (4.6) when $d = 2$:

Lemma 2.5. *Given any constants $C, r_0 > 0$, there exists a positive constant $\tau_1 = \tau_1(C, E, r_0)$ such that for τ satisfying (2.7) with $\tau_0 \ge \tau_1$ and for all $0 < h \le h_0$, $0 < h_0 < 1$ being a constant depending on E, r_0 and τ_0, we have the inequality*

$$A(r) - h^2 r^{-3}\mu(r) - C B(r) \ge -\frac{2E}{3}\mu'(r) \tag{2.21}$$

for all $r \ge r_0$, $r \ne a$.

Proof. For $r_0 \le r < a$, we have

$$h^2 r^{-3}\mu(r) \lesssim h^2 (r+1)^{-3}\mu(r) \lesssim h^2 (r+1)^{-2}\mu'(r) \le \frac{E}{6}\mu'(r),$$

provided h is taken small enough. For $r > a$, in view of (2.6) with $j = 1$, we have

$$h^2 r^{-3}\mu(r) \lesssim h^2 a^{2k}(r+1)^{2s-3}\mu'(r) \lesssim h^2 a^{2k+2s-3}\mu'(r) \lesssim h^{2-m(2k+2s-3)} a_0^{2k+2s-3}\mu'(r) \le \frac{E}{6}\mu'(r),$$

provided h is taken small enough, depending on a_0. Clearly, (2.21) follows from these inequalities and (2.9). □

It is easy to see from the proof that when V satisfies (1.3), the inequality (2.21) holds also for $h_0 < h \le 1$. This is no longer true when V satisfies (1.8), because in this case $2k + 2s - 3$ does not have the right sign. Therefore, to make (2.21) hold for h not necessarily small, we need to make a new choice of the parameters k and k_0 in order to change the sign of $2k + 2s - 3$ and for which Lemma 2.3 still holds.

Thus, in view of Remark 2.4, in the semiclassical regime ($0 < h \le h_0$) we take $k = 1$, $k_0 = \frac{1}{2}$, and in the classical regime ($h_0 < h \le 1$) we take $k = \frac{1}{2}$, $k_0 = 0$. To cover the second case we need the following:

Lemma 2.6. *If V satisfies* (1.8), *we take $k = \frac{1}{2}$ and $k_0 = 0$. Then, given any constants $C, r_0 > 0$, there exists a positive constant $\tau_1 = \tau_1(C, E, r_0)$ such that for τ satisfying* (2.7) *with $\tau_0 \ge \tau_1$ the inequality* (2.21) *holds for all $r \ge r_0$, $r \ne a$, and all $0 < h \le 1$.*

Proof. For $r_0 \le r \le a/2$, we have

$$h^2 r^{-3}\mu(r) \lesssim (r+1)^{-3}\mu(r) \lesssim (r+1)^{-3+2k} \lesssim (r+1)^{-2(k-k_0)-1}.$$

For $a/2 < r < a$, we have

$$h^2 r^{-3}\mu(r) \lesssim (r+1)^{-2}\mu'(r) \lesssim a^{-2}\mu'(r) \lesssim a_0^{-2}\mu'(r) \le \frac{E}{6}\mu'(r),$$

provided a_0 is taken big enough. For $r > a$, we have

$$h^2 r^{-3}\mu(r) \lesssim a^{2k}(r+1)^{2s-3}\mu'(r) \lesssim a^{2k+2s-3}\mu'(r) \lesssim a_0^{2k+2s-3}\mu'(r) \le \frac{E}{6}\mu'(r),$$

provided a_0 is taken big enough. Then, (2.21) easily follows from these inequalities and Remark 2.4. □

3. Carleman estimates for Hölder potentials on bounded domains

Throughout this section $X \subset \mathbb{R}^d$, $d \ge 2$, will be a bounded, connected domain with a smooth boundary ∂X. Introduce the operator

$$P(h) = -h^2\Delta + V(x),$$

where $0 < h \le 1$ is a semiclassical parameter and $V \in L^\infty(X)$ is a real-valued potential. Let $U \subset X$, $U \ne \varnothing$, be an arbitrary open domain, independent of h, such that $\partial U \cap \partial X = \varnothing$, and let $z \in \mathbb{C}$, $|z| \le C_0$, $C_0 > 0$ be a constant independent of h. We will also denote by H_h^1 the Sobolev space equipped with the semiclassical norm. Given any $0 < \alpha \le 1$, denote by $C^\alpha(\overline{X})$ the space of all functions a such that

$$\|a\|_{C^\alpha} := \sup_{x', x \in \overline{X}\,:\,0<|x-x'|\le 1} \frac{|a(x)-a(x')|}{|x-x'|^\alpha} < +\infty.$$

Theorem 3.1. *Let $V \in C^\alpha(\overline{X})$ with $0 < \alpha \le 1$. Then, there exists a positive constant γ depending on U, $\|V\|_{C^\alpha}$ and C_0, but independent of h, such that for all $0 < h \le 1$, we have the estimate*

$$\|u\|_{H_h^1(X)} \le e^{\gamma h^{-4/(\alpha+3)}}\|(P(h)-z)u\|_{L^2(X)} + e^{\gamma h^{-4/(\alpha+3)}}\|u\|_{H_h^1(U)} \tag{3.1}$$

for every $u \in H^2(X)$ such that $u|_{\partial X} = 0$.

It is proved in Section 2 of [Vodev 2020b] that for complex-valued potentials $V \in L^\infty(X)$, the estimate (3.1) holds with $\alpha = 0$. The proof is based on the local Carleman estimates proved in [Lebeau and Robbiano 1995]. We will follow the same strategy in the case of Hölder potentials as well. For such potentials we will get new local Carleman estimates by making use of the results of [Lebeau and Robbiano 1995]. To be more precise, we let $W \subset X$ be a small open domain and let x be local coordinates in W. If $\Gamma := \overline{W} \cap \partial X$ is not empty, we choose $x = (x_1, x')$, $x_1 > 0$ being the normal coordinate in W and x'

the tangential ones. Thus, in these coordinates Γ is given by $\{x_1 = 0\}$. Let $\phi, \phi_1 \in C^\infty(\overline{W})$ be real-valued functions such that $\operatorname{supp}\phi \subset \operatorname{supp}\phi_1 \subset \overline{W}$, $\phi_1 = 1$ on $\operatorname{supp}\phi$. When $V \in C^\alpha(\overline{X})$ with $0 < \alpha < 1$, we approximate the function $\phi_1 V$ by the smooth function

$$V_\theta(x) = \theta^{-1} \int_X \rho\Big(\frac{x'-x}{\theta}\Big)(\phi_1 V)(x')\, dx',$$

where $\rho \in C_0^\infty(|x| \le 1)$ is a real-valued function such that $\int_{\mathbb{R}^d} \rho(x)\, dx = 1$ and $0 < \theta < 1$ is a small parameter to be fixed later on. The fact that $V \in C^\alpha(\overline{X})$ implies the bounds

$$|(\phi_1 V)(x) - V_\theta(x)| \lesssim \theta^\alpha, \tag{3.2}$$

$$|\partial_x^\beta V_\theta(x)| \lesssim \theta^{\alpha-1}, \tag{3.3}$$

for all multi-indices β such that $|\beta| = 1$. Set $\widetilde{V} = \theta^{1-\alpha}(V_\theta - z)$ if $V \in C^\alpha(\overline{X})$ with $0 < \alpha < 1$ and $\widetilde{V} = V - z$ if $V \in C^1(\overline{X})$. In view of (3.2) and (3.3), we have $\partial_x^\beta \widetilde{V}(x) = \mathcal{O}(1)$ uniformly in θ, for all multi-indices β such that $|\beta| \le 1$.

Now, let $\psi \in C^\infty(\overline{W})$ be a real-valued function independent of h and θ such that

$$\nabla\psi \neq 0 \quad \text{in } \overline{W}. \tag{3.4}$$

If $\Gamma \neq \varnothing$, we also suppose that

$$\frac{\partial\psi}{\partial x_1}(0, x') > 0 \quad \text{for all } x'. \tag{3.5}$$

We set $\varphi = e^{\lambda\psi}$, where $\lambda > 0$ is a big parameter to be fixed later on, independent of h and θ. Let $p(x,\xi) \in C^\infty(T^*W)$ be the principal symbol of the operator $-\Delta$, and let $0 < \tilde{h} \ll 1$ be a new semiclassical parameter. Then the principal symbol, $\tilde{p}_\varphi$, of the operator

$$e^{\varphi/\tilde{h}}\big(-\tilde{h}^2\Delta + \widetilde{V}\,\big)e^{-\varphi/\tilde{h}}$$

is given by the formula

$$\tilde{p}_\varphi(x,\xi) = p(x, \xi + i\nabla\varphi(x)) + \widetilde{V}(x).$$

An easy computation shows that given any constant $C > 0$, there is $\lambda = \lambda(C)$ such that the condition (3.4) for the function ψ implies the following condition for the function φ:

$$\{\operatorname{Re}\tilde{p}_\varphi, \operatorname{Im}\tilde{p}_\varphi\}(x,\xi) \ge c_1 \quad \text{for } |\xi| \le C, \tag{3.6}$$

with some constant $c_1 > 0$ independent of θ. On the other hand, if C is taken large enough, we can arrange the lower bound

$$|\tilde{p}_\varphi(x,\xi)| \ge c_2|\xi|^2 \quad \text{for } |\xi| \ge C, \tag{3.7}$$

with some constant $c_2 > 0$ independent of θ. If $\Gamma \neq \varnothing$, the condition (3.5) implies

$$\frac{\partial\varphi}{\partial x_1}(0, x') > 0 \quad \text{for all } x'. \tag{3.8}$$

Now, we are in position to use Propositions 1 and 2 of [Lebeau and Robbiano 1995], where the proof is based on the properties (3.6), (3.7) and (3.8).

Proposition 3.2. *Let the function u be as in Theorem 3.1. Then there exist constants $C_1, \tilde{h}_0 > 0$ such that for all $0 < \tilde{h} \le \tilde{h}_0$, we have the estimate*

$$\int_X \big(|\phi u|^2 + |\tilde{h}\nabla(\phi u)|^2\big) e^{2\varphi/\tilde{h}}\, dx \le C_1 \tilde{h}^{-1} \int_X \big|\big(-\tilde{h}^2\Delta + \widetilde{V}\big)(\phi u)\big|^2 e^{2\varphi/\tilde{h}}\, dx. \tag{3.9}$$

We take $\tilde{h} = h\theta^{(1-\alpha)/2}$ when $\alpha < 1$, and we rewrite the inequality (3.9) as follows:

$$\begin{aligned}
&\int_X \big(|\phi u|^2 + \theta^{1-\alpha}|h\nabla(\phi u)|^2\big) e^{2\varphi/h\theta^{(1-\alpha)/2}}\, dx \\
&\quad\le C_1 h^{-1}\theta^{3(1-\alpha)/2} \int_X |(-h^2\Delta + V_\theta - z)(\phi u)|^2 e^{2\varphi/h\theta^{(1-\alpha)/2}}\, dx \\
&\quad\le C_1 h^{-1}\theta^{3(1-\alpha)/2} \int_X |(P(h) - z)(\phi u)|^2 e^{2\varphi/h\theta^{(1-\alpha)/2}}\, dx \\
&\qquad\qquad + C_1 h^{-1}\theta^{3(1-\alpha)/2} \sup|\phi_1 V - V_\theta|^2 \int_X |\phi u|^2 e^{2\varphi/h\theta^{(1-\alpha)/2}}\, dx \\
&\quad\le C_1 h^{-1}\theta^{3(1-\alpha)/2} \int_X |(P(h) - z)(\phi u)|^2 e^{2\varphi/h\theta^{(1-\alpha)/2}}\, dx + C_2 h^{-1}\theta^{(3+\alpha)/2} \int_X |\phi u|^2 e^{2\varphi/h\theta^{(1-\alpha)/2}}\, dx.
\end{aligned}$$

We now take $\theta = h^{2/(\alpha+3)}\kappa^{2/(1-\alpha)}$, where $\kappa > 0$ is a small parameter independent of h. Thus, taking κ small enough we can absorb the last term in the right-hand side of the above inequality. When $\alpha = 1$, we take $\tilde{h} = h\kappa$. Thus, we deduce the following from Proposition 3.2:

Proposition 3.3. *Let the function u be as in Theorem 3.1. Then there exist constants $\widetilde{C}, \kappa_0 > 0$ such that for all $0 < \kappa \le \kappa_0$ and all $0 < h \le 1$, we have the estimate*

$$\int_X \big(|\phi u|^2 + |h\nabla(\phi u)|^2\big) e^{2\varphi/\kappa h^{4/(\alpha+3)}}\, dx \le \widetilde{C}\kappa h^{-2(\alpha+1)/(\alpha+3)} \int_X |(P(h) - z)(\phi u)|^2 e^{2\varphi/\kappa h^{4/(\alpha+3)}}\, dx. \tag{3.10}$$

Now Theorem 3.1 follows from Proposition 3.3 in precisely the same way as in Section 2 of [Vodev 2020b], where the analysis is carried out in the particular case $\alpha = 0$. It is an easy observation that the general case requires no changes in the arguments, and therefore we omit the details.

4. Resolvent estimates

The following global Carlemann estimate is similar to that of [Vodev 2020c, Section 3] and can be proved in the same way. The proof will be carried out in Section 5. In what follows, we set $\mathcal{D}_r = -ih\partial_r$:

Theorem 4.1. *Let $d \ge 3$, and let the potential V satisfy* (1.1). *Let also V satisfy either* (1.3) *or* (1.8), *and let s satisfy* (2.4). *Then, for all $0 < h \le 1$, $0 < \varepsilon \le 1$ and for all functions $f \in H^2(\mathbb{R}^d)$ such that*

$$(|x|+1)^s (P(h) - E \pm i\varepsilon) f \in L^2(\mathbb{R}^d),$$

we have the estimate

$$\begin{aligned}\|(|x|+1)^{-s}e^{\varphi/h}f\|_{L^2(\mathbb{R}^d)}+\|(|x|+1)^{-s}e^{\varphi/h}\mathcal{D}_r f\|_{L^2(\mathbb{R}^d)}\\ \le Ca^2h^{-1}\|(|x|+1)^{s}e^{\varphi/h}(P(h)-E\pm i\varepsilon)f\|_{L^2(\mathbb{R}^d)}+C\tau a(\varepsilon/h)^{1/2}\|e^{\varphi/h}f\|_{L^2(\mathbb{R}^d)},\end{aligned}\tag{4.1}$$

with a constant $C>0$ *independent of* h, ε *and* f.

Theorems 1.1 and 1.2 can be obtained from Theorem 4.1 in the same way as in Section 4 of [Vodev 2020c]. We will sketch the proof for the sake of completeness. It follows from the estimate (4.1) and Lemma 2.2 that for $0<h\le 1$ and s satisfying (2.4), we have the estimate

$$\|(|x|+1)^{-s}f\|_{L^2}\le M\|(|x|+1)^{s}(P(h)-E\pm i\varepsilon)f\|_{L^2}+M\varepsilon^{1/2}\|f\|_{L^2},\tag{4.2}$$

where $M>0$ is given by

$$\log M=\begin{cases}Ch^{-1} & \text{if } V \text{ satisfies (1.3)},\\ Ch^{-4/(\alpha+3)}\log(h^{-1})+C & \text{if } V \text{ satisfies (1.8)},\end{cases}$$

with a constant $C>0$ independent of h and ε. On the other hand, since the operator $P(h)$ is symmetric, we have

$$\begin{aligned}\varepsilon\|f\|_{L^2}^2&=\pm\operatorname{Im}\langle(P(h)-E\pm i\varepsilon)f,f\rangle_{L^2}\\&\le(2M)^{-2}\|(|x|+1)^{-s}f\|_{L^2}^2+(2M)^2\|(|x|+1)^{s}(P(h)-E\pm i\varepsilon)f\|_{L^2}^2,\end{aligned}$$

which yields

$$M\varepsilon^{1/2}\|f\|_{L^2}\le\tfrac12\|(|x|+1)^{-s}f\|_{L^2}+2M^2\|(|x|+1)^{s}(P(h)-E\pm i\varepsilon)f\|_{L^2}.\tag{4.3}$$

By (4.2) and (4.3), we get

$$\|(|x|+1)^{-s}f\|_{L^2}\le 4M^2\|(|x|+1)^{s}(P(h)-E\pm i\varepsilon)f\|_{L^2}.\tag{4.4}$$

It follows from (4.4) that the resolvent estimate

$$\left\|(|x|+1)^{-s}(P(h)-E\pm i\varepsilon)^{-1}(|x|+1)^{-s}\right\|_{L^2\to L^2}\le 4M^2\tag{4.5}$$

holds for all $0<h\le 1$ and s satisfying (2.4), and hence for all $s>\frac12$ independent of h. Clearly, (4.5) implies the desired bounds for $g_s^{\pm}$.

Given any $r_0>0$, we denote $Y_{r_0}:=\{x\in\mathbb{R}^d:|x|\ge r_0\}$, and we let $\eta_{r_0}\in C^\infty(\mathbb{R})$ be such that $\eta_{r_0}(r)=0$ for $r\le r_0/3$ and $\eta_{r_0}(r)=1$ for $r\ge r_0/2$. We set $V_\eta(x):=\eta_{r_0}(|x|)V(x)$. To prove Theorem 1.3 we need the following:

Theorem 4.2. *Let* $d\ge 3$, *and let the potential* V *satisfy* (1.1) *for* $|x|\ge r_0$. *Let also* V_η *satisfy either* (1.3) *or* (1.8), *and let* s *satisfy* (2.4). *Then, for all* $0<h\le 1$, $0<\varepsilon\le 1$ *and for all functions* $f\in H^2(Y_{r_0})$ *such that* $f=\partial_r f=0$ *on* ∂Y_{r_0} *and*

$$(|x|+1)^{s}(P(h)-E\pm i\varepsilon)f\in L^2(Y_{r_0}),$$

we have the estimate

$$\|(|x|+1)^{-s}e^{\varphi/h}f\|_{L^2(Y_{r_0})}+\|(|x|+1)^{-s}e^{\varphi/h}\mathcal{D}_r f\|_{L^2(Y_{r_0})} \\ \le Ca^2h^{-1}\|(|x|+1)^{s}e^{\varphi/h}(P(h)-E\pm i\varepsilon)f\|_{L^2(Y_{r_0})}+C\tau a(\varepsilon/h)^{1/2}\|e^{\varphi/h}f\|_{L^2(Y_{r_0})}, \quad (4.6)$$

with a constant $C>0$ independent of h, ε and f.

Let $d=2$. If V_η satisfies (1.8) *and $k=1$, $k_0=\frac{1}{2}$, then* (4.6) *holds for $0<h\le h_0$ with some constant $0<h_0\ll 1$ depending on τ_0. If V_η satisfies* (1.8) *and $k=\frac{1}{2}$, $k_0=0$, or V_η satisfies* (1.3), *then* (4.6) *holds for all $0<h\le 1$.*

The proof of Theorem 4.2 is similar to that of Theorem 4.1 with some suitable modifications when $d=2$ and will be carried out in Section 5.

Theorem 1.3 can be derived from Theorems 3.1 and 4.2 in a way similar to the one developed in Section 5 of [Vodev 2020b]. Let $r_0>0$ be such that $Y_{r_0/3}\subset\Omega$. Fix r_j, $j=1,2,3,4$, such that $r_0<r_1<r_2<r_3<r_4$. Choose functions $\psi_1,\psi_2\in C^\infty(\mathbb{R}^d)$, depending only on the radial variable r, such that $\psi_1=1$ in $\mathbb{R}^d\setminus Y_{r_1}$, $\psi_1=0$ in Y_{r_2}, $\psi_2=1$ in $\mathbb{R}^d\setminus Y_{r_3}$, $\psi_2=0$ in Y_{r_4}. If s satisfies (2.4), we choose a function $\chi_s\in C^\infty(\overline{\Omega})$, $\chi_s>0$, such that $\chi_s(x)=|x|^{-s}$ on Y_{r_0}. Let $f\in H^2(\Omega)$ be such that $\chi_s^{-1}(P(h)-E\pm i\varepsilon)f\in L^2(\Omega)$ and $f|_{\partial\Omega}=0$. Set

$$\mathcal{Q}_0=\|\chi_s^{-1}(P(h)-E\pm i\varepsilon)f\|_{L^2(\Omega)},$$
$$\mathcal{Q}_1=\|f\|_{L^2(Y_{r_1}\setminus Y_{r_2})}+\|\mathcal{D}_r f\|_{L^2(Y_{r_1}\setminus Y_{r_2})},$$
$$\mathcal{Q}_2=\|f\|_{L^2(Y_{r_3}\setminus Y_{r_4})}+\|\mathcal{D}_r f\|_{L^2(Y_{r_3}\setminus Y_{r_4})},$$

and observe that

$$\|[P(h),\psi_j]f\|_{L^2}\lesssim\mathcal{Q}_j,\quad j=1,2.$$

We now apply Theorem 3.1 to the function $\psi_2 f$ with $X=\Omega\setminus Y_{r_4}$ and $U\subset X$ such that $U\cap\operatorname{supp}\psi_2=\varnothing$. Thus, we obtain

$$\|f\|_{H_h^1(\Omega\setminus Y_{r_3})}\le\|\psi_2 f\|_{H_h^1(\Omega\setminus Y_{r_4})} \\ \le e^{\gamma h^{-4/(\alpha+3)}}\|(P(h)-E\pm i\varepsilon)\psi_2 f\|_{L^2(\Omega\setminus Y_{r_4})} \\ \le e^{\gamma h^{-4/(\alpha+3)}}\|(P(h)-E\pm i\varepsilon)f\|_{L^2(\Omega\setminus Y_{r_4})}+e^{\gamma h^{-4/(\alpha+3)}}\mathcal{Q}_2, \quad (4.7)$$

with a constant $\gamma>0$ independent of h and τ_0. In particular, (4.7) implies

$$\mathcal{Q}_1\le e^{\gamma h^{-4/(\alpha+3)}}\mathcal{Q}_0+e^{\gamma h^{-4/(\alpha+3)}}\mathcal{Q}_2. \quad (4.8)$$

On the other hand, it is clear that if V satisfies (1.10) with $\alpha=1$ and $\beta>1$ (respectively, $0<\alpha<1$ and $\beta=4$), then V_η satisfies (1.3) (respectively, (1.8)). Therefore, we can apply Theorem 4.2 to the function $(1-\psi_1)f$ to obtain

$$\begin{aligned}
&\|(|x|+1)^{-s}e^{\varphi/h}f\|_{L^2(Y_{r_2})}+\|(|x|+1)^{-s}e^{\varphi/h}\mathcal{D}_r f\|_{L^2(Y_{r_2})}\\
&\quad\le \|(|x|+1)^{-s}e^{\varphi/h}(1-\psi_1)f\|_{L^2(Y_{r_1})}+\|(|x|+1)^{-s}e^{\varphi/h}\mathcal{D}_r(1-\psi_1)f\|_{L^2(Y_{r_1})}\\
&\quad\le Ca^2h^{-1}\|(|x|+1)^{s}e^{\varphi/h}(P(h)-E\pm i\varepsilon)(1-\psi_1)f\|_{L^2(Y_{r_1})}+C\tau a(\varepsilon/h)^{1/2}\|e^{\varphi/h}f\|_{L^2(Y_{r_1})}\\
&\quad\le Ca^2h^{-1}\|(|x|+1)^{s}e^{\varphi/h}(P(h)-E\pm i\varepsilon)f\|_{L^2(Y_{r_1})}+Ca^2h^{-1}e^{\varphi(r_2)/h}\mathcal{Q}_1\\
&\qquad\qquad +C\tau a(\varepsilon/h)^{1/2}\|e^{\varphi/h}f\|_{L^2(Y_{r_1})} \qquad (4.9)
\end{aligned}$$

for all $0<h\le 1$. In particular, (4.9) implies

$$e^{\varphi(r_3)/h}\mathcal{Q}_2\le Ca^2h^{-1}e^{\max\varphi/h}\mathcal{Q}_0+C\tau a(\varepsilon/h)^{1/2}e^{\max\varphi/h}\|f\|_{L^2(\Omega)}+Ca^2h^{-1}e^{\varphi(r_2)/h}\mathcal{Q}_1. \qquad (4.10)$$

We have

$$\varphi(r_3)-\varphi(r_2)=\tau\int_{r_2}^{r_3}\big((r+1)^{-k}-(a+1)^{-k}\big)\,dr\ge c\tau,$$

with some constant $c>0$. We deduce from (4.10)

$$\begin{aligned}
\mathcal{Q}_2\le \exp\Big(\tilde\beta h^{-4/(\alpha+3)}+\frac{\max\varphi}{h}\Big)\mathcal{Q}_0+\varepsilon^{1/2}\exp\Big(\tilde\beta h^{-4/(\alpha+3)}+\frac{\max\varphi}{h}\Big)\|f\|_{L^2(\Omega)}\\
+\tau_0^{2\ell}\exp\big((\beta-c\tau_0)h^{-4/(\alpha+3)}\big)\mathcal{Q}_1, \qquad (4.11)
\end{aligned}$$

with a constant $\tilde\beta>0$ independent of h and a constant $\beta>0$ independent of h and τ_0. Combining (4.8) and (4.11) we get

$$\begin{aligned}
\mathcal{Q}_2\le \exp\Big((\tilde\beta+\gamma)h^{-4/(\alpha+3)}+\frac{\max\varphi}{h}\Big)\mathcal{Q}_0+\varepsilon^{1/2}\exp\Big(\tilde\beta h^{-4/(\alpha+3)}+\frac{\max\varphi}{h}\Big)\|f\|_{L^2(\Omega)}\\
+\tau_0^{2\ell}\exp\big((\beta+\gamma-c\tau_0)h^{-4/(\alpha+3)}\big)\mathcal{Q}_2. \qquad (4.12)
\end{aligned}$$

Taking τ_0 big enough, independent of h, we can arrange that

$$\tau_0^{2\ell}\exp\big((\beta+\gamma-c\tau_0)h^{-4/(\alpha+3)}\big)\le\tau_0^{2\ell}\exp\big(-c\tau_0h^{-4/(\alpha+3)}/2\big)\le\tau_0^{2\ell}\exp\big(-c\tau_0/2\big)\le\tfrac12$$

for all $0<h\le 1$. Thus, we can absorb the last term in the right-hand side of (4.12) to conclude that

$$\mathcal{Q}_1+\mathcal{Q}_2\le\exp\Big(\beta_1h^{-4/(\alpha+3)}+\frac{\max\varphi}{h}\Big)\mathcal{Q}_0+\varepsilon^{1/2}\exp\Big(\beta_1h^{-4/(\alpha+3)}+\frac{\max\varphi}{h}\Big)\|f\|_{L^2(\Omega)}, \qquad (4.13)$$

with a constant $\beta_1>0$ independent of h. By (4.7), (4.9) and (4.13) we obtain

$$\|\chi_s f\|_{L^2(\Omega)}\le N\mathcal{Q}_0+\varepsilon^{1/2}N\|f\|_{L^2(\Omega)}, \qquad (4.14)$$

where

$$N=\exp\Big(\beta_2h^{-4/(\alpha+3)}+\frac{\max\varphi}{h}\Big),$$

with a constant $\beta_2 > 0$ independent of h. In the same way as above, using the fact that the operator $P(h)$ is symmetric, we get from (4.14) that the resolvent estimate

$$\left\| \chi_s (P(h) - E \pm i\varepsilon)^{-1} \chi_s \right\|_{L^2(\Omega) \to L^2(\Omega)} \leq 4N^2 \tag{4.15}$$

holds for all $0 < h \leq 1$, $0 < \varepsilon \leq 1$ and s satisfying (2.4), which together with Lemma 2.2 clearly imply the desired bound.

5. Proofs of Theorems 4.1 and 4.2

The main point is to work with the polar coordinates $(r, w) \in \mathbb{R}^+ \times \mathbb{S}^{d-1}$, $r = |x|$, $w = x/|x|$ and to use that $L^2(\mathbb{R}^d) = L^2(\mathbb{R}^+ \times \mathbb{S}^{d-1}, r^{d-1}\, dr\, dw)$. In what follows in this section, we denote by $\|\cdot\|$ and $\langle \cdot, \cdot \rangle$ the norm and the scalar product in $L^2(\mathbb{S}^{d-1})$. We will make use of the identity

$$r^{(d-1)/2} \Delta r^{-(d-1)/2} = \partial_r^2 + \frac{\widetilde{\Delta}_w}{r^2}, \tag{5.1}$$

where $\widetilde{\Delta}_w = \frac{1}{4}(d-1)(d-3)$ and Δ_w denotes the negative Laplace–Beltrami operator on $\mathbb{S}^{d-1}$. Set $u = r^{(d-1)/2} e^{\varphi/h} f$ and

$$\mathcal{P}^{\pm}(h) = r^{(d-1)/2}(P(h) - E \pm i\varepsilon) r^{-(d-1)/2},$$
$$\mathcal{P}_{\varphi}^{\pm}(h) = e^{\varphi/h} \mathcal{P}^{\pm}(h) e^{-\varphi/h}.$$

Using (5.1) we can write the operator $\mathcal{P}^{\pm}(h)$ in the coordinates (r, w) as follows:

$$\mathcal{P}^{\pm}(h) = \mathcal{D}_r^2 + \frac{\Lambda_w}{r^2} - E \pm i\varepsilon + V,$$

where we have put $\mathcal{D}_r = -ih\partial_r$ and $\Lambda_w = -h^2 \widetilde{\Delta}_w$. Since the function φ depends only on the variable r, we get

$$\mathcal{P}_{\varphi}^{\pm}(h) = \mathcal{D}_r^2 + \frac{\Lambda_w}{r^2} - E \pm i\varepsilon - \varphi'^2 + h\varphi'' + 2i\varphi' \mathcal{D}_r + V.$$

We write $V = V_L + V_S$ with $V_L := V_\theta$ and $V_S := V - V_\theta$ if V satisfies (1.8), and $V_L := V$ and $V_S := 0$ if V satisfies (1.3). For $r > 0$, $r \neq a$, introduce the function

$$F(r) = -\langle (r^{-2}\Lambda_w - E - \varphi'(r)^2 + V_L(r, \cdot)) u(r, \cdot), u(r, \cdot) \rangle + \|\mathcal{D}_r u(r, \cdot)\|^2,$$

where $V_L(r, w) := V_L(rw)$. Then its first derivative is given by

$$\begin{aligned} F'(r) = {} & \frac{2}{r} \langle r^{-2}\Lambda_w u(r, \cdot), u(r, \cdot) \rangle + ((\varphi')^2 - V_L)' \|u(r, \cdot)\|^2 - 2h^{-1} \operatorname{Im} \langle \mathcal{P}_{\varphi}^{\pm}(h) u(r, \cdot), \mathcal{D}_r u(r, \cdot) \rangle \\ & \pm 2\varepsilon h^{-1} \operatorname{Re} \langle u(r, \cdot), \mathcal{D}_r u(r, \cdot) \rangle + 4h^{-1}\varphi' \|\mathcal{D}_r u(r, \cdot)\|^2 + 2h^{-1} \operatorname{Im} \langle (V_S + h\varphi'') u(r, \cdot), \mathcal{D}_r u(r, \cdot) \rangle. \end{aligned}$$

Thus, we obtain the identity

$$\begin{aligned}(\mu F)' &= \mu' F + \mu F' \\ &= (2r^{-1}\mu - \mu')\langle r^{-2}\Lambda_w u(r,\cdot), u(r,\cdot)\rangle + (E\mu' + (\mu(\varphi')^2 - \mu V_L)')\|u(r,\cdot)\|^2 \\ &\qquad - 2h^{-1}\mu \operatorname{Im}\langle \mathcal{P}_\varphi^{\pm}(h)u(r,\cdot), \mathcal{D}_r u(r,\cdot)\rangle \pm 2\varepsilon h^{-1}\mu \operatorname{Re}\langle u(r,\cdot), \mathcal{D}_r u(r,\cdot)\rangle \\ &\qquad + 2h^{-1}\mu \operatorname{Im}\langle (V_S + h\varphi'')u(r,\cdot), \mathcal{D}_r u(r,\cdot)\rangle.\end{aligned}$$

Using that $\Lambda_w \geq 0$ as long as $d \geq 3$ together with (2.5), we get the inequality

$$\begin{aligned}&\mu' F + \mu F' \\ &\geq (E\mu' + (\mu(\varphi')^2 - \mu V_L)')\|u(r,\cdot)\|^2 + (\mu' + 4h^{-1}\varphi'\mu)\|\mathcal{D}_r u(r,\cdot)\|^2 \\ &\quad - \frac{3h^{-2}\mu^2}{\mu'}\|\mathcal{P}_\varphi^{\pm}(h)u(r,\cdot)\|^2 - \frac{\mu'}{3}\|\mathcal{D}_r u(r,\cdot)\|^2 - \varepsilon h^{-1}\mu\big(\|u(r,\cdot)\|^2 + \|\mathcal{D}_r u(r,\cdot)\|^2\big) \\ &\quad - 3h^{-2}\mu^2(\mu' + 4h^{-1}\varphi'\mu)^{-1}\|(V_S + h\varphi'')u(r,\cdot)\|^2 - \frac{1}{3}(\mu' + 4h^{-1}\varphi'\mu)\|\mathcal{D}_r u(r,\cdot)\|^2 \\ &\geq (E\mu' + (\mu(\varphi')^2)' - T_L\mu - Z_L\mu')\|u(r,\cdot)\|^2 + \frac{\mu'}{3}\|\mathcal{D}_r u(r,\cdot)\|^2 - \frac{3h^{-2}\mu^2}{\mu'}\|\mathcal{P}_\varphi^{\pm}(h)u(r,\cdot)\|^2 \\ &\quad - \varepsilon h^{-1}\mu\big(\|u(r,\cdot)\|^2 + \|\mathcal{D}_r u(r,\cdot)\|^2\big) - 3h^{-2}\mu^2(\mu' + 4h^{-1}\varphi'\mu)^{-1}(Q_S + h|\varphi''|)^2\|u(r,\cdot)\|^2,\end{aligned}$$

where

$$T_L = \mathcal{O}\big((r+1)^{-\beta}\big), \quad Z_L = p(r), \quad Q_S = 0$$

if V satisfies (1.3),

$$T_L = \mathcal{O}\big(\theta^{-1+\alpha}(r+1)^{-4}\big), \quad Z_L = p(r) + \mathcal{O}\big((r+1)^{-4}\big), \quad Q_S = \mathcal{O}\big(\theta^{\alpha}(r+1)^{-4}\big),$$

if V satisfies (1.8), and we have used the bounds (2.1),(2.2) and (2.3) in the second case. Hence, we can rewrite the above inequality in the form

$$\begin{aligned}\mu' F + \mu F' &\geq \big(E\mu' + A(r) - CB(r)\big)\|u(r,\cdot)\|^2 + \frac{\mu'}{3}\|\mathcal{D}_r u(r,\cdot)\|^2 \\ &\quad - \frac{3h^{-2}\mu^2}{\mu'}\|\mathcal{P}_\varphi^{\pm}(h)u(r,\cdot)\|^2 - \varepsilon h^{-1}\mu\big(\|u(r,\cdot)\|^2 + \|\mathcal{D}_r u(r,\cdot)\|^2\big),\end{aligned}$$

with a suitable constant $C > 0$. Now we use Lemma 2.3 to conclude that

$$\begin{aligned}\mu' F + \mu F' &\geq \frac{E}{2}\mu'\|u(r,\cdot)\|^2 + \frac{\mu'}{3}\|\mathcal{D}_r u(r,\cdot)\|^2 - \frac{3h^{-2}\mu^2}{\mu'}\|\mathcal{P}_\varphi^{\pm}(h)u(r,\cdot)\|^2 \\ &\quad - \varepsilon h^{-1}\mu\big(\|u(r,\cdot)\|^2 + \|\mathcal{D}_r u(r,\cdot)\|^2\big). \qquad (5.2)\end{aligned}$$

We integrate this inequality with respect to r and use that $\mu(0) = 0$. We have

$$\int_0^\infty (\mu' F + \mu F')\, dr = 0.$$

Thus, we obtain the estimate

$$\frac{E}{2}\int_0^\infty \mu'\|u(r,\cdot)\|^2\,dr+\int_0^\infty \frac{\mu'}{3}\|\mathcal{D}_r u(r,\cdot)\|^2\,dr \le 3h^{-2}\int_0^\infty \frac{\mu^2}{\mu'}\|\mathcal{P}_\varphi^\pm(h)u(r,\cdot)\|^2\,dr$$
$$+\varepsilon h^{-1}\int_0^\infty \mu\big(\|u(r,\cdot)\|^2+\|\mathcal{D}_r u(r,\cdot)\|^2\big)\,dr. \quad (5.3)$$

Using that $\mu=\mathcal{O}(a^2)$ together with (2.6), we get from (5.3)

$$\int_0^\infty (r+1)^{-2s}\big(\|u(r,\cdot)\|^2+\|\mathcal{D}_r u(r,\cdot)\|^2\big)\,dr \le Ca^4h^{-2}\int_0^\infty (r+1)^{2s}\|\mathcal{P}_\varphi^\pm(h)u(r,\cdot)\|^2\,dr$$
$$+C\varepsilon h^{-1}a^2\int_0^\infty \big(\|u(r,\cdot)\|^2+\|\mathcal{D}_r u(r,\cdot)\|^2\big)\,dr, \quad (5.4)$$

with some constant $C>0$ independent of h and ε. On the other hand, we have the identity

$$\operatorname{Re}\int_0^\infty \langle 2i\varphi'\mathcal{D}_r u(r,\cdot), u(r,\cdot)\rangle\,dr=\int_0^\infty h\varphi''\|u(r,\cdot)\|^2\,dr,$$

and hence,

$$\operatorname{Re}\int_0^\infty \langle \mathcal{P}_\varphi^\pm(h)u(r,\cdot), u(r,\cdot)\rangle\,dr=\int_0^\infty \|\mathcal{D}_r u(r,\cdot)\|^2\,dr+\int_0^\infty \langle r^{-2}\Lambda_w u(r,\cdot), u(r,\cdot)\rangle\,dr$$
$$-\int_0^\infty (E+\varphi'^2)\|u(r,\cdot)\|^2\,dr+\int_0^\infty \langle Vu(r,\cdot), u(r,\cdot)\rangle\,dr$$
$$\ge \int_0^\infty \|\mathcal{D}_r u(r,\cdot)\|^2\,dr-\mathcal{O}(\tau^2)\int_0^\infty \|u(r,\cdot)\|^2\,dr.$$

This implies

$$\varepsilon h^{-1}a^2\int_0^\infty \|\mathcal{D}_r u(r,\cdot)\|^2\,dr \le \mathcal{O}(\tau^2)\varepsilon h^{-1}a^2\int_0^\infty \|u(r,\cdot)\|^2\,dr$$
$$+\gamma\int_0^\infty (r+1)^{-2s}\|u(r,\cdot)\|^2\,dr+\gamma^{-1}h^{-2}a^4\int_0^\infty (r+1)^{2s}\|\mathcal{P}_\varphi^\pm(h)u(r,\cdot)\|^2\,dr \quad (5.5)$$

for every $\gamma>0$. Taking γ small enough, independent of h, τ and a and combining the estimates (5.4) and (5.5), we get

$$\int_0^\infty (r+1)^{-2s}\big(\|u(r,\cdot)\|^2+\|\mathcal{D}_r u(r,\cdot)\|^2\big)\,dr \le Ca^4h^{-2}\int_0^\infty (r+1)^{2s}\|\mathcal{P}_\varphi^\pm(h)u(r,\cdot)\|^2\,dr$$
$$+C\varepsilon h^{-1}a^2\tau^2\int_0^\infty \|u(r,\cdot)\|^2\,dr, \quad (5.6)$$

with a new constant $C>0$ independent of h and ε. Clearly, the estimate (5.6) implies (4.1).

The proof of Theorem 4.2 in the case when $d\ge 3$ goes very much like the proof of Theorem 4.1 above. The only difference in this case is that we have to integrate the function $F(r)$ from r_0 to ∞ and use that $F(r_0)=0$ by assumption. Thus, by Lemma 2.3 we conclude that the inequality (5.2) holds for all $r\ge r_0$.

When $d = 2$, the operator Λ_w is no longer nonnegative. Instead, we will use that so is the operator $-\Delta_w$. Thus, it is easy to see that the above inequalities still hold with V_L replaced by $V_L - h^2(2r)^{-2}$. Since

$$h^2(\mu(r)(2r)^{-2})' = h^2\mu'(r)(2r)^{-2} - 2^{-1}h^2r^{-3}\mu(r) > -h^2r^{-3}\mu(r),$$

we can use Lemmas 2.5 and 2.6, instead of Lemma 2.3, to conclude that the inequality (5.2) remains valid for $r \geq r_0$ with $E/2$ replaced by $E/3$.

References

[Burq 1998] N. Burq, "Décroissance de l'énergie locale de l'équation des ondes pour le problème extérieur et absence de résonance au voisinage du réel", *Acta Math.* **180**:1 (1998), 1–29. MR Zbl

[Burq 2002] N. Burq, "Lower bounds for shape resonances widths of long range Schrödinger operators", *Amer. J. Math.* **124**:4 (2002), 677–735. MR Zbl

[Cardoso and Vodev 2002] F. Cardoso and G. Vodev, "Uniform estimates of the resolvent of the Laplace–Beltrami operator on infinite volume Riemannian manifolds. II", *Ann. Henri Poincaré* **3**:4 (2002), 673–691. MR Zbl

[Datchev 2014] K. Datchev, "Quantitative limiting absorption principle in the semiclassical limit", *Geom. Funct. Anal.* **24**:3 (2014), 740–747. MR Zbl

[Galkowski and Shapiro 2020] J. Galkowski and J. Shapiro, "Semiclassical resolvent bounds for weakly decaying potentials", preprint, 2020. arXiv

[Klopp and Vogel 2019] F. Klopp and M. Vogel, "Semiclassical resolvent estimates for bounded potentials", *Pure Appl. Anal.* **1**:1 (2019), 1–25. MR Zbl

[Lebeau and Robbiano 1995] G. Lebeau and L. Robbiano, "Contrôle exact de l'équation de la chaleur", *Comm. Partial Differential Equations* **20**:1-2 (1995), 335–356. MR Zbl

[Shapiro 2018] J. Shapiro, "Local energy decay for Lipschitz wavespeeds", *Comm. Partial Differential Equations* **43**:5 (2018), 839–858. MR Zbl

[Shapiro 2019] J. Shapiro, "Semiclassical resolvent bounds in dimension two", *Proc. Amer. Math. Soc.* **147**:5 (2019), 1999–2008. MR Zbl

[Shapiro 2020] J. Shapiro, "Semiclassical resolvent bound for compactly supported L^∞ potentials", *J. Spectr. Theory* **10**:2 (2020), 651–672. MR Zbl

[Vodev 2019] G. Vodev, "Semiclassical resolvent estimates for short-range L^∞ potentials", *Pure Appl. Anal.* **1**:2 (2019), 207–214. MR Zbl

[Vodev 2020a] G. Vodev, "Improved resolvent bounds for radial potentials", preprint, 2020. To appear in *Lett. Math. Phys.* arXiv

[Vodev 2020b] G. Vodev, "Semiclassical resolvent estimates for L^∞ potentials on Riemannian manifolds", *Ann. Henri Poincaré* **21**:2 (2020), 437–459. MR Zbl

[Vodev 2020c] G. Vodev, "Semiclassical resolvent estimates for short-range L^∞ potentials. II", *Asymptot. Anal.* **118**:4 (2020), 297–312. MR Zbl

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RESONANCES AND VISCOSITY LIMIT FOR THE WIGNER–VON NEUMANN-TYPE HAMILTONIAN

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The resonances for the Wigner–von Neumann-type Hamiltonian are defined by the periodic complex distortion in the Fourier space. Also, following Zworski, we characterize resonances as the limit points of discrete eigenvalues of the Hamiltonian with a quadratic complex-absorbing potential in the viscosity-type limit.

1. Introduction

We consider the one-dimensional Schrödinger operator

$$P=-\frac{d^2}{dx^2}+V(x)\quad \text{on } L^2(\mathbb{R})$$

and its resonances, where $V(x)$ is an oscillatory and slowly decaying potential. A typical example is

$$P=-\frac{d^2}{dx^2}+a\frac{\sin 2x}{x}\quad \text{on } L^2(\mathbb{R}),$$

where $a\in\mathbb{R}$. We note that P is not dilation-analytic in this case since the potential is exponentially growing in the complex direction. More generally, we consider the following class of potentials.

Assumption A. The potential $V(x)$ has the form

$$V(x)=\sum_{j=1}^{J}s_j(x)W_j(x),$$

where $J\in\mathbb{N}$, $s_j\in C(\mathbb{R};\mathbb{R})$ are periodic functions with period π whose Fourier series converge absolutely, and $W_j\in C^\infty(\mathbb{R};\mathbb{R})$ have analytic continuations to the region $\{z=x+iy\mid |x|>R_0,\ |y|<K|x|\}$ for some $R_0>0$ and $K>0$ with the bound $|W_j(z)|\le C|z|^{-\mu}$ for some $\mu>0$ in this region; see Figure 1, left.

We note that $V(x)=a(\sin 2x)/x$ satisfies Assumption A for any $K>0$. We also note that dilation-analytic potentials satisfy Assumption A by setting $s_j(x)=1$. We first show that resonances can be defined for this class of potentials. We write the set of threshold by $\mathcal{T}=\{n^2\mid n\in\mathbb{N}\cup\{0\}\}$ (see Remark 2.2 for the necessity of $\mathcal{T}$). The resolvent on the upper half-plane is denoted by $R_+(z)=(z-P)^{-1}$, $\operatorname{Im} z>0$.

Theorem 1.1. *Under Assumption A, there exists a complex neighborhood $\Omega\subset\mathbb{C}$ of $[0,\infty)\setminus\mathcal{T}$ such that the following holds: for any $f,g\in L^2_{\mathrm{comp}}(\mathbb{R})$, the matrix element $(f,R_+(z)g)$ has a meromorphic continuation to Ω.*

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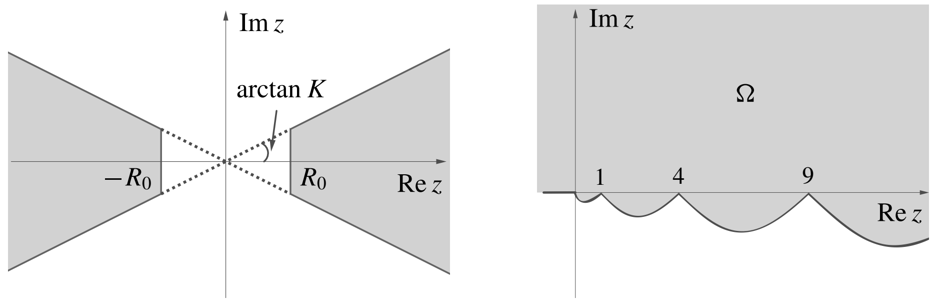

Figure 1. Left: the domain of analyticity of W_j from Assumption A. Right: the domain Ω in Theorem 1.1 and Theorem 1.6.

Remark 1.2. The neighborhoods Ω in Theorems 1.1 and 1.6 are given explicitly in Sections 2 and 3; see also Figure 1, right.

Remark 1.3. Unfortunately, the original Wigner–von Neumann potential [von Neumann and Wigner 1929], see also [Reed and Simon 1978, Section XIII.13],

$$V(x) = (1+g(x)^2)^{-2}(-32\sin x)(g(x)^3\cos x - 3g(x)^2\sin^3 x + g(x)\cos x + \sin^3 x),$$

where $g(x) = 2x - \sin 2x$, does not seem to satisfy Assumption A. In fact, the argument principle implies that if $\nu > \frac{1}{2}$ and $\ell \gg 1$ with $\ell \in \mathbb{Z}$, then $g(z) \pm i$ have two zeros in the region

$$\bigl\{z \in \mathbb{C} \bigm| \bigl(\ell - \tfrac{1}{2}\bigr)\pi \le \operatorname{Re} z \le \bigl(\ell + \tfrac{1}{2}\bigr)\pi,\ -\nu \log \ell \le \operatorname{Im} z \le \nu \log \ell\bigr\}.$$

Thus another method is needed to study the complex resonances for the original Wigner–von Neumann Hamiltonian.

Following the standard theory of resonances, the complex resonances are defined using this meromorphic continuation.

Definition 1.4. Let $R_+(z)$ be the meromorphic continuation of the resolvent for P as in Theorem 1.1. A complex number $z \in \Omega$ is called a resonance if z is a pole of $(f, R_+(z)g)$ for some $f, g \in L^2_{\mathrm{comp}}(\mathbb{R})$ and the multiplicity m_z is defined as the maximal number m such that there exist $f_1, \dots, f_m, g_1, \dots, g_m \in L^2_{\mathrm{comp}}(\mathbb{R})$ with

$$\det\biggl(\frac{1}{2\pi i}\oint_{C(z)} (f_i, R_+(\zeta)g_j)\,d\zeta\biggr)_{i,j=1}^{m} \neq 0,$$

where $C(z)$ is a small circle around z. The set of resonances is denoted by $\operatorname{Res}(P)$.

Remark 1.5. $\operatorname{Res}(P)$ is discrete in Ω and $m_z < \infty$ for any $z \in \Omega$ (see Remark 2.3).

We prove Theorem 1.1 by introducing the periodic complex distortion in the Fourier space (see Section 2 for the definition and the underlying idea).

We now introduce the complex dissipative potential

$$P_\varepsilon = -\frac{d^2}{dx^2} + V(x) - i\varepsilon x^2, \quad \varepsilon > 0.$$

We easily see that $P_\varepsilon,\ \varepsilon > 0$, has purely discrete spectrum on $L^2(\mathbb{R})$. Zworski [2018] proved that the set of resonances can be characterized as limit points of the eigenvalues of P_ε as $\varepsilon \to 0$, namely $\lim_{\varepsilon\to 0}\sigma_d(P_\varepsilon) = \mathrm{Res}(P)$ for compactly supported potentials employing the dilation-analytic method. Zworski [2018] also proposed a problem of finding a potential $V(x)$ such that the limit set of $\sigma_d(P_\varepsilon)$ when $\varepsilon \to 0$ is not discrete, and suggested $V(x) = (\sin x)/x$ as a candidate for such a $V(x)$. Our next result disproves this conjecture (away from the thresholds).

Theorem 1.6. *Under Assumption A, there exists a complex neighborhood* $\Omega \subset \mathbb{C}$ *of* $[0,\infty)\setminus\mathcal{T}$ *such that* $\lim_{\varepsilon\to 0}\sigma_d(P_\varepsilon) = \mathrm{Res}(P)$ *in* Ω *including multiplicities. In particular,* $\lim_{\varepsilon\to 0}\sigma_d(P_\varepsilon)$ *is discrete in* Ω*. More precisely, for any* $z \in \Omega$ *there exists* $\rho_0 > 0$ *such that for any* $0 < \rho < \rho_0$ *there exists* $\varepsilon_0 > 0$ *such that for any* $0 < \varepsilon < \varepsilon_0$

$$\#\sigma_d(P_\varepsilon)\cap B(z,\rho) = m_z,$$

where $B(z,\rho) = \{w \in \mathbb{C} \mid |w - z| \le \rho\}$.

Wigner–von Neumann-type Hamiltonians have been investigated by many authors. See for instance [Behncke 1991; 1994; Cruz-Sampedro et al. 2002; Devinatz et al. 1991; Froese and Herbst 1982; Hinton et al. 1991; Klaus 1991; Lukic 2013; Rejto and Taboada 1997; Richard et al. 2016]. To our knowledge, the definition of the complex resonances based on the complex distortion for Schrödinger operators with oscillatory and slowly decaying potentials is new. The complex distortion in the momentum variables is studied in [Cycon 1985; Sigal 1984] for radially symmetric dilation-analytic or sufficiently smooth exponentially decaying potentials. In [Nakamura 1990], this method is extended to the not necessarily radially symmetric case. See the references in that work for related earlier works on the complex distortion.

Stefanov [2005] studied the approximation of resonances by the fixed complex-absorbing potential method in the semiclassical limit. Similar methods are used in generalized geometric settings in [Nonnenmacher and Zworski 2009; 2015; Vasy 2013]. As mentioned above, Theorem 1.6 was proved by Zworski [2018] for compactly supported potentials. This was extended to more general dilation-analytic potentials in [Xiong 2020]. Analogous results were proved for Pollicott–Ruelle resonances in [Dyatlov and Zworski 2015] (see also [Dang and Riviere 2017; Drouot 2017]), and for 0th-order pseudodifferential operators in [Galkowski and Zworski 2019]. For the numerical results and original approach in physical chemistry, see the references in [Stefanov 2005; Zworski 2018].

This paper is organized as follows. In Section 2, we present the proofs of the theorems for the model case $V(x) = a(\sin 2x)/x$, which contain all the essential ideas for the general case. In Section 3, we present technical arguments which complete the proofs for the general case.

2. The model case

In this section, we explain the general ideas for the proofs and give the full proofs for the model case $V(x) = a(\sin 2x)/x,\ a \in \mathbb{R}$.

2A. ***Periodic distortion in the Fourier space.*** The main idea of Theorem 1.1 is as follows: We note the standard dilation-analytic method for the complex resonances does not apply to our potentials. On the other hand, it is known that if we set

$$A' = \tfrac{1}{2}(x \cdot D' + D' \cdot x), \quad D'u(x) = \tfrac{1}{2\pi i}(u(x+\pi) - u(x-\pi)),$$

then we can construct a Mourre theory with this conjugate operator; see [Nakamura 2014]. We can use this operator as the generator of complex distortion to define the resonances for our model. Actually, in the Fourier space, A' is a differential operator

$$\widetilde{A}' = \tfrac{1}{2\pi}((i\partial_\xi) \cdot \sin(\pi\xi) + \sin(\pi\xi) \cdot (i\partial_\xi)),$$

and this generates a periodic complex distortion in the Fourier space; see [Nakamura 1990] for Hunziker-type local distortion in the Fourier space.

Thus we introduce the periodic distortion in the Fourier space

$$\Phi_\theta(\xi) = \xi + \theta \sin(\pi\xi), \quad U_\theta f(\xi) = \Phi'_\theta(\xi)^{\frac{1}{2}} f(\Phi_\theta(\xi)),$$

where $\theta \in (-\pi^{-1}, \pi^{-1})$. In the Fourier space, P has the form $\widetilde{P} = \xi^2 + \widetilde{V}$, where $\widetilde{V} = (2\pi)^{-1/2}\widehat{V} *$ is a convolution operator and $\widehat{V}$ is the Fourier transform $\widehat{V}(\xi) = (2\pi)^{-1/2} \int V(x) e^{-ix\xi}\, dx$. Hence we have

$$\widetilde{P}_\theta := U_\theta \widetilde{P} U_\theta^{-1} = (\xi + \theta \sin(\pi\xi))^2 + \widetilde{V}_\theta, \quad \widetilde{V}_\theta = U_\theta \widetilde{V} U_\theta^{-1}.$$

Lemma 2.1. *Let $V(x) = a(\sin 2x)/x$ for $a \in \mathbb{R}$. Then $\widetilde{V}_\theta = (\Phi'_\theta)^{1/2} \widetilde{V} (\Phi'_\theta)^{1/2}$, where $(\Phi'_\theta)^{1/2}$ is a multiplication operator by $\Phi'_\theta(\xi)^{1/2}$, and $\widetilde{V} = (a/2)\chi_{[-2,2]} *$, where $\chi_{[-2,2]}$ denotes the characteristic function of $[-2, 2]$. In particular, $\widetilde{V}_\theta$ is analytic with respect to θ and ξ^2-compact for $\theta \in \mathbb{C} \setminus ((-\infty, -\pi^{-1}] \cup [\pi^{-1}, \infty))$.*

Proof. By direct computation, we immediately have $\widetilde{V} = (a/2)\chi_{[-2,2]} *$. Thus we have, for $\theta \in (-\pi^{-1}, \pi^{-1})$,

$$\begin{aligned}\widetilde{V}_\theta f(\xi) &= U_\theta \widetilde{V} U_\theta^{-1} f(\xi) \\ &= \int_{\mathbb{R}} \Phi'_\theta(\xi)^{\frac{1}{2}} \frac{a}{2} \chi_{[-2,2]}(\Phi_\theta(\xi) - \eta)(\Phi_\theta^{-1})'(\eta)^{\frac{1}{2}} f(\Phi_\theta^{-1}(\eta))\, d\eta \\ &= \int_{\mathbb{R}} \Phi'_\theta(\xi)^{\frac{1}{2}} \frac{a}{2} \chi_{[-2,2]}(\Phi_\theta(\xi) - \Phi_\theta(\eta)) \Phi'_\theta(\eta)^{\frac{1}{2}} f(\eta)\, d\eta.\end{aligned}$$

On the other hand, we note

$$\frac{d}{d\xi}(\Phi_\theta(\xi) - \Phi_\theta(\eta)) = 1 + \theta\pi \cos(\pi\xi) > 0$$

for $\theta \in (-\pi^{-1}, \pi^{-1})$. Moreover, we have

$$\Phi_\theta(\eta \pm 2) - \Phi_\theta(\eta) = \pm 2 + \theta(\sin(\pi(\eta \pm 2)) - \sin(\pi\eta)) = \pm 2.$$

These imply that $-2 \le \Phi_\theta(\xi) - \Phi_\theta(\eta) \le 2$ if and only if $-2 \le \xi - \eta \le 2$. Thus we have

$$\begin{aligned}\widetilde{V}_\theta f(\xi) &= \int_{\mathbb{R}} \Phi'_\theta(\xi)^{\frac{1}{2}} \frac{a}{2} \chi_{[-2,2]}(\xi - \eta) \Phi'_\theta(\eta)^{\frac{1}{2}} f(\eta)\, d\eta \\ &= (\Phi'_\theta)^{\frac{1}{2}} \widetilde{V} (\Phi'_\theta)^{\frac{1}{2}} f(\xi).\end{aligned}$$

The second part of Lemma 2.1 follows from the first part. We note that $(\Phi'_\theta)^{\frac{1}{2}}$ is well-defined for $\theta \in \mathbb{C} \setminus ((-\infty, -\pi^{-1}] \cup [\pi^{-1}, \infty))$ since $\Phi'_\theta(\xi) = 1 + \theta\pi \cos(\pi\xi) \ne 0$ and $\mathbb{C} \setminus ((-\infty, -\pi^{-1}] \cup [\pi^{-1}, \infty))$ is simply connected. □

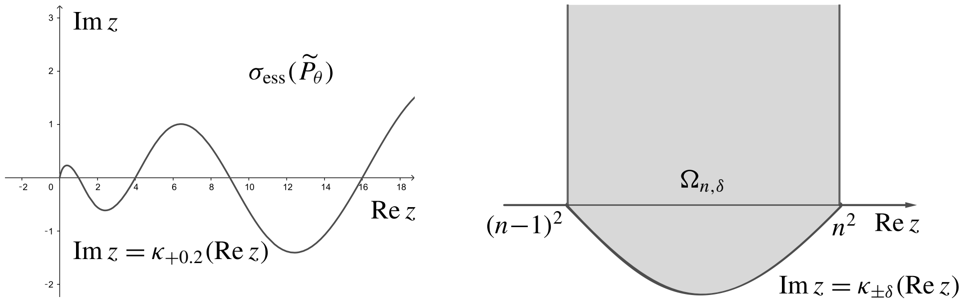

Figure 2. Left: $\sigma_{\text{ess}}(\widetilde{P}_\theta)$ for $\theta = 0.2i$. Right: the region $\Omega_{n,\delta}$.

2B. *Definition of resonances.* In Sections 2B and 2C, we assume that $V(x) = a(\sin 2x)/x$ for $a \in \mathbb{R}$. The modifications needed for the general case are explained in Section 3.

By Lemma 2.1 we learn that $\widetilde{P}_\theta$ is analytic with respect to θ in the sense of Kato, and the essential spectrum of $\widetilde{P}_\theta$ is given by

$$\sigma_{\text{ess}}(\widetilde{P}_\theta) = \{(\xi + \theta \sin(\pi\xi))^2 \mid \xi \in \mathbb{R}\};$$

see Figure 2, left.

Remark 2.2. We note that, for complex θ,

$$\sigma_{\text{ess}}(\widetilde{P}_\theta) \cap [0, \infty) = \{n^2 \mid n \in \mathbb{N} \cup \{0\}\}.$$

Thus $\mathcal{T} = \{n^2 \mid n \in \mathbb{N} \cup \{0\}\} \subset [0, \infty)$ is considered as the set of thresholds with respect to our periodic complex distortion in the Fourier space and is analogous to the set of threshold $\{0\} \subset [0, \infty)$ in the case of the usual complex scaling. In addition to the usual threshold 0, the set $\mathcal{T}$ contains energy n^2, $n \in \mathbb{N}$, at which corresponding plane waves $e^{\pm inx}$ are half-harmonics, i.e., the waves of half-multiple frequencies of the oscillating part of the potential.

We fix $n \in \mathbb{N}$, and for the energy interval $((n-1)^2, n^2)$ we take $\theta = (-1)^n i\delta = \pm i\delta$. We easily see that for $0 < \delta < \pi^{-1}$ the essential spectrum of $\widetilde{P}_{\pm i\delta}$ is the graph of a function $\kappa_{\pm\delta} : [0, \infty) \to \mathbb{R}$ in $\mathbb{R}^2 \cong \mathbb{C}$. Namely, we may define $\kappa_{\pm\delta}(x)$, $x = \text{Re}\, z \geq 0$, by the relation

$$\sigma_{\text{ess}}(\widetilde{P}_{\pm i\delta}) = \{z \in \mathbb{C} \mid \text{Im}\, z = \kappa_{\pm\delta}(\text{Re}\, z),\ \text{Re}\, z \geq 0\}.$$

More explicitly, if $x = \xi^2 - \delta^2 \sin^2(\pi\xi)$ for $\xi \in \mathbb{R}$, then $\kappa_{\pm\delta}(x) = \pm 2\delta\xi \sin(\pi\xi)$. A important fact is that $\kappa_{(-1)^n\delta}(x) < 0$ for $x \in ((n-1)^2, n^2)$.

We set $\delta_0 = \pi^{-1}$ and take any $0 < \delta < \delta_0$. We also set

$$\Omega_{n,\delta} = \{z = x + iy \mid (n-1)^2 < x < n^2,\ y > \kappa_{(-1)^n\delta}(x)\};$$

see Figure 2, right. Note that $\Omega_{n,\delta} \subset \Omega_{n,\delta'}$ if $0 < \delta < \delta' < \delta_0$.

Proof of Theorem 1.1 for the model case. We fix $n \in \mathbb{N}$ and $\delta > 0$ as above, and we write $\mathcal{A} = L^2_{\text{comp}}(\mathbb{R})$. We first note that $U_\theta \hat{f}$ $(f \in \mathcal{A})$ has an analytic continuation for complex θ. We denote the resolvent

$R_+(z)$ on the Fourier space by $\widetilde{R}_+(z)$. For $f, g \in \mathcal{A}$, we have

$$(\hat{f}, \widetilde{R}_+(z)\hat{g}) = (U_\theta \hat{f}, U_\theta \widetilde{R}_+(z) U_\theta^{-1} U_\theta \hat{g}) = (U_{\bar{\theta}} \hat{f}, (z - \widetilde{P}_\theta)^{-1} U_\theta \hat{g}),$$

where $\theta \in \mathbb{R}$ and $\operatorname{Im} z > 0$. The right-hand side is analytic with respect to θ by Lemma 2.1, where θ ranges over a complex neighborhood of $\{(-1)^n i\delta \mid 0 \le \delta < \delta_0\}$. This in turn implies that the left-hand side has a meromorphic continuation to Ω_{n,δ_0} with respect to z. Thus Theorem 1.1 is proved for $\Omega = \bigcup_{n\in\mathbb{N}} \Omega_{n,\delta_0}$. $\square$

Remark 2.3. We set

$$\Pi_z^\theta = \frac{1}{2\pi i} \oint_{C(z)} (\zeta - \widetilde{P}_\theta)^{-1}\, d\zeta$$

to be the spectral projection for $\widetilde{P}_\theta$. Then we have

$$\frac{1}{2\pi i} \oint_{C(z)} (f, R_+(\zeta) g)\, d\zeta = \frac{1}{2\pi i} \oint_{C(z)} (U_{\bar{\theta}} \hat{f}, (\zeta - \widetilde{P}_\theta)^{-1} U_\theta \hat{g})\, d\zeta = (U_{\bar{\theta}} \hat{f}, \Pi_z^\theta U_\theta \hat{g}).$$

We note that $\{U_\theta \hat{f} \mid f \in \mathcal{A}\}$ is dense in L^2, which is proved by an argument similar to [Hunziker 1986, Theorem 3]. This implies that $m_z = \operatorname{rank}[\Pi_z^\theta]$. Namely, the resonances coincide with the discrete eigenvalues of $\widetilde{P}_\theta$ including multiplicities. In particular, $\operatorname{Res}(P)$ is discrete and $m_z < \infty$ for any $z \in \Omega$.

2C. *Viscosity limit.* As in [Zworski 2018], the essential ingredient of the proof of Theorem 1.6 is the resolvent estimate of the distorted operator which is uniform with respect to ε in the case of $V = 0$. We prove this by employing the semiclassical analysis in the Fourier space with the semiclassical parameter $h = \sqrt{\varepsilon}$. Since we work in the Fourier space, the term $-i\varepsilon x^2 = i\varepsilon \partial_\xi^2$ is the usual viscosity term (multiplied by i) and the viscosity limit corresponds to the semiclassical limit.

For notational simplicity, we set $P_0 = P$, $\widetilde{P}_0 = \widetilde{P}$ and $\widetilde{P}_{0,\theta} = \widetilde{P}_\theta$. In the Fourier space, P_ε, $\varepsilon \ge 0$, has the form

$$\widetilde{P}_\varepsilon = \xi^2 + \widetilde{V} + i\varepsilon \partial_\xi^2.$$

Hence the distorted operator $\widetilde{P}_{\varepsilon,\theta} = U_\theta \widetilde{P}_\varepsilon U_\theta^{-1}$ is given by

$$\widetilde{P}_{\varepsilon,\theta} = (\xi + \theta \sin(\pi\xi))^2 + \widetilde{V}_\theta - i\varepsilon D_\xi (1 + \pi\theta \cos(\pi\xi))^{-2} D_\xi - i\varepsilon r_\theta(\xi),$$

where $r_\theta(\xi) = -\Phi_\theta'(\xi)^{-1/2} \partial_\xi (\Phi_\theta'(\xi)^{-1} \partial_\xi (\Phi_\theta'(\xi)^{-1/2}))$ is a function which is analytic with respect to θ and bounded with respect to ξ. Since $\widetilde{P}_{\varepsilon,\theta}$ has a compact resolvent, $\widetilde{P}_{\varepsilon,\theta}$, $\varepsilon > 0$, has purely discrete spectrum. Moreover, for fixed $\varepsilon > 0$, $\widetilde{P}_{\varepsilon,\theta}$ is analytic with respect to θ in the sense of Kato. These imply that the eigenvalues of $\widetilde{P}_{\varepsilon,\theta}$ coincide with those of $\widetilde{P}_\varepsilon$ including multiplicities by the same argument as in Remark 2.3. Thus it is enough to show that the eigenvalues of $\widetilde{P}_{\varepsilon,\theta}$ converge to those of $\widetilde{P}_\theta$ as $\varepsilon \to +0$.

Proof of Theorem 1.6 for the model case. We first prove the resolvent estimate (2-1) for the distorted free Hamiltonian

$$\widetilde{Q}_{\varepsilon,\theta} = (\xi + \theta \sin(\pi\xi))^2 - i\varepsilon D_\xi (1 + \pi\theta \cos(\pi\xi))^{-2} D_\xi - i\varepsilon r_\theta(\xi), \quad \varepsilon \ge 0.$$

In the following, we fix $n \in \mathbb{N}$, and set $\theta = (-1)^n i\delta = \pm i\delta$, $0 < \delta < \delta_0$, as in Section 2B.

We set $h = \sqrt{\varepsilon}$ and view $\widetilde{Q}_{\varepsilon,\theta}$ as an h-pseudodifferential operator in the Fourier space. Recall that $\Omega_{n,\delta}$ is defined in Section 2B; see Figure 2, right. We easily see that the numerical range of the h-principal symbol of $\widetilde{Q}_{\varepsilon,\theta}$, i.e.,

$$\{(\xi + \theta \sin(\pi\xi))^2 - i(1 + \pi\theta \cos(\pi\xi))^{-2}x^2 \mid x, \xi \in \mathbb{R}\},$$

is disjoint from $\Omega_{n,\delta}$ for small $\delta > 0$. For instance, this is true for $0 < \delta \le \delta_1$, where $\delta_1 = (\sqrt{2} - 1)\pi^{-1}$. The constant δ_1 comes from requiring

$$\sup_{x \ge 0} \left| \frac{d}{dx} \kappa_{\pm\delta}(x) \right| = \left| \frac{d}{dx} \kappa_{\pm\delta}(0) \right| = \frac{2\pi\delta}{1 - \pi^2\delta^2}$$

is less than or equal to the minimal value $\frac{1}{2}(1/(\pi\delta) - \pi\delta)$ with respect to $\xi \in \mathbb{R}$ of the absolute value of the slope of the half-line $\{-i(1 \pm \pi\delta i \cos(\pi\xi))^{-2}x^2 \mid x \in \mathbb{R}\}$ in the complex plane. For simplicity, we consider $0 < \delta < \delta_1$ and do not pursue the optimal δ. Now we fix $0 < \delta < \delta_1$ and $z \in \Omega_{n,\delta}$. Then there exists $\rho_0 > 0$ such that there is no resonance in $B(z, \rho_0) \Subset \Omega_{n,\delta}$ possibly expect for z, where $B(z, \rho)$ denotes the ball of radius ρ with the center at z. In the following, we fix $0 < \rho < \rho_0$, and let $w \in B_z = B(z, \rho)$. By the standard semiclassical calculus we learn $(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1}$ exists and

$$\|(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1}\|_{L^2 \to L^2} \le C \tag{2-1}$$

for $w \in B_z$ and for sufficiently small $\varepsilon > 0$. We note that it also holds for $\varepsilon = 0$.

We next employ the perturbation argument. Since $(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1}$ exists, we have

$$\widetilde{P}_{\varepsilon,\theta} - w = (1 + \widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1})(\widetilde{Q}_{\varepsilon,\theta} - w).$$

By Lemma 2.1 and the boundedness of $(\xi^2 + i)(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1}$, we learn $\widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1}$ is compact for $\varepsilon \ge 0$. Thus the analytic Fredholm theory can be applied. We have

$$\begin{aligned}(w - \widetilde{P}_{\varepsilon,\theta})^{-1} &= (\partial_w(\widetilde{P}_{\varepsilon,\theta} - w))(\widetilde{P}_{\varepsilon,\theta} - w)^{-1} \\ &= (\partial_w \widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1})(1 + \widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1})^{-1} \\ &\qquad + (1 + \widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1})(w - \widetilde{Q}_{\varepsilon,\theta})^{-1}(1 + \widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1})^{-1}.\end{aligned}$$

The Gohberg–Sigal factorization [1971, Theorem 3.1] applied to $1 + \widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1}$, Cauchy's theorem and the cyclicity of the trace imply that

$$\operatorname{tr} \oint_{\partial B_z} (1 + \widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1})(w - \widetilde{Q}_{\varepsilon,\theta})^{-1}(1 + \widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1})^{-1}\, dw = 0.$$

Thus the number of the eigenvalues of $P_{\varepsilon,\theta},\ \varepsilon \ge 0$, in B_z is given by

$$\operatorname{tr} \frac{1}{2\pi i} \oint_{\partial B_z} (w - \widetilde{P}_{\varepsilon,\theta})^{-1}\, dw = \operatorname{tr} \frac{1}{2\pi i} \oint_{\partial B_z} (\partial_w \widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1})(1 + \widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1})^{-1}\, dw.$$

Note that the right-hand side of this equality is the number of zeros of $1 + \widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta} - w)^{-1}$ in B_z in the sense of [Gohberg and Sigal 1971, Theorem 2.1]. Thus the operator-valued Rouché theorem [Gohberg and Sigal 1971, Theorem 2.2] implies that in order to prove Theorem 1.6, it suffices to show

$$\|((1+\widetilde{V}_\theta(\widetilde{Q}_{0,\theta}-w)^{-1})-(1+\widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta}-w)^{-1}))(1+\widetilde{V}_\theta(\widetilde{Q}_{0,\theta}-w)^{-1})^{-1}\|_{L^2\to L^2}<1$$

for $w\in\partial B_z$ and small $\varepsilon>0$. Since $(1+\widetilde{V}_\theta(\widetilde{Q}_{0,\theta}-w)^{-1})^{-1}$ exists and independent of $\varepsilon>0$ for $w\in\partial B_z$, the above estimate holds if we show

$$\lim_{\varepsilon\to 0}\|\widetilde{V}_\theta(\widetilde{Q}_{0,\theta}-w)^{-1}-\widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta}-w)^{-1}\|_{L^2\to L^2}=0 \tag{2-2}$$

uniformly for $w\in\partial B_z$.

Let $\gamma>0$. We claim that we can decompose $\widetilde{V}_\theta=\widetilde{V}_{\theta,1}+\widetilde{V}_{\theta,2}$, where $\widetilde{V}_{\theta,1}$ is a smoothing pseudodifferential operator in the Fourier space and $\|\widetilde{V}_{\theta,2}\|_{L^2\to L^2}<\gamma$. To see this, we take the decomposition

$$\widetilde{V}_\theta=(\Phi'_\theta)^{\frac12}\widetilde{V}(\Phi'_\theta)^{\frac12}=(\Phi'_\theta)^{\frac12}\widetilde{V}_{1,R}(\Phi'_\theta)^{\frac12}+(\Phi'_\theta)^{\frac12}\widetilde{V}_{2,R}(\Phi'_\theta)^{\frac12}=\widetilde{V}_{\theta,1}+\widetilde{V}_{\theta,2}$$

for large $R>0$, where $\widetilde{V}_{j,R}$ is the Fourier multiplier on the Fourier space by $V_{j,R}$, $\chi\in C_c^\infty(\mathbb{R})$ such that $\chi=1$ near $x=0$, and

$$a\frac{\sin 2x}{x}=a\frac{\sin 2x}{x}\chi\Big(\frac{x}{R}\Big)+a\frac{\sin 2x}{x}\Big(1-\chi\Big(\frac{x}{R}\Big)\Big)=V_{1,R}+V_{2,R}.$$

Then the claimed properties are easily verified.

Since $\|(\widetilde{Q}_{\varepsilon,\theta}-w)^{-1}\|_{L^2\to L^2}\le C$ for small $\varepsilon\ge 0$ and $w\in B_z$, we have

$$\|\widetilde{V}_{\theta,2}(\widetilde{Q}_{0,\theta}-w)^{-1}-\widetilde{V}_{\theta,2}(\widetilde{Q}_{\varepsilon,\theta}-w)^{-1}\|_{L^2\to L^2}\le 2C\gamma,$$

where C is independent of γ. By the resolvent equation, we also learn

$$\begin{aligned}&\widetilde{V}_{\theta,1}(\widetilde{Q}_{0,\theta}-w)^{-1}-\widetilde{V}_{\theta,1}(\widetilde{Q}_{\varepsilon,\theta}-w)^{-1}\\&\qquad=-i\varepsilon\widetilde{V}_{\theta,1}(\widetilde{Q}_{0,\theta}-w)^{-1}(D_\xi(1+\pi\theta\cos(\pi\xi))^{-2}D_\xi+r_\theta(\xi))(\widetilde{Q}_{\varepsilon,\theta}-w)^{-1}.\end{aligned}$$

Since $\widetilde{V}_{\theta,1}$ is a smoothing pseudodifferential operator and $(\widetilde{Q}_{0,\theta}-w)^{-1}$ is also a pseudodifferential operator with a bounded symbol, $\widetilde{V}_{\theta,1}(\widetilde{Q}_{0,\theta}-w)^{-1}D_\xi^2$ is L^2-bounded. Thus we have

$$\|\widetilde{V}_{\theta,1}(\widetilde{Q}_{0,\theta}-w)^{-1}-\widetilde{V}_{\theta,1}(\widetilde{Q}_{\varepsilon,\theta}-w)^{-1}\|_{L^2\to L^2}\le C_\gamma\varepsilon,$$

with some (γ-dependent) constant $C_\gamma>0$. If ε is so small that $\varepsilon\le(C/C_\gamma)\gamma$, we have

$$\|\widetilde{V}_\theta(\widetilde{Q}_{0,\theta}-w)^{-1}-\widetilde{V}_\theta(\widetilde{Q}_{\varepsilon,\theta}-w)^{-1}\|_{L^2\to L^2}\le 2C\gamma+C_\gamma\varepsilon\le 3C\gamma$$

and thus (2-2) is proved since $\gamma>0$ may be arbitrary small. Thus Theorem 1.6 is proved for $\Omega=\bigcup_{n\in\mathbb{N}}\Omega_{n,\delta_1}$. □

3. The general case

3A. *Analyticity of $\widetilde{V}_\theta$.* We recall that $\widetilde{V}_\theta$ was defined in Section 2A.

Lemma 3.1. *Under Assumption A, $\widetilde{V}_\theta$ is analytic with respect to θ and ξ^2-compact for θ in some complex neighborhood of $\{i\delta\mid -K\pi^{-1}<\delta<K\pi^{-1}\}$, where K is the constant in Assumption A.*

Proof of Lemma 3.1. For real θ, the integral kernel $\widetilde{V}_\theta(\xi,\eta)$ of $\widetilde{V}_\theta$ is given by

$$\widetilde{V}_\theta(\xi,\eta)=\frac{1}{\sqrt{2\pi}}\Phi'_\theta(\xi)^{\frac12}\widehat{V}(\Phi_\theta(\xi)-\Phi_\theta(\eta))\Phi'_\theta(\eta)^{\frac12},\quad \xi,\eta\in\mathbb{R}.$$

We first consider the case of $V\in C_c^\infty(\mathbb{R};\mathbb{R})$. Then the Paley–Wiener estimate implies that $\widetilde{V}_\theta(\xi,\eta)$ is analytic with respect to $\theta\in\mathbb{C}$ and has the off-diagonal decay bounds

$$|\partial_\xi^\alpha\partial_\eta^\beta\widetilde{V}_\theta(\xi,\eta)|\le C_{\alpha,\beta,N}\langle\xi-\eta\rangle^{-N},\quad \xi,\eta\in\mathbb{R},$$

for any α, β and N, where $C_{\alpha,\beta,N}$ is independent of θ when $\theta\in\mathbb{C}$ ranges over a bounded set. We also recall the formula, see, e.g., [Zworski 2012, Section 8.1],

$$\widetilde{V}_\theta=b^{\mathrm{w}}(\xi,D_\xi;\theta),\quad b(\xi,x;\theta)=\int_{\mathbb{R}}\widetilde{V}_\theta\Big(\xi+\frac{\eta}{2},\xi-\frac{\eta}{2}\Big)e^{-i\langle\eta,x\rangle}\,d\eta,$$

where b^{w} denotes the Weyl quantization

$$b^{\mathrm{w}}(\xi,D_\xi;\theta)f(\xi)=\frac{1}{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}}b\Big(\frac{\xi+\eta}{2},x;\theta\Big)e^{i\langle\xi-\eta,x\rangle}f(\eta)\,d\eta\,dx.$$

In fact, the integral kernel of $b^{\mathrm{w}}(\xi,D_\xi;\theta)$ is

$$\frac{1}{2\pi}\int_{\mathbb{R}}b\Big(\frac{\xi+\eta}{2},x;\theta\Big)e^{i\langle\xi-\eta,x\rangle}\,dx$$

and this coincides with $\widetilde{V}_\theta(\xi,\eta)$ by simple computations. These imply that $\widetilde{V}_\theta$ is a pseudodifferential operator in the Fourier space with a symbol rapidly decaying with respect to x (that is,

$$|\partial_\xi^\alpha\partial_x^\beta b(\xi,x;\theta)|\le C_{\alpha,\beta,N}\langle x\rangle^{-N},\quad \xi,x\in\mathbb{R},$$

for any α, β and N, where $C_{\alpha,\beta,N}$ is independent of θ when $\theta\in\mathbb{C}$ ranges over a bounded set) and analytic with respect to θ. Thus Lemma 3.1 is proved in this case.

We next consider the case of $V(x)=s(x)W(x)$, where $s(x)$ and $W(x)$ satisfy the condition in Assumption A; see Figure 1, left. We first estimate the Fourier transform of $W(x)$. By the deformation of the integral (see Figure 3, left), we have

$$\widehat{W}(\xi)=\frac{1}{\sqrt{2\pi}}\int_{C_{\pm,\tau}}W(z)e^{-iz\xi}\,dz,\quad \pm\xi>0,$$

where

$$C_{\pm,\tau}=(e^{\pm i\tau}(-\infty,0]-2R_0)\cup[-2R_0,2R_0]\cup(2R_0+e^{\mp i\tau}[0,\infty)),$$

$0<\tau<\arctan K$, and R_0 is that in Assumption A. This expression shows that $\widehat{W}(\xi)$ has an analytic continuation to

$$S_\tau=\{z\in\mathbb{C}^*\mid-\tau<\arg z<\tau\}\cup\{z\in\mathbb{C}^*\mid-\tau<\arg z-\pi<\tau\};$$

see Figure 3, right. We see that $\widehat{W}(\xi)$ decays rapidly in S_τ when $|\xi|\to\infty$ thanks to the smoothness of W. For small $\xi\in S_\tau$, we have $|\widehat{W}(\xi)|\le C|\xi|^{-1/(1+\mu)}$, where $\mu>0$ is the constant in Assumption A. To see

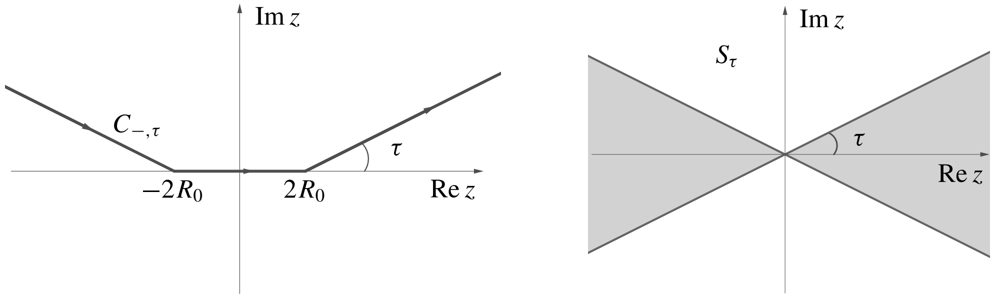

Figure 3. Left: the curve $C_{-,\tau}$, and $C_{+,\tau}$ is its reflection with respect to the real axis. Right: the domain S_τ.

this, we take $C_{\pm,\tau'}$ for $0 < \tau < \tau' < \arctan K$ and estimate

$$|\widehat{W}(\xi)| \le C \int_0^\infty e^{-cx|\xi|} \langle x \rangle^{-\mu}\, dx = C|\xi|^{-1} \int_0^\infty e^{-c|x|} \langle x/|\xi| \rangle^{-\mu}\, dx.$$

We divide the integral into $\int_0^\varepsilon + \int_\varepsilon^\infty$ and we obtain the bound

$$\frac{\varepsilon}{|\xi|} + \frac{1}{|\xi|} \langle \varepsilon/|\xi| \rangle^{-\mu}.$$

Taking $\varepsilon = |\xi|^{\mu/(1+\mu)}$, we have $|\widehat{W}(\xi)| \le C|\xi|^{-1/(1+\mu)}$.

We next claim that the Fourier transform $\widehat{V}(\xi)$ has an analytic continuation to the region $T_\tau = \bigcup_{k\in\mathbb{Z}} T_{\tau,k}$, where (see Figure 4)

$$T_{\tau,k} = \{z \in \mathbb{C} \setminus \{0, 2\} \mid -\tau < \arg z < \tau,\ -\tau < \arg(2 - z) < \tau\} + 2k,$$

and the estimate

$$\sum_{k\in\mathbb{Z}} \sup_{\xi\in T_{\tau,k}} |\xi - 2k|^{\frac{1}{1+\mu}} |\xi - 2k - 2|^{\frac{1}{1+\mu}} |\widehat{V}(\xi)| < \infty \tag{3-1}$$

holds. To see this, we first denote the Fourier transform of s by $\hat{s}(\xi) = \sqrt{2\pi} \sum_{k\in\mathbb{Z}} a_k \delta(\xi - 2k)$. Then we have

$$\widehat{V}(\xi) = \sum_{k\in\mathbb{Z}} a_k \widehat{W}(\xi - 2k).$$

By Assumption A, we have $\sum_{k\in\mathbb{Z}} |a_k| < \infty$. The estimates on $\widehat{W}(\xi)$ above show

$$\sum_{k\in\mathbb{Z}} \sup_{\xi\in T_{\tau,k}} |\xi - 2k|^{\frac{1}{1+\mu}} |\xi - 2k - 2|^{\frac{1}{1+\mu}} |\widehat{W}(\xi)| < \infty.$$

Then the estimate (3-1) follows from Young's inequality in $\ell^1(\mathbb{Z})$ applied to sequences $\{a_k\}_{k\in\mathbb{Z}}$ and

$$\Big\{ \sup_{\xi\in T_{\tau,k}} |\xi - 2k|^{\frac{1}{1+\mu}} |\xi - 2k - 2|^{\frac{1}{1+\mu}} |\widehat{W}(\xi)| \Big\}_{k\in\mathbb{Z}}.$$

By (3-1), we have $|\widetilde{V}_\theta(\xi, \eta)| \le g(\xi - \eta)$ for some integrable function g. This is also true for $(\partial/\partial\theta)\widetilde{V}_\theta(\xi, \eta)$ by Cauchy's formula with respect to θ. Thus Young's inequality implies that the

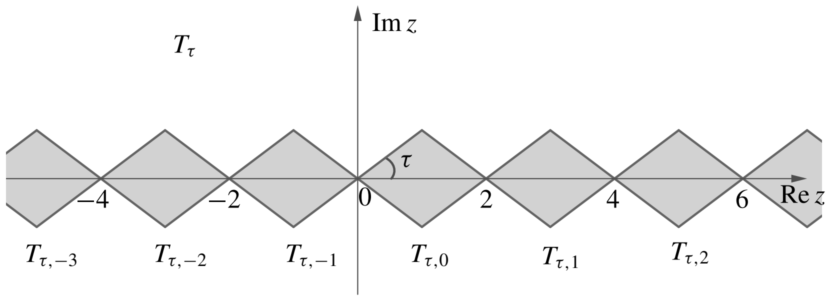

Figure 4. The domains T_τ and $T_{\tau,k}$.

operator $\widetilde{V}_\theta$ with integral kernel $\widetilde{V}_\theta(\xi,\eta)$ is L^2-bounded and analytic with respect to θ. We note that if θ is purely imaginary, we have

$$|\operatorname{Im}(\Phi_\theta(\xi)-\Phi_\theta(\eta))|\le\pi|\theta||\operatorname{Re}(\Phi_\theta(\xi)-\Phi_\theta(\eta))-2k|,$$

with any $k\in\mathbb{Z}$, in particular k such that $|\xi-\eta-2k|\le 1$. Thus θ may be taken from a complex neighborhood of $\{i\delta\mid -\pi^{-1}\tan\tau<\delta<\pi^{-1}\tan\tau\}$. Since $0<\tau<\arctan K$ is arbitrary, $\widetilde{V}_\theta$ is analytic for θ as claimed in Lemma 3.1.

To see ξ^2-compactness, we approximate V by C_c^∞ functions. Take $\chi\in C_c^\infty(\mathbb{R})$ such that $\chi=1$ near $x=0$. We take the decomposition $V(x)=V_{1,R}+V_{2,R}$, where $R>0$,

$$V_{1,R}=\chi\Big(\frac{x}{R}\Big)W(x)\sum_{|k|\le R}a_ke^{2ikx},$$

$$V_{2,R}=W(x)\sum_{|k|>R}a_ke^{2ikx}+\Big(1-\chi\Big(\frac{x}{R}\Big)\Big)W(x)\sum_{|k|\le R}a_ke^{2ikx}.$$

We also denote the corresponding distorted operators on the Fourier space by $\widetilde{V}_{\theta,1,R}$ and $\widetilde{V}_{\theta,2,R}$. Since $V_{1,R}\in C_c^\infty$, we know $\widetilde{V}_{\theta,1,R}$ is ξ^2-compact. We also see that $\lim_{R\to\infty}\|\widetilde{V}_{\theta,2,R}\|_{L^2\to L^2}=0$ by the estimate for $V=s(x)W(x)$ as above. This completes the proof of Lemma 3.1. □

3B. ***Proofs of theorems for the general case.*** Although we set $\delta_0=\pi^{-1}$ for the model case in Section 2, we set $\delta_0=\min\{\pi^{-1},K\pi^{-1}\}$ for the general case in this subsection in view of Lemma 3.1. Similarly we set $\delta_1=\min\{(\sqrt{2}-1)\pi^{-1},K\pi^{-1}\}$ in this subsection. Then all the statements in Sections 2B and 2C remain true for these δ_0 and δ_1.

Proof of Theorem 1.1 for the general case. The proof is exactly the same as that for the model case in Section 2 if we replace Lemma 2.1 by Lemma 3.1. □

Proof of Theorem 1.6 for the general case. The proof is almost the same as that for the model case in Section 2. The only necessary change is the following: In the claim that we can take the decomposition $\widetilde{V}_\theta=\widetilde{V}_{\theta,1}+\widetilde{V}_{\theta,2}$, where $\widetilde{V}_{\theta,1}$ is a smoothing pseudodifferential operator in the Fourier space and $\|\widetilde{V}_{\theta,2}\|_{L^2\to L^2}<\gamma$, we set $\widetilde{V}_{\theta,1}=\widetilde{V}_{\theta,1,R}$ and $\widetilde{V}_{\theta,2}=\widetilde{V}_{\theta,2,R}$ for large $R>0$, where $\widetilde{V}_{\theta,j,R}$ was defined in the ξ^2-compactness part of the proof of Lemma 3.1. □

Remark 3.2. In the case of $V = a(\sin 2x)/x + V_0$, $V_0 \in C_c^\infty(\mathbb{R};\mathbb{R})$, Lemma 2.1 and the proof of Lemma 3.1 show that Lemma 3.1 holds for $\theta \in \mathbb{C} \setminus ((-\infty, -\pi^{-1}] \cup [\pi^{-1}, \infty))$. Thus the set of resonances $\mathrm{Res}_n(P)$ is defined in $\mathbb{C} \setminus (0, \infty)$ for any $n \in \mathbb{N}$ including multiplicities by the meromorphic continuation of $(f, R_+(z)g)$ from $\{z \mid 0 < \arg z < \pi\}$ to

$$\{z \mid 0 < \arg z < \pi\} \cup \{z \mid \arg z = 0, (n-1)^2 < |z| < n^2\} \cup \{z \mid -2\pi < \arg z < 0\}.$$

This poses the problem of whether $\mathrm{Res}_n(P) \neq \mathrm{Res}_{n'}(P)$ when $n \neq n'$.

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References

[Behncke 1991] H. Behncke, "Absolute continuity of Hamiltonians with von Neumann–Wigner potentials", *Proc. Amer. Math. Soc.* **111**:2 (1991), 373–384. MR Zbl

[Behncke 1994] H. Behncke, "The *m*-function for Hamiltonians with Wigner–von Neumann potentials", *J. Math. Phys.* **35**:4 (1994), 1445–1462. MR Zbl

[Cruz-Sampedro et al. 2002] J. Cruz-Sampedro, I. Herbst, and R. Martínez-Avendaño, "Perturbations of the Wigner–von Neumann potential leaving the embedded eigenvalue fixed", *Ann. Henri Poincaré* **3**:2 (2002), 331–345. MR Zbl

[Cycon 1985] H. L. Cycon, "Resonances defined by modified dilations", *Helv. Phys. Acta* **58**:6 (1985), 969–981. MR

[Dang and Riviere 2017] N. V. Dang and G. Riviere, "Pollicott–Ruelle spectrum and Witten Laplacians", preprint, 2017. To appear in *J. Eur. Math. Soc.* arXiv

[Devinatz et al. 1991] A. Devinatz, R. Moeckel, and P. Rejto, "A limiting absorption principle for Schrödinger operators with von Neumann–Wigner type potentials", *Integral Equations Operator Theory* **14**:1 (1991), 13–68. MR Zbl

[Drouot 2017] A. Drouot, "Stochastic stability of Pollicott–Ruelle resonances", *Comm. Math. Phys.* **356**:2 (2017), 357–396. MR Zbl

[Dyatlov and Zworski 2015] S. Dyatlov and M. Zworski, "Stochastic stability of Pollicott–Ruelle resonances", *Nonlinearity* **28**:10 (2015), 3511–3533. MR Zbl

[Froese and Herbst 1982] R. Froese and I. Herbst, "Exponential bounds and absence of positive eigenvalues for *N*-body Schrödinger operators", *Comm. Math. Phys.* **87**:3 (1982), 429–447. MR Zbl

[Galkowski and Zworski 2019] J. Galkowski and M. Zworski, "Viscosity limits for 0th order pseudodifferential operators", preprint, 2019. arXiv

[Gohberg and Sigal 1971] I. C. Gohberg and E. I. Sigal, "An operator generalization of the logarithmic residue theorem and the theorem of Rouché", *Mat. Sb.* (*N.S.*) **84(126)** (1971), 607–629. In Russian; translated in *Math. USSR-Sb.* **13** (1971), 603–625. MR Zbl

[Hinton et al. 1991] D. B. Hinton, M. Klaus, and J. K. Shaw, "Embedded half-bound states for potentials of Wigner–von Neumann type", *Proc. Lond. Math. Soc.* (3) **62**:3 (1991), 607–646. MR Zbl

[Hunziker 1986] W. Hunziker, "Distortion analyticity and molecular resonance curves", *Ann. Inst. H. Poincaré Phys. Théor.* **45**:4 (1986), 339–358. MR Zbl

[Klaus 1991] M. Klaus, "Asymptotic behavior of Jost functions near resonance points for Wigner–von Neumann type potentials", *J. Math. Phys.* **32**:1 (1991), 163–174. MR Zbl

[Lukic 2013] M. Lukic, "Schrödinger operators with slowly decaying Wigner–von Neumann type potentials", *J. Spectr. Theory* **3**:2 (2013), 147–169. MR Zbl

[Nakamura 1990] S. Nakamura, "Distortion analyticity for two-body Schrödinger operators", *Ann. Inst. H. Poincaré Phys. Théor.* **53**:2 (1990), 149–157. MR Zbl

[Nakamura 2014] S. Nakamura, "A remark on the Mourre theory for two body Schrödinger operators", *J. Spectr. Theory* **4**:3 (2014), 613–619. MR Zbl

[von Neumann and Wigner 1929] J. von Neumann and E. Wigner, "Über merkwürdige diskrete Eigenwerte", *Phys. Z.* **30** (1929), 465–467. Zbl

[Nonnenmacher and Zworski 2009] S. Nonnenmacher and M. Zworski, "Quantum decay rates in chaotic scattering", *Acta Math.* **203**:2 (2009), 149–233. MR Zbl

[Nonnenmacher and Zworski 2015] S. Nonnenmacher and M. Zworski, "Decay of correlations for normally hyperbolic trapping", *Invent. Math.* **200**:2 (2015), 345–438. MR Zbl

[Reed and Simon 1978] M. Reed and B. Simon, *Methods of modern mathematical physics, IV*: *Analysis of operators*, Academic, New York, 1978. MR Zbl

[Rejto and Taboada 1997] P. Rejto and M. Taboada, "A limiting absorption principle for Schrödinger operators with generalized von Neumann–Wigner potentials, I: Construction of approximate phase", *J. Math. Anal. Appl.* **208**:1 (1997), 85–108. MR Zbl

[Richard et al. 2016] S. Richard, J. Uchiyama, and T. Umeda, "Schrödinger operators with n positive eigenvalues: an explicit construction involving complex-valued potentials", *Proc. Japan Acad. Ser. A Math. Sci.* **92**:1 (2016), 7–12. MR Zbl

[Sigal 1984] I. M. Sigal, "Complex transformation method and resonances in one-body quantum systems", *Ann. Inst. H. Poincaré Phys. Théor.* **41**:1 (1984), 103–114. MR Zbl

[Stefanov 2005] P. Stefanov, "Approximating resonances with the complex absorbing potential method", *Comm. Partial Differential Equations* **30**:10-12 (2005), 1843–1862. MR Zbl

[Vasy 2013] A. Vasy, "Microlocal analysis of asymptotically hyperbolic and Kerr–de Sitter spaces", *Invent. Math.* **194**:2 (2013), 381–513. MR Zbl

[Xiong 2020] H. Xiong, "Resonances as viscosity limits for exterior dilation analytic potentials", preprint, 2020. arXiv

[Zworski 2012] M. Zworski, *Semiclassical analysis*, Grad. Studies Math. **138**, Amer. Math. Soc., Providence, RI, 2012. MR Zbl

[Zworski 2018] M. Zworski, "Scattering resonances as viscosity limits", pp. 635–654 in *Algebraic and analytic microlocal analysis* (Evanston, IL, 2012/2013), edited by M. Hitrik et al., Springer Proc. Math. Stat. **269**, Springer, 2018. MR Zbl

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A FREE BOUNDARY PROBLEM DRIVEN BY THE BIHARMONIC OPERATOR

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We consider the minimization of the functional

$$J[u] := \int_\Omega \big(|\Delta u|^2 + \chi_{\{u>0\}}\big)$$

in the admissible class of functions

$$\mathcal{A} := \big\{u \in W^{2,2}(\Omega) : u - u_0 \in W_0^{1,2}(\Omega)\big\}.$$

Here, Ω is a smooth and bounded domain of $\mathbb{R}^n$ and $u_0 \in W^{2,2}(\Omega)$ is a given function defining the Navier type boundary condition.

When $n = 2$, the functional J can be interpreted as a sum of the linearized Willmore energy of the graph of u and the area of $\{u > 0\}$ on the xy-plane.

The regularity of a minimizer u and that of the free boundary $\partial\{u > 0\}$ are very complicated problems. The most intriguing part of this is to study the structure of $\partial\{u > 0\}$ near singular points, where $\nabla u = 0$ (of course, at the nonsingular free boundary points where $\nabla u \neq 0$, the free boundary is locally C^1 smooth).

The scale invariance of the problem suggests that, at the singular points of the free boundary, quadratic growth of u is expected. We prove that u is quadratically nondegenerate at the singular free boundary points using a refinement of Whitney's cube decomposition, which applies, if, for instance, the set $\{u > 0\}$ is a John domain.

The optimal growth is linked with the approximate symmetries of the free boundary. More precisely, if at small scales the free boundary can be approximated by zero level sets of a quadratic degree two homogeneous polynomial, then we say that $\partial\{u > 0\}$ is rank-2 flat.

Using a dichotomy method for nonlinear free boundary problems, we also show that, at the free boundary points $x \in \Omega$, where $\nabla u(x) = 0$, the free boundary is either well approximated by zero sets of quadratic polynomials, i.e., $\partial\{u > 0\}$ is rank-2 flat, or u has quadratic growth.

More can be said if $n = 2$, in which case we obtain a monotonicity formula and show that, at the singular points of the free boundary where the free boundary is not well approximated by level sets of quadratic polynomials, the blow-up of the minimizer is a homogeneous function of degree two.

In particular, if $n = 2$ and $\{u > 0\}$ is a John domain, then we get that the blow-up of the free boundary is a cone; and in the one-phase case, it follows that $\partial\{u > 0\}$ possesses a tangent line in the measure theoretic sense.

Differently from the classical free boundary problems driven by the Laplacian operator, the one-phase minimizers present structural differences with respect to the minimizers, and one notion is not included into the other. In addition, one-phase minimizers arise from the combination of a volume type free boundary problem and an obstacle type problem, hence their growth condition is influenced in a nonstandard way by these two ingredients.

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Keywords: biharmonic operator, free boundary, regularity theory, monotonicity formula, free boundary conditions.

1. Introduction

1A. ***Mathematical framework and motivations.*** In this paper we consider the problem of minimizing the functional

$$J[u] = J[u, \Omega] := \int_\Omega \big(|\Delta u|^2 + \chi_{\{u>0\}}\big) \tag{1-1}$$

over the admissible class of functions

$$\mathcal{A} := \big\{u \in W^{2,2}(\Omega) : u - u_0 \in W^{1,2}_0(\Omega)\big\}. \tag{1-2}$$

Here, Ω is a smooth and bounded domain of $\mathbb{R}^n$ and $u_0 \in W^{2,2}(\Omega)$ is a given function defining the Navier type boundary condition (see, e.g., the "hinged problem" on the right-hand side of Figure 1(a) and on page 84 of [Sweers 2009], or Figure 1.5 on page 6 of [Ganguli 2017], or the monograph [Gazzola et al. 2010] for additional information on this condition, which can be interpreted as a weak form of two boundary conditions: $u = u_0$ along $\partial\Omega$ and $\Delta u = 0$ along $\partial\Omega \cap \{u \neq 0\}$).

More precisely, we study here two different types of minimization problems related to the functional in (1-1), namely the *minimizers* in the class $\mathcal{A}$ introduced in (1-2), as well as the minimizers among all the nonnegative functions in $\mathcal{A}$ (that will be called *one-phase minimizers* and thoroughly discussed from Definition 1.2 on). An important feature of the problem that we study is that these two types of minimizers are different and exhibit different[1] features.

[1] As a matter of fact, most of the results presented here will concern minimizers (see in particular Theorems 1.1, 1.7, 1.8, 1.10, and 1.11); some results will include, basically at the same time, both minimizers and one-phase minimizers (see Theorems 1.3, 1.12, and 1.13), and one result (namely Theorem 1.14) will focus specifically on the case of one-phase minimizers. Yet, we believe it was worth stressing the distinction between minimizers and one-phase minimizers, since it is a special characteristic of the fourth order equations and provides a conceptual difference with respect to the more extensively studied case of second order

The functional in (1-1) is clearly related to the biharmonic operator, which provides classical models for rigidity problems with concrete applications, for instance, in the construction of suspension bridges, see, e.g., [McKenna and Walter 1987]. Other classical applications of the biharmonic operator arise in the study of steady state incompressible fluid flows at small Reynolds numbers under the Stokes flow approximation assumption, see, e.g., formula (1) in [Mardanov and Zaripov 2016].

Moreover, the functional in (1-1) provides a linearized model for the Willmore problem which asks to find an immersion/embedding M in $\mathbb{R}^3$ that minimizes the Willmore energy

$$W(M)=\int_M H^2\,dA,$$

where H denotes the mean curvature. The linearization of this energy density gives

$$H^2\,dA=\tfrac{1}{4}(\Delta u)^2\,dx\,dy+\text{lower order terms}.$$

In this context, our problem can be regarded as a free boundary problem for the linearized Willmore energy, where the surface M has a flat part on the xy-plane.

We also refer to the very recent work in [Da Lio et al. 2020] for a problem related to the minimization of the Willmore energy functional with prescribed boundary, boundary Gauss map, and area. See also the recent contributions in [Miura 2016; 2017] for the one-dimensional analysis of the global properties of the solutions of free boundary problems involving the curvature of a curve.

In the setting of (1-1), an additional motivation for us comes from the study of the degenerate/unstable obstacle problem, see [Caffarelli 1980; Monneau and Weiss 2007]. Indeed, we will see in Corollary 4.2 that u is globally almost subharmonic in Ω, i.e., there exists $\hat{C}>0$ (possibly depending also on the energy of the minimizer) such that $\Delta u\geqslant-\hat{C}$. Therefore, the function $\Delta u:=f$ is bounded from below. Accordingly, we can relate our problem to an obstacle problem with unknown right-hand side, namely determine u and $f\geqslant-\hat{C}$ such that

$$\begin{cases}\Delta u=f & \text{in } \Omega,\\ u=|\nabla u|=0 & \text{on } \partial\{u>0\},\\ f=1 & \text{on } \partial\{u>0\}.\end{cases}\tag{1-3}$$

The principal difference from the classical obstacle problem is that f may change sign in Ω and degenerate on the free boundary points, since the last condition in (1-3) is satisfied in a generalized sense: for this reason, it does not follow from the classical obstacle problem theory that u is quadratically nondegenerate.

Motivation for (1-1) also comes from the limit as $\varepsilon\to0$ of the singularly perturbed bi-Laplacian equation

$$\Delta^2u^\varepsilon=-\frac{1}{\varepsilon}\beta\Big(\frac{u^\varepsilon}{\varepsilon}\Big),\tag{1-4}$$

where β is a compactly supported nonnegative function with finite total mass, see [Dipierro et al. 2019]. Equation (1-4) can be seen as the biharmonic counterpart to classical combustion models, see, e.g., [Petrosyan 2002].

equations. In particular, while one-phase minimizers exhibit nontrivial zero sets, the same does not happen for the minimizers (see Proposition B.1). Let us also mention that one-phase minimizers are perhaps less justified by physical motivations, since one is adding an extra "obstacle condition" precisely at the discontinuity level of the potential, nevertheless we think they also deserve further mathematical investigation besides the one carried out in the present paper.

1B. ***Comparison with the existing literature.*** Free boundary problems are, of course, a classical topic of investigation, nevertheless only few results are available concerning the case of equations of order higher than two, and there seems to be no investigation at all for the free boundary problem in (1-1).

Other types of free boundary problems for higher order operators have been considered in [Mawi 2014]. Moreover, obstacle problems involving biharmonic operators have been studied in [Frehse 1973; Caffarelli and Friedman 1979; Caffarelli et al. 1981; 1982; Adams and Vandenhouten 2000; Pozzolini and Léger 2008; Novaga and Okabe 2015; 2016; Aleksanyan 2019]; but, till now, we are not aware of any previous investigation of free boundary problems dealing with higher order operators combined with "bulk" volume terms as in (1-1) here.

Of course, one of the striking differences in our framework, as opposed to the case of the Alt–Caffarelli functional (see [Alt and Caffarelli 1981])

$$J_{\mathrm{AC}}[u] := \int_\Omega \bigl(|\nabla u|^2 + \chi_{\{u>0\}}\bigr),$$

is the lack of a maximum principle and the Harnack inequality for higher order operators. This, in our setting, reflects to the fact that the set $\{u<0\}$ may be nonempty, even under the boundary condition $u_0 \geqslant 0$. This is one of the peculiarities of the situation involving the bi-Laplacian, and it makes the mathematical treatment of the problem extremely difficult (and this is likely to be the reason for which there are not many results in the direction of free boundary regularity in the framework that we consider here).

Thus, the main difficulties in our setting, in comparison with the existing literature, follow from the fact that major elliptic methods based on a maximum principle, the Harnack inequality, and propagation of ellipticity cannot be applied. Moreover, many classical tools, such as domain variations, have not been fully analyzed yet; and, in any case, cannot provide consequences which are as strong as in the classical framework. For instance, the main result that we obtain by domain variation (given in details in Lemma 4.4) is that, for any $\phi = (\phi^1, \dots, \phi^n) \in C_0^\infty(\Omega)$,

$$2\int_\Omega \Delta u(x) \sum_{m=1}^{n} (2\nabla u_m(x)\cdot\nabla\phi^m(x) + u_m(x)\Delta\phi^m(x))\,dx = \int_\Omega \bigl(|\Delta u(x)|^2 + \chi_{\{u>0\}}(x)\bigr)\,\mathrm{div}\,\phi(x)\,dx. \tag{1-5}$$

As customary, we denote by $u_m = \partial_m u = \partial_{x_m} u$ the partial derivative of u with respect to the mth variable. Then, in the classical literature, the standard argument leading to the monotonicity formula for the Alt–Caffarelli problem would be to choose ϕ of a particular form, see [Weiss 1998]. More precisely, for $\varepsilon > 0$, the classical idea would be to consider

$$\eta(x) := \begin{cases} 1 & \text{if } x \in B_r(x_0), \\ \dfrac{r+\varepsilon-|x-x_0|}{\varepsilon} & \text{if } x \in B_{r+\varepsilon}(x_0) \setminus B_r(x_0), \\ 0 & \text{otherwise,} \end{cases}$$

where $x_0 \in \partial\{u>0\}$, and take $\phi(x) := x\eta(x)$ in identity (1-5). Note that

$$\nabla\phi(x) = \begin{cases} \mathbb{I} & \text{if } x \in B_r(x_0), \\ \mathbb{I}\eta - \dfrac{1}{\varepsilon}\dfrac{(x-x_0)\otimes(x-x_0)}{|x-x_0|} & \text{if } x \in B_{r+\varepsilon}(x_0) \setminus B_r(x_0), \\ 0 & \text{otherwise,} \end{cases}$$

where $\mathbb{I} \in \mathrm{Mat}_{n\times n}$ is the identity matrix. However, in our case, identity (1-5) contains the term $\Delta\phi$ which is not defined on the boundary of the ring $B_{r+\varepsilon}(x_0) \setminus B_r(x_0)$, and this creates an important conceptual difficulty. Thus, to overcome this issue, one needs to perform a series of ad hoc integration by parts. This strategy, however, has to deal with the possible generation of third order derivatives of the minimizers, which also cannot be controlled. Therefore, these terms need to be suitably smoothened and simplified via appropriate cancellations.

In this setting, the lack of monotonicity formulas can also be seen as a counterpart to the lack of Pohozhaev type inequalities, and our approach bypasses this kind of difficulty.

As a matter of fact, we will establish a new monotonicity formula in dimension 2, which will lead to Theorem 1.12. In addition, differently from the harmonic case, there are no estimates available in the literature for the biharmonic measure, and this makes the free boundary analysis significantly more complicated. We will overcome these difficulties by Theorem 1.10.

Moreover, in terms of barrier and test functions, an additional difficulty of the biharmonic setting is given by the fact that the function $\max\{u, v\}$ is not an admissible competitor, having possibly infinite energy, so we cannot consider the maximal and minimal solutions.

The analysis of nondegeneracy and optimal regularity of minimizers and of their free boundary is also a novel ingredient with respect to the classical literature, and nothing seemed to be known before about these important questions.

1C. *Main results.* In what follows, we will denote by $\{u > 0\}$ the positivity set of u and by $\partial\{u > 0\}$ its free boundary. The main results of this paper are the following:

- If $z \in \partial\{u > 0\}$ and $\nabla u(z) = 0$, then either $\partial\{u > 0\}$ can be approximated by the zero level sets of a quadratic homogeneous polynomial of degree two, or u has quadratic growth at z.
- If $n = 2$, there exists a monotonicity formula, and we can classify the homogeneous one-phase solutions of degree two.
- We provide various sufficient conditions for strong nondegeneracy in terms of a suitable refinement of Whitney's cube decomposition (c-covering). For instance, we show that if $\{u > 0\}$ is a John domain (see the definition in Section 7B), then $\partial\{u > 0\}$ possesses a measure theoretic tangent line.

A road map of this article is displayed in Figure 1.

1C.1. *BMO estimates for the Laplacian of the minimizers and free boundary conditions.* In further details, the first regularity result that we establish is a BMO estimate on the Laplacian of the minimizers.

Theorem 1.1. *Let u be a minimizer of the functional J defined in* (1-1). *Then, we have* $\Delta u \in BMO_{\mathrm{loc}}(\Omega)$.

We also introduce a notion of one-phase minimizer, in the following setting:

Definition 1.2. We say that u is a one-phase minimizer of J if it minimizes the functional J in (1-1) among the nonnegative admissible functions $\mathcal{A}_+ := \{u \in \mathcal{A} : u \geqslant 0 \text{ in } \Omega\}$, $\mathcal{A}$ being as in (1-2).

Interestingly, one-phase minimizers, as given in Definition 1.2, arise from a combination of a biharmonic free boundary problem and an obstacle problem. We also observe that, in general, minimizers of J which

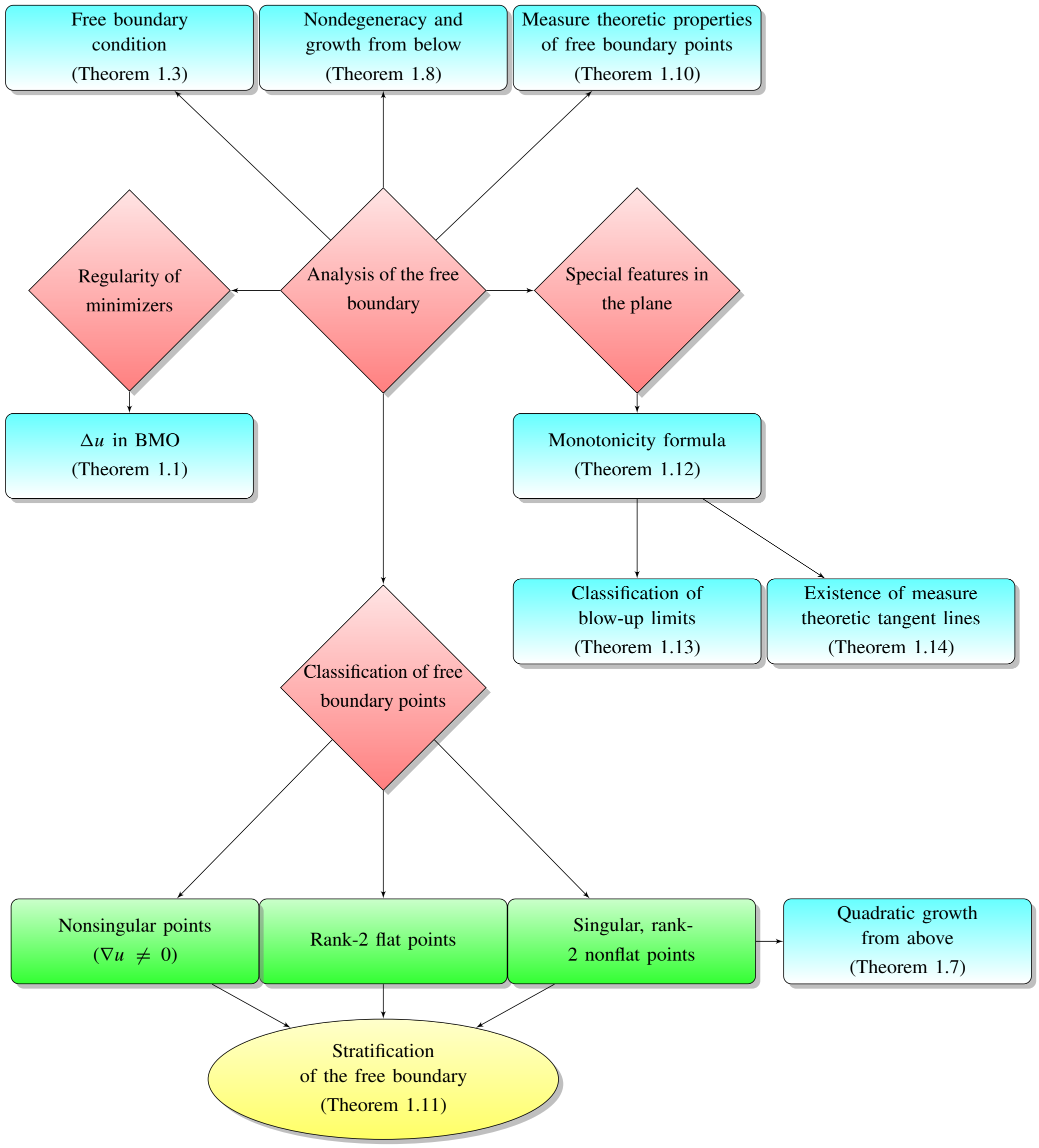

Figure 1. A road map of this article.

happen to be nonnegative do not naturally develop open regions in which the minimizer vanishes (see Proposition B.1 for a concrete result), while one-phase minimizers do (hence, the notion of minimizers that are nonnegative and the notion of one-phase minimizers are structurally very different in this framework, due to the lack of a maximum principle).

We stress that one-phase minimizers, as given in Definition 1.2, are not necessarily minimizers over $\mathcal{A}$. This fact produces significant differences, with respect to the classical case of free boundary problems driven by the Laplacian, and requires some nonstandard techniques to overcome the lack of structure provided, in the classical case, by super-harmonic functions.

We also observe that, in the classical Alt–Caffarelli problem [Alt and Caffarelli 1981] a nonnegative boundary datum produces, in general, considerable portions of the domain in which the minimizer vanishes, but in our case minimizers with nonnegative (and even strictly positive) boundary data may produce regions with considerable negative phases. This difference between zero and strictly negative phases is indeed one of the typical features of our problem, and it is also due to the characteristic function in (1-1). Specifically, the Alt–Caffarelli problem [Alt and Caffarelli 1981] with nonnegative datum typically produces large zero phases, while in most of the situations that one can imagine, our minimizers with nonnegative data have negligible zero sets (but nonnegligible negative sets): the role of one-phase minimizers in our setting is precisely to create natural conditions to produce nonnegligible zero sets (the reader may also consider looking immediately at the examples in Section 5 to see these phenomena of zero and negative phases in simple, but concrete, cases).

Given the higher order structure of the biharmonic functional, the minimizers satisfy a free boundary condition which is richer, and more complicated, than in the harmonic case. To express it in a general form, suppose that the free boundary (locally) separates two regions, say $\Omega^{(1)}$ and $\Omega^{(2)}$, of the domain Ω, with $\partial\Omega^{(1)} = \partial\Omega^{(2)} = \partial\{u > 0\}$: in this case, the minimizer u can be seen as the result of the junction of two functions, say $u^{(1)}$ and $u^{(2)}$, from each side of the free boundary, with $u^{(1)}$ and $u^{(2)}$ not changing sign. In this notation, for $i \in \{1, 2\}$, we set

$$\lambda^{(i)} := \begin{cases} 1 & \text{if } u^{(i)} > 0 \text{ in } \Omega^{(i)}, \\ 0 & \text{if } u^{(i)} \leqslant 0 \text{ in } \Omega^{(i)}. \end{cases} \tag{1-6}$$

Then, we have the following result describing the free boundary condition in this framework:

Theorem 1.3. *Let u be either a minimizer or a continuous one-phase minimizer of the functional J defined in* (1-1). *Assume that*

$$\partial\{|u| > \varepsilon\} \text{ is of class } C^1, \tag{1-7}$$

for all $\varepsilon \in (0, \varepsilon_0)$, for some $\varepsilon_0 > 0$. Then, for any $\phi = (\phi^1, \dots, \phi^n) \in C_0^\infty(\Omega)$,

$$\begin{aligned} &\lim_{\varepsilon\to 0}\int_{\partial(\Omega\cap\{|u|>\varepsilon\})}\Big(\big(|\Delta u^{(1)}|^2+\lambda^{(1)}\big)\phi\cdot\nu-2\sum_{m=1}^{n}\big(\phi^m(\Delta u^{(1)}\nabla u_m^{(1)}-u_m^{(1)}\nabla\Delta u^{(1)})\cdot\nu+\Delta u^{(1)}u_m^{(1)}\nabla\phi^m\cdot\nu\big)\Big) \\ &=\lim_{\varepsilon\to 0}\int_{\partial(\Omega\cap\{|u|>\varepsilon\})}\Big(\big(|\Delta u^{(2)}|^2+\lambda^{(2)}\big)\phi\cdot\nu-2\sum_{m=1}^{n}\big(\phi^m(\Delta u^{(2)}\nabla u_m^{(2)}-u_m^{(2)}\nabla\Delta u^{(2)})\cdot\nu+\Delta u^{(2)}u_m^{(2)}\nabla\phi^m\cdot\nu\big)\Big), \end{aligned} \tag{1-8}$$

where ν is the exterior normal to $\Omega^{(1)}$.

Furthermore, if $u \in C^1(\Omega) \cap C^3(\overline{\Omega^{(1)}}) \cap C^3(\overline{\Omega^{(2)}})$ and $\partial\{|u| > \varepsilon\}$ approaches $\partial\{|u| > 0\} = \partial\{u > 0\} = \partial\{u < 0\} = \{u = 0\}$ in the C^1-sense, we have that

$$\begin{cases} \Delta u^{(1)} u_m^{(1)} = \Delta u^{(2)} u_m^{(2)} \\ \big(|\Delta u^{(1)}|^2 + \lambda^{(1)}\big)\nu_m - 2(\Delta u^{(1)}\nabla u_m^{(1)} - u_m^{(1)}\nabla\Delta u^{(1)})\cdot\nu \\ \qquad\qquad = \big(|\Delta u^{(2)}|^2 + \lambda^{(2)}\big)\nu_m - 2(\Delta u^{(2)}\nabla u_m^{(2)} - u_m^{(2)}\nabla\Delta u^{(2)})\cdot\nu, \end{cases} \tag{1-9}$$

for any $m \in \{1, \dots, n\}$, on $\partial\{u > 0\}$.

Concrete examples of this free boundary condition will also be presented in Section 5 (of course, the reader is welcome to jump to these examples, before diving into all the rather technical details of this paper, if she or he wants to immediately have a close-to-intuition approach to the model and the problems discussed in this paper, as well as to develop some feeling on how minimizers may be expected to look).

As already discussed in Section 1B, one of the principal features of the problem that we consider in the present work is that it does not share the standard properties of its "sibling" Alt–Caffarelli problem [Alt and Caffarelli 1981], such as nondegeneracy, linear growth, etc. Moreover, the existing techniques fail because of the involvement of higher order derivatives.

However, the scale invariance of the functional suggests that the optimal regularity of u must be $C^{1,1}$. This is also supported by the computations that we have for the one-dimensional case (see Remark 4.5 and the explicit examples in Section 5).

1C.2. *Notion of rank-2 flatness, the role played by quadratic polynomials, and dichotomy arguments.* To study the free boundary points of the minimizers, it is useful to distinguish between regular and singular points. Related to this, suppose that $x \in \partial\{u > 0\}$, then there are two possible cases:

- $\nabla u(x) \neq 0$, then $\partial\{u > 0\}$ is C^1 near x.
- $\nabla u(x) = 0$, then we expect u to grow quadratically, and the free boundary may have self-intersections.

To analyze these situations, we introduce the following setting:

Definition 1.4. If $x \in \partial\{u > 0\}$ and $\nabla u(x) = 0$, then we say that x is a singular free boundary point. The set of singular points is denoted by $\partial_{\text{sing}}\{u > 0\}$.

Clearly the singular points are the most interesting points of the free boundary to study. In order to overcome all the difficulties mentioned in Section 1B and to study the regularity of u and that of the free boundary $\partial\{u > 0\}$, we employ a dichotomy argument which was introduced in [Dipierro and Karakhanyan 2018]. The idea is to exploit a suitable notion[2] of "flatness" and distinguish between points where the free boundary is flat and points where it is nonflat, according to this *new notion*.

To this aim, we let

$$\mathrm{HD}(A, B) := \max\Big\{ \sup_{a\in A} \mathrm{dist}(a, B),\ \sup_{b\in B} \mathrm{dist}(b, A)\Big\} \tag{1-10}$$

be the Hausdorff distance of two sets $A, B \subset \mathbb{R}^n$.

We also let P_2 be the set of all homogeneous polynomials of degree two, i.e.,

$$P_2 := \left\{ p(x) = \sum_{i,j=1}^{n} a_{ij} x_i x_j,\ \text{for any } x \in \mathbb{R}^n \text{ with } \|p\|_{L^\infty(B_1)} = 1 \right\}, \tag{1-11}$$

[2] We stress that the "flatness" condition that we consider here is not related to a geometric idea of flatness as being close to a hyperplane. In general, the "flat" objects that we consider look like boundaries of cones and their special feature is related to the "rank-2" notion of flatness, that is being close to zero sets of homogeneous polynomials of degree 2. With this respect, the usual notion of flatness intended as proximity to hyperplanes can be interpreted as a "rank-1 flatness". We maintained the name of "flatness" also for the rank-2 case in order to make the comparison with the classical elliptic free boundary theory easier and more transparent.

where a_{ij} is a symmetric $n\times n$ matrix. Moreover, given $p\in P_2$ and $x_0\in\mathbb{R}^n$, we set $p_{x_0}(x):=p(x-x_0)$ and

$$S(p, x_0) := \{x \in \mathbb{R}^n : p_{x_0}(x) = 0\}. \tag{1-12}$$

We observe that the set $S(p, x_0)$ defined in (1-12) is a cone with vertex at x_0, i.e., if $x \in S(p, x_0)$ then, for every $t > 0$, it holds that $x_0 + t(x - x_0) \in S(p, x_0)$.

With this notation, we set:

Definition 1.5. Let $\delta > 0$, $R > 0$, and $x_0 \in \partial\{u > 0\}$. We say that $\partial\{u > 0\}$ is (δ, R)-rank-2 flat at x_0 if, for every $r \in (0, R]$, there exists $p \in P_2$ such that

$$\mathrm{HD}\big(\partial\{u > 0\} \cap B_r(x_0), S(p, x_0) \cap B_r(x_0)\big) < \delta r.$$

Now, given $r > 0$, $x_0 \in \partial\{u > 0\}$, and $p \in P_2$, we let

$$h_{\min}(r, x_0, p) := \mathrm{HD}\big(\partial\{u > 0\} \cap B_r(x_0), S(p, x_0) \cap B_r(x_0)\big). \tag{1-13}$$

Then, we define the rank-2 flatness at level $r > 0$ of $\partial\{u > 0\}$ at x_0 as follows: We set

$$h(r, x_0) := \inf_{p\in P_2} h_{\min}(r, x_0, p), \tag{1-14}$$

and we introduce the following notation:

Definition 1.6. Let $\delta > 0$, $r > 0$, and $x_0 \in \partial\{u > 0\}$. We say that $\partial\{u > 0\}$ is δ-rank-2 flat at level r at x_0 if $h(r, x_0) < \delta r$.

In view of Definitions 1.5 and 1.6, we can say that $\partial\{u > 0\}$ is (δ, R)-rank-2 flat at $x_0 \in \partial\{u > 0\}$ if and only if, for every $r \in (0, R]$, it is δ-rank-2 flat at level r at x_0.

We stress that the notion of "flatness" introduced in Definitions 1.5 and 1.6 does not refer to a geometric property of being "close to linear," but rather to a proximity to level sets of quadratic polynomials (that is, from the linguistic perspective, one should not separate the adjective "flat" from its own specification "rank-2"). Roughly speaking, our objective is to exploit quadratic objects to describe the minimizers, and our typical strategy would be to distinguish between points of the free boundary where the free boundary itself "looks like the level set of a quadratic polynomial" (i.e., it is in some sense rank-2 flat), and the "other points" of the free boundary, proving in the latter case that then it is the minimizer itself to possess some similarities, in terms of growth, with "quadratic objects". The reason for which we used the terminology of "flatness" to describe these "quadratic" (rather than "linear") scenarios is to maintain some jargon coming from the classical case in [Alt and Caffarelli 1981] and to interpret the notion of flatness as the one describing the "deviation" from a well-understood case (that is, the linear case in [Alt and Caffarelli 1981] and the quadratic case here).

Of course, making precise these results in our setting requires the development of a rather technical terminology, and detailed formulations of these ideas will be provided in Theorems 1.7, 1.8, 1.10, and 1.11.

In this framework, we now state the following result concerning the quadratic growth of u at δ-rank-2 nonflat points of the free boundary:

Theorem 1.7. *Let $n \geqslant 2$ and u be a minimizer of the functional J defined in* (1-1). *Let $D \subset\subset \Omega$, $\delta > 0$, and let $x_0 \in \partial\{u > 0\} \cap D$ such that $|\nabla u(x_0)| = 0$ and $\partial\{u > 0\}$ is not δ-rank-2 flat at x_0 at any level $r > 0$.*

Then, u has at most quadratic growth at x_0, bounded from above in dependence on δ.

1C.3. *Further results on the quadratic growth of the minimizers.* Now we turn our attention to the nondegeneracy properties of the minimizers. First of all, setting as usual $u^+(x) := \max\{u(x), 0\}$, we provide a weak form of nondegeneracy, investigating the validity of statements of this form:

$$\text{If } B \subset \{u > 0\} \text{ is a ball touching } \partial\{u > 0\}, \text{ then } \sup_B u^+ \geqslant C[\operatorname{diam}(B)]^2 \tag{1-15}$$

for some $C > 0$ (possibly depending on dimension, on the domain, and on the datum u_0).

We consider this as a weak form of nondegeneracy as opposed to the one in which B is centered at free boundary points, which we call strong nondegeneracy.

We establish that (1-15) is satisfied, and, more generally, that the positive density of the positivity set is sufficient to ensure at least quadratic growth from the free boundary. The precise result we obtain is:

Theorem 1.8. *Let u be a minimizer of the functional J defined in* (1-1). *Then*:

1° *If $x_0 \in \partial\{u > 0\}$ and*

$$\liminf_{\rho \to 0} \frac{|B_\rho(x_0) \cap \{u > 0\}|}{|B_\rho|} \geqslant \theta_* \tag{1-16}$$

for some $\theta_* > 0$, then

$$\sup_{B_r(x_0)} |u| \geqslant \bar{c} r^2,$$

as long as $B_r(x_0) \subset\subset \Omega$, for some $\bar{c} > 0$ depending on θ_*, n, $\operatorname{dist}(B_r(x_0), \Omega)$, and $\|u_0\|_{W^{2,2}(\Omega)}$.

2° *If $x_0 \in \{u > 0\}$ and $r := \operatorname{dist}(x_0, \partial\{u > 0\})$, then*

$$\sup_{B_r(x_0)} u^+ \geqslant \bar{c} r^2,$$

as long as $B_r(x_0) \subset\subset \Omega$, for some $\bar{c} > 0$ depending on n, $\operatorname{dist}(B_r(x_0), \Omega)$, and $\|u_0\|_{W^{2,2}(\Omega)}$.

We observe that the claim in **2°** is exactly the statement in (1-15).

Sufficient conditions for the density estimate in (1-16) to hold will be discussed in Section 7B, where we also recall and compare the notions of the weak c-covering condition and Whitney's covering. In addition, in Section 7C we will relate the nondegeneracy properties with a fine analysis of the biharmonic measure, which in turn produces some regularity results on the free boundary.

It is also convenient to consider "vanishing" free boundary points, in the following sense:

Definition 1.9. Let u be a minimizer of the functional J defined in (1-1), and let $x_0 \in \partial\{u > 0\} \cap B_1$. We say that $\partial\{u > 0\}$ is vanishing rank-2 flat at x_0 if there exist sequences $\delta_k \to 0$ and $r_k \to 0$ such that

$$h(r_k, x_0) \leqslant \delta_k r_k, \tag{1-17}$$

where h is defined in (1-14).

Notice, in particular, that condition (1-17) is equivalent to $\lim_{k\to+\infty} \dfrac{h(r_k, x_0)}{r_k} = 0$, and this justifies the name of "vanishing" in Definition 1.9.

Theorem 1.10. *Let u be a minimizer of the functional J defined in* (1-1). *Then*:

1° *The set of vanishing rank-2 flat points of the free boundary has zero measure in Ω.*

2° *If $D \subset\subset \Omega$ and there exists $\bar{c} > 0$ such that*

$$\liminf_{r\to 0} \frac{\sup_{B_r(x)} |u|}{r^2} \geqslant \bar{c} \tag{1-18}$$

for every $x \in \partial\{u > 0\} \cap \overline{D}$, then $\partial\{u > 0\}$ has zero measure, and for any $\delta > 0$, the set of free boundary points that are not δ-rank-2 flat has finite $(n-2)$-dimensional Hausdorff measure.

In general, we can restate the previous results in a dichotomy form: roughly speaking, the free boundary in the vicinity of singular points is either "flat" with respect to the level sets of homogeneous polynomial of degree two, being "close" to the level sets of quadratic polynomials, or "nonflat" and in this case the growth from the free boundary is quadratic. To formalize these notions, we decompose the class P_2 introduced in (1-11) as

$$P_2 = \bigcup_{i=1}^{n} P_2^i,$$

where $P_2^i := \{p \in P_2 : \mathrm{Rank}(D^2 p) = i\}$. As we will see, in our setting, the above notion will play a useful role since if $x_0 \in \partial\{u > 0\}$, with $|\nabla u(x_0)| = 0$, and $\partial\{u > 0\}$ is rank-2 flat at x_0, then there exists $p \in P_2$ such that the blow-up of $\partial\{u > 0\}$ at x_0 is the zero set of p. We separate out some interesting cases:

- If $\mathrm{Rank}(D^2 p) = n$ and $D^2 p \geqslant 0$, then the free boundary is a singleton.
- If $\mathrm{Rank}(D^2 p) = 1$, then the free boundary is a hyperplane in $\mathbb{R}^n$, i.e., a codimension 1 plane in $\mathbb{R}^n$ and after some rotation of coordinates we can write $p(x) = \alpha(x_1^+)^2$, where $\alpha \in \mathbb{R}$ is a normalizing constant.
- If $\mathrm{Rank}(D^2 p) = n$ and $D^2 p$ has eigenvalues of opposite signs, then the free boundary has self intersection. For instance, if $n = 2$, then $p(x) = \alpha(x_1^2 - x_2^2)$, where $\alpha \in \mathbb{R}$ is a normalizing constant.

Roughly speaking, in this setting the classes P_2^i detect the approximate symmetries of the free boundary at small scales.

Now, let $\mathcal{F} \subseteq \partial_{\mathrm{sing}}\{u > 0\}$ be the set of singular free boundary points that are vanishing rank-2 flat and

$$\mathcal{N} := (\partial\{u > 0\} \setminus \mathcal{F}) \cap \big\{|\nabla u| = 0\big\} = \partial_{\mathrm{sing}}\{u > 0\} \setminus \mathcal{F}.$$

In this framework, the main result in the stratification setting reads as follows:

Theorem 1.11. *Let u be a minimizer of J. We have*:

- *For any $z \in \mathcal{F}$, there exist $r_k \to 0$ and $p \in P_2^i$, for some $i \in \{1, \dots, n\}$, such that*

$$\lim_{k\to+\infty} \mathrm{HD}\big((\partial E_k) \cap B_R, \{p = 0\} \cap B_R\big) = 0 \tag{1-19}$$

for every fixed $R > 0$, where

$$E_k := \{x \in \mathbb{R}^n : z + r_k x \in \{u > 0\}\}.$$

Furthermore, u^+ is strongly nondegenerate at z, namely

$$\sup_{B_r(z)} u^+ \geqslant cr^2$$

for some $c > 0$, as long as $B_r(z) \subset\subset \Omega$, with c possibly depending on n, $\operatorname{dist}(z, \partial\Omega)$ *and u.*

- *For any $z \in \mathcal{N}$, there exists $C_z > 0$, possibly depending on n,* $\operatorname{dist}(z, \partial\Omega)$*, and $\|u\|_{W^{2,2}(\Omega)}$, such that*

$$|u(x)| \leqslant C_z |x - z|^2 \tag{1-20}$$

near z.

1C.4. *Monotonicity formula and classification of blow-up limits.* To analyze and classify the free boundary properties of the minimizers of J and their blow-up limits, it would be extremely desirable to have suitable monotonicity formulas. Different from the classical case, in our setting no general result of this type is known. To overcome this difficulty, we focus on the two-dimensional case, for which we prove:

Theorem 1.12. *Let $n = 2$ and $\tau > 0$ such that $B_\tau \subset\subset \Omega$. Let $u : \Omega \to \mathbb{R}$, with $0 \in \partial\{u > 0\}$ and $\nabla u(0) = 0$, be*

- *either: a minimizer of the functional J, with 0 not (δ, τ)-rank-2 flat in the sense of Definition 1.5,*
- *or: a one-phase minimizer of the functional J with $u \in C^{1,1}(\Omega)$, and such that $\partial\{u > 0\}$ has null Lebesgue measure.*

Then, there exists a function $E : (0, \tau) \to \mathbb{R}$, which is bounded, nondecreasing, and such that, for any $\tau_2 > \tau_1 > 0$,

$$E(\tau_2) - E(\tau_1) = \int_{\tau_1}^{\tau_2} \left\{ \frac{1}{r^2} \int_{\partial B_r} \left[\left(\frac{u_{\theta r}}{r} - \frac{2u_\theta}{r^2} \right)^2 + \left(u_{rr} - \frac{3u_r}{r} + \frac{4u}{r^2} \right)^2 \right] \right\} dr. \tag{1-21}$$

The explicit value of the function E is given by

$$E(r) = \int_{\partial B_r} \left(\frac{\Delta u\, u_r}{2r^2} - \frac{5u_r^2}{2r^3} - \frac{\Delta u u}{r^3} + \frac{6uu_r}{r^4} + \frac{u_\theta u_{\theta r}}{r^4} - \frac{4u^2}{r^5} - \frac{3u_\theta^2}{2r^5} \right) + \frac{1}{4r^2} \int_{B_r} \left(|\Delta u|^2 + \chi_{\{u>0\}} \right). \tag{1-22}$$

Furthermore, if E is constant in $(0, \tau)$, then u is a homogeneous function of degree two in B_τ.

We stress that the C^1 assumption on u in Theorem 1.12 is taken only in the case of one-phase minimizers, while for minimizers no additional regularity assumption is required in Theorem 1.12.

Given $x_0 \in \partial\{u > 0\}$, we consider the blow-up sequence of u at x_0, defined as

$$u_k(x) := \frac{u(x_0 + \rho_k x)}{\rho_k^2}, \tag{1-23}$$

where $\rho_k \to 0$ as $k \to +\infty$.

In this setting, we can classify blow-up limits of minimizers in the plane.

Theorem 1.13. *Let $n = 2$. Let $B_r \subset\subset \Omega$. Let $x_0 \in \Omega$ and $u : \Omega \to \mathbb{R}$, with $x_0 \in \partial_{\text{sing}}\{u > 0\}$. Assume that either u is a minimizer of the functional J, with*

$$\partial\{u > 0\} \text{ not } \delta\text{-rank-2 flat at } x_0 \text{ at any level} \tag{1-24}$$

for some $\delta > 0$, *or that* u *is a one-phase minimizer of the functional* J *with* $u \in C^{1,1}(\Omega)$, *and such that* $\partial\{u > 0\}$ *has null Lebesgue measure. Then every blow-up limit of* u *at* x_0 *is either a homogeneous function of degree two*, *or it is identically zero.*

One of the main issues in the free boundary analysis is that, even in the one-phase problem, the topological and measure theoretic boundaries of $\{u > 0\}$ may not coincide. On the other hand, the following is a regularity result for the one-phase free boundary in the plane:

Theorem 1.14. *Let* $n = 2$. *Suppose that* $B_1 \subset\subset \Omega$. *Assume that* u *is a one-phase minimizer for* J, *that*

$$u \in C^{1,1}(B_1), \tag{1-25}$$

and that $\partial\{u > 0\}$ *has null Lebesgue measure. Suppose that* $0 \in \partial_{\text{sing}}\{u > 0\}$. *Assume also that*, *for every* $\bar{x} \in \partial\{u > 0\} \cap B_1$,

$$\liminf_{\rho \to 0^+} \frac{\sup_{B_\rho(\bar{x})} u}{\rho^2} \geqslant c \tag{1-26}$$

for some $c > 0$, *for all* $\rho \in (0, 1)$, *and that*

$$\limsup_{\rho \to 0} \frac{|B_\rho \cap \{u > 0\}|}{|B_\rho|} < 1. \tag{1-27}$$

Then there exists $r_0 > 0$ *such that at every point* $\bar{x}$ *of* $\partial\{u > 0\} \cap B_{r_0}$ *the free boundary possesses a unique approximate tangent line in measure theoretic sense*, *namely if* D *is the symmetric difference of the sets* $\{u > 0\}$ *and a suitable rotation of* $\{(x - \bar{x}) \cdot e_1 > 0\}$, *we have that*

$$\lim_{\rho \to 0^+} \frac{|B_\rho(\bar{x}) \cap D|}{|B_\rho(\bar{x})|} = 0.$$

We think that it is an interesting open problem to detect suitable conditions guaranteeing that the $C^{1,1}$-assumptions taken in Theorems 1.12, 1.13, and 1.14 are fulfilled.

Moreover, in our setting, Theorems 1.1, 1.7, 1.8, 1.10, and 1.11 are obtained specifically for the minimizers, and Theorem 1.14 specifically for the one -phase minimizers, while Theorems 1.3, 1.12, and 1.13 are valid for both minimizers and one-phase minimizers. Though the minimization setting is, in our case, structurally different from that of one-phase minimization due to the lack of Maximum Principle, we think that it is an interesting open problem to unify as much as possible the theory of minimizers with that of one-phase minimizers.

It is also an interesting problem to detect the optimal regularity of the solutions and their free boundaries.

1D. ***Organization of the paper.*** The rest of the paper is organized as follows: Section 2 contains the main existence result. In Section 3 we provide the proof of the local BMO estimate for the Laplacian of the minimizers, as given by Theorem 1.1. In Section 4 we present some structural properties of the minimizers which are based on the first variation of the functional J. As a consequence, we also obtain the free boundary condition, and we prove Theorem 1.3. In Section 5, we discuss some one-dimensional examples. Section 6 contains a dichotomy argument which leads to the proof of Theorem 1.7. Section 7 is devoted to nondegeneracy considerations and to the proof of Theorems 1.8 and 1.10. In Section 8 we consider the stratification of the free boundary, reformulating some results obtained in Section 6, and, in particular, we prove Theorem 1.11. Section 9 focuses on the monotonicity formula and contains the proof of Theorem 1.12. In Section 10 we present an application of such a monotonicity formula, proving the homogeneity of the blow-up limits, and establishing Theorem 1.13. Then, Section 11 focuses on explicit two-dimensional regularity and classification results and contains the proof of Theorem 1.14. The paper ends with two appendices which collect some ancillary observations.

2. Existence of minimizers

The following result exploits the direct method of the calculus of variations to obtain the existence of the minimizers for our problem. Due to the presence of several technical aspects in the proof, we provide the argument in full details.

Lemma 2.1. *The functional in* (1-1) *attains a minimum over* $\mathcal{A}$.

Proof. Let $u_k \in \mathcal{A}$ be a minimizing sequence, namely

$$\lim_{k\to+\infty} J[u_k] = \inf_{v\in\mathcal{A}} J[v]. \tag{2-1}$$

For large k, we can suppose that

$$J[u_k] \leqslant J[u_0]+1 \leqslant \int_\Omega \big(|\Delta u_0|^2+1\big) \leqslant C \tag{2-2}$$

for some $C>0$. Also, since $u_k\in\mathcal{A}$, we know from (1-2) that $u_k^* := u_k - u_0 \in W^{2,2}(\Omega)\cap W_0^{1,2}(\Omega)$. Let also $v_k^* := \Delta u_k^* \in L^2(\Omega)$. In this way, we have that

$$\begin{cases} \Delta u_k^* = v_k^* & \text{in } \Omega,\\ u_k^* = 0 & \text{on } \partial\Omega. \end{cases}$$

Consequently, by elliptic regularity (see Theorem 4 on page 317 of [Evans 1998]), we know that

$$\|u_k^*\|_{W^{2,2}(\Omega)} \leqslant C'\big(\|v_k^*\|_{L^2(\Omega)} + \|u_k^*\|_{L^2(\Omega)}\big) \tag{2-3}$$

for some $C'>0$. Also (see Theorem 6 on page 306 of [Evans 1998]), one has that

$$\|u_k^*\|_{L^2(\Omega)} \leqslant C''\|v_k^*\|_{L^2(\Omega)} \tag{2-4}$$

for some $C''>0$. Therefore, in light of (2-3) and (2-4) we conclude

$$\|u_k^*\|_{W^{2,2}(\Omega)} \leqslant C'''\|v_k^*\|_{L^2(\Omega)} = C'''\|\Delta u_k^*\|_{L^2(\Omega)}$$

for some $C'''>0$. This and (2-2) imply

$$\|u_k^*\|_{W^{2,2}(\Omega)} \leqslant C''''$$

for some $C''''>0$. Therefore, we can suppose, up to a subsequence, that

$$u_k^* \text{ converges to some } u^* \text{ weakly in } W^{2,2}(\Omega), \tag{2-5}$$

and then, by compact embedding,

$$u_k^* \text{ converges strongly to } u^* \text{ in } W^{1,2}(\Omega). \tag{2-6}$$

Since $u_k^* \in W_0^{1,2}(\Omega)$, this implies that also $u^* \in W_0^{1,2}(\Omega)$. As a consequence, recalling (1-2), we know

$$u := u^* + u_0 \text{ belongs to } \mathcal{A}. \tag{2-7}$$

Furthermore, by (2-5), it holds that u_k converges to u weakly in $W^{2,2}(\Omega)$. In particular, u_k is bounded in $W^{2,2}(\Omega)$, and therefore, for any $i \in \{1, \dots, n\}$, it holds that $\partial_i^2 u_k$ is bounded in $L^2(\Omega)$. This yields that $\partial_i^2 u_k$ converges to some w_i weakly in $L^2(\Omega)$. This and

$$\text{the strong convergence of } u_k \text{ to } u \text{ in } W_0^{1,2}(\Omega) \subset L^2(\Omega) \tag{2-8}$$

(recall (2-6)) imply that, for any $\varphi \in C_0^\infty(\Omega)$,

$$\int_\Omega w_i\,\varphi = \lim_{k\to+\infty} \int_\Omega \partial_i^2 u_k\,\varphi = \lim_{k\to+\infty} \int_\Omega u_k\,\partial_i^2\varphi = \int_\Omega u\,\partial_i^2\varphi,$$

which shows that $w_i = \partial_i^2 u$.

Accordingly, we have that $\partial_i^2 u_k$ converges to $\partial_i^2 u$ weakly in $L^2(\Omega)$. Therefore, we have

$$\begin{aligned} 0 &\leqslant \lim_{k\to+\infty} \int_\Omega |\Delta(u_k - u)|^2 \\ &= \lim_{k\to+\infty} \int_\Omega |\Delta u_k|^2 + \int_\Omega |\Delta u|^2 - 2\int_\Omega \Delta u_k \Delta u = \lim_{k\to+\infty} \int_\Omega |\Delta u_k|^2 - \int_\Omega |\Delta u|^2. \end{aligned} \tag{2-9}$$

Now, up to a subsequence, recalling (2-8), we can suppose that u_k converges to u a.e. in Ω, and therefore, $\liminf_{k\to+\infty} \chi_{\{u_k>0\}} \geqslant \chi_{\{u>0\}}$ a.e. in Ω. Consequently, by Fatou's Lemma,

$$\liminf_{k\to+\infty} \int_\Omega \chi_{\{u_k>0\}} \geqslant \int_\Omega \chi_{\{u>0\}}.$$

Combining this with (2-9), we see that (2-1) provides

$$J[u] \leqslant \liminf_{k\to+\infty} J[u_k] = \inf_{v\in\mathcal{A}} J[v].$$

This and (2-7) imply that u is the desired minimizer. □

By taking into account a nonnegative constraint in the minimizing sequence in the proof of Lemma 2.1, one also obtains an existence result for the one-phase problem[3] with datum $u_0 \geqslant 0$.

[3]To prove the existence of one-phase minimizers, one can proceed as in the proof of Lemma 2.1, but considering in this case a minimizing sequence $u_k \in \mathcal{A}_+$: notice that $\mathcal{A}_+$ was introduced in Definition 1.2, and this space is nonempty due to the sign of u_0. Also, the sequence $u_k \in \mathcal{A}_+$ is not obtained by a minimizing sequence in $\mathcal{A}$ by taking its positive part, but simply by the usual procedure of minimizing the energy functional in the given domain $\mathcal{A}_+$. The argument given in the proof of Lemma 2.1 leads to a function $u \in \mathcal{A}$ such that $u_k \to u$ weakly in $W^{2,2}(\Omega)$, strongly to u^* in $W^{1,2}(\Omega)$, and a.e. in Ω, up to a subsequence, with $J[u] \leqslant \liminf_{k\to+\infty} J[u_k] = \inf_{v\in\mathcal{A}_+} J[v]$. Since $u(x) = \lim_{k\to+\infty} u_k(x) \geqslant 0$ for a.e. $x \in \Omega$, it follows that $u \in \mathcal{A}_+$, hence u is the desired one-phase minimizer.

3. BMO estimates and proof of Theorem 1.1

The goal of this section is to show that the minimizers of (1-1) have a Laplacian which is a function of locally bounded mean oscillation, and thus prove Theorem 1.1.

Proof of Theorem 1.1. We fix $R_0 > R > r > 0$ and $x_0 \in \Omega$ such that the ball $B_{2R_0}(x_0)$ is contained in Ω, and we consider the function h that solves

$$\begin{cases} \Delta^2 h = 0 & \text{in } B_{2R}(x_0), \\ h = u & \text{on } \partial B_{2R}(x_0), \\ \nabla h = \nabla u & \text{on } \partial B_{2R}(x_0). \end{cases}$$

The existence of h follows from Green's formula for biharmonic functions, see page 48 in [Gazzola et al. 2010], or by minimizing energy with

$$h - u \in W_0^{2,2}(B_{2R}(x_0)). \tag{3-1}$$

We also extend h outside $B_{2R}(x_0)$ to be equal to u in $\Omega \setminus B_{2R}(x_0)$. We observe that the function h is an admissible competitor for u, since

$$h \in W^{2,2}(\Omega). \tag{3-2}$$

Indeed, if $v := h - u$, we see from (3-1) and the extension results in classical Sobolev spaces (see, e.g., Proposition IX.18 in [Brezis 1983]) that $v \in W^{2,2}(\Omega)$. Since $u \in W^{2,2}(\Omega)$, the claim in (3-2) follows.

Then, by the minimality of u, we have that $J[u] \leqslant J[h]$; that is,

$$\int_{B_{2R}(x_0)} |\Delta u|^2 + \chi_{\{u>0\}} \leqslant \int_{B_{2R}(x_0)} |\Delta h|^2 + \chi_{\{h>0\}},$$

which in turn yields

$$\int_{B_{2R}(x_0)} |\Delta u|^2 - |\Delta h|^2 \leqslant C R^n \tag{3-3}$$

for some $C > 0$. Also, by (3-1), and since $\Delta^2 h = 0$ in $B_{2R}(x_0)$, we get

$$\begin{aligned} \int_{B_{2R}(x_0)} |\Delta u|^2 - |\Delta h|^2 &= \int_{B_{2R}(x_0)} (\Delta u - \Delta h)(\Delta u + \Delta h) \\ &= \int_{B_{2R}(x_0)} (\Delta u - \Delta h)\Delta u = \int_{B_{2R}(x_0)} |\Delta u - \Delta h|^2. \end{aligned}$$

From this and (3-3), we obtain

$$\int_{B_{2R}(x_0)} |\Delta u - \Delta h|^2 \leqslant C R^n. \tag{3-4}$$

Now we introduce the notation

$$(\Delta u)_{x_0,r} := \fint_{B_r(x_0)} \Delta u(x)\, dx,$$

and we observe that, by Hölder's inequality,

$$|(\Delta u)_{x_0,r} - (\Delta h)_{x_0,r}|^2 \leqslant \left(\fint_{B_r(x_0)} |\Delta u - \Delta h| \right)^2 \leqslant \fint_{B_r(x_0)} |\Delta u - \Delta h|^2,$$

which implies that

$$\int_{B_r(x_0)} |(\Delta h)_{x_0,r} - (\Delta u)_{x_0,r}|^2 \leqslant \int_{B_r(x_0)} |\Delta u - \Delta h|^2. \tag{3-5}$$

Moreover, since the function $H := \Delta h$ is harmonic in $B_{2R}(x_0)$, we have the following Campanato type estimate: there exists $\alpha > 0$ and a universal constant $C > 0$ such that

$$\fint_{B_r(x_0)} |\Delta h - (\Delta h)_{x_0,r}|^2 \leqslant C\Big(\frac{r}{R}\Big)^{\alpha} \fint_{B_R} |\Delta h - (\Delta h)_{x_0,R}|^2,$$

see, e.g., formula (1.13) on page 96 in [Giaquinta 1983] (see also the notation on page 92 there).

Hence, using also the triangle inequality and recalling (3-4) and (3-5),

$$\begin{aligned}
&\int_{B_r(x_0)} |\Delta u - (\Delta u)_{x_0,r}|^2 \\
&= \int_{B_r(x_0)} |\Delta u - \Delta h + \Delta h - (\Delta h)_{x_0,r} + (\Delta h)_{x_0,r} - (\Delta u)_{x_0,r}|^2 \\
&\leqslant C\bigg(\int_{B_r(x_0)} |\Delta u - \Delta h|^2 + \int_{B_r(x_0)} |\Delta h - (\Delta h)_{x_0,r}|^2 + \int_{B_r(x_0)} |(\Delta h)_{x_0,r} - (\Delta u)_{x_0,r}|^2\bigg) \\
&\leqslant C\bigg(R^n + \Big(\frac{r}{R}\Big)^{\alpha+n} \int_{B_R(x_0)} |\Delta h - (\Delta h)_{x_0,R}|^2\bigg) \\
&= C\bigg(R^n + \Big(\frac{r}{R}\Big)^{\alpha+n} \int_{B_R(x_0)} |\Delta h - \Delta u + \Delta u - (\Delta u)_{x_0,R} + (\Delta u)_{x_0,R} - (\Delta h)_{x_0,R}|^2\bigg) \\
&\leqslant C\bigg[R^n + \Big(\frac{r}{R}\Big)^{\alpha+n} \bigg(\int_{B_R(x_0)} |\Delta h - \Delta u|^2 + \int_{B_R(x_0)} |\Delta u - (\Delta u)_{x_0,R}|^2 + \int_{B_R(x_0)} |(\Delta u)_{x_0,R} - (\Delta h)_{x_0,R}|^2\bigg)\bigg] \\
&\leqslant C\bigg[R^n + \Big(\frac{r}{R}\Big)^{\alpha+n} \bigg(\int_{B_R(x_0)} |\Delta h - \Delta u|^2 + \int_{B_R(x_0)} |\Delta u - (\Delta u)_{x_0,R}|^2\bigg)\bigg] \\
&\leqslant C\bigg[R^n + \Big(\frac{r}{R}\Big)^{\alpha+n} \bigg(R^n + \int_{B_R(x_0)} |\Delta u - (\Delta u)_{x_0,R}|^2\bigg)\bigg] \leqslant C\bigg[R^n + \Big(\frac{r}{R}\Big)^{\alpha+n} \int_{B_R(x_0)} |\Delta u - (\Delta u)_{x_0,R}|^2\bigg].
\end{aligned} \tag{3-6}$$

We can therefore exploit Lemma 2.1 in Chapter 3 on page 86 of [Giaquinta 1983] (see also Lemma 3.1 in [Dipierro and Karakhanyan 2018] and Theorem 1.1 in [Dipierro et al. 2017]), used here with

$$\phi(\rho) := \int_{B_\rho(x_0)} |\Delta u - (\Delta u)_{x_0,\rho}|^2, \quad \beta := n, \quad a := \alpha + n, \quad \beta := n, \quad A := C, \quad \text{and} \quad B := C.$$

Thus writing (3-6) in the form

$$\phi(r) \leqslant C\Big[R^\beta + \Big(\frac{r}{R}\Big)^a \phi(R)\Big] = A\Big[\Big(\frac{r}{R}\Big)^a + \varepsilon\Big]\phi(R) + BR^\beta,$$

and hence deducing that $\phi(r) \leqslant C\big[\big(\frac{r}{R}\big)^\beta \phi(R) + r^\beta\big]$, up to renaming constants, that provides

$$\int_{B_r(x_0)} |\Delta u - (\Delta u)_{x_0,r}|^2 \leqslant Cr^n, \tag{3-7}$$

for a suitable $C > 0$, possibly depending on u, x_0, R_0, which gives the desired result. □

4. First variation of J, free boundary condition, and proof of Theorem 1.3

We consider the first variation of the functional in (1-1). Of course, the main problem is to take into account variations performed by a test function whose support intersects the free boundary of u, since in this case the lack of regularity of the characteristic function plays an important role. Therefore, it is useful to know that the set $\{u > 0\}$ is an open subset of Ω, which, in the case of minimizers, follows from

$$u \in C^{1,\alpha}_{\mathrm{loc}}(\Omega) \text{ for any } \alpha \in (0, 1), \tag{4-1}$$

which, in turn, follows from the fact that

$$u \in W^{2,p}_{\mathrm{loc}}(\Omega) \text{ for any } p \in (1, +\infty), \tag{4-2}$$

in virtue of Theorem 1.1 and the Calderón–Zygmund regularity theory (we think that it is an interesting open problem to establish whether (4-1) and (4-2) are also fulfilled by one-phase minimizers).

The main structural properties of the minimizers which are based on the first variation of the functional are given by the following result:

Lemma 4.1. *Let u be a minimizer of J. Then u is weakly super-biharmonic in Ω (i.e., $\Delta^2 u \leqslant 0$ in the sense of distributions) and biharmonic in $\{u > 0\} \cup \{u < 0\}^\circ$, where E° denotes the interior of E.*

Similarly, if u is a one-phase minimizer of J and B is an open ball contained in $\{u \geqslant a\}$, with $a > 0$, then u is biharmonic in B.

Proof. We prove the claims assuming that u is a minimizer (the one-phase problem can be treated similarly). Define $u_\varepsilon := u - \varepsilon\phi$, where $0 \leqslant \phi \in W^{2,2}(\Omega) \cap W^{1,2}_0(\Omega)$ and ε is a small parameter to be fixed below. Using the comparison of the energies of u and u_ε, and recalling (1-1), we get

$$\int_\Omega \big(|\Delta u|^2 - |\Delta u - \varepsilon\Delta\phi|^2\big) \leqslant \int_\Omega (\chi_{\{u-\varepsilon\phi>0\}} - \chi_{\{u>0\}}).$$

Note that $\{u - \varepsilon\phi > 0\} \subset \{u > 0\}$, provided that $\varepsilon > 0$. Consequently, we have

$$0 \geqslant \int_\Omega \big(|\Delta u|^2 - |\Delta u - \varepsilon\phi|^2\big) = 2\varepsilon \int_\Omega \Delta u\, \Delta\phi - \varepsilon^2 \int_\Omega (\Delta u)^2. \tag{4-3}$$

Dividing both sides of the last inequality by $\varepsilon > 0$ and then letting $\varepsilon \to 0$, we get that $\int_\Omega \Delta u\, \Delta\phi \leqslant 0$. If we take $\phi \in C^\infty_0(\Omega)$, this gives that u is super-biharmonic. In addition, if we suppose that $\operatorname{supp}\phi \subset \{u > 0\}$, then from (4-3) we deduce, without any sign assumption on ε, that $\int_\Omega \Delta u\, \Delta\phi = 0$. □

Concerning the statement of Lemma 4.1, it is interesting to remark that one-phase minimizers are not necessarily super-biharmonic (an explicit counterexample to this fact is discussed on page 898).

The basic analytic structure of the minimizers is then completed by the following result:

Corollary 4.2. *Let u be a minimizer of J. For every bounded subdomain $\Omega' \subset\subset \Omega$, there exists $C > 0$, depending only on n, such that*

$$\Delta u \geqslant -\frac{C\|\Delta u\|_{L^1(\Omega)}}{(\operatorname{dist}(\Omega', \partial\Omega))^n} \quad \text{in } \Omega'.$$

Proof. Let $r := \frac{1}{2}\,\mathrm{dist}(\Omega', \partial\Omega)$ and, for all $y \in \Omega'$, define the function

$$\phi(y) := \fint_{B_r(y)} \Delta u(x)\,dx.$$

Thanks to (4-2), we see that ϕ is continuous on the compact set $\overline{\Omega}'$. Therefore, there exists $y_0 \in \overline{\Omega}'$ such that $\min_{\overline{\Omega}'} \phi(y) = \phi(y_0)$. Then, for any $y \in \Omega'$,

$$\phi(y) \geqslant \phi(y_0) \geqslant -\fint_{B_r(y_0)} |\Delta u(x)|\,dx \geqslant -\frac{\|\Delta u\|_{L^1(\Omega)}}{|B_r|}. \tag{4-4}$$

As a consequence, since u is super-biharmonic, thanks to Lemma 4.1, we obtain the desired estimate by the mean value inequality for weak subsolutions of the Laplace equation (see, e.g., [Serrin 2011] and [Littman 1963]). More precisely, if v is weakly super-harmonic in Ω, we know from Theorem A in [Littman 1963] that there exists a sequence of smooth super-harmonic functions v_h in Ω' that converge to v a.e. in Ω' and in $L^1(\Omega')$. Consequently, a.e. $y \in \Omega'$,

$$v(y) = \lim_{h\to 0} v_h(y) \geqslant \lim_{h\to 0} \fint_{B_r(y_0)} v_h(x)\,dx = \fint_{B_r(y_0)} v(x)\,dx. \tag{4-5}$$

Then, choosing $v := \Delta u$ and applying (4-4), we find that

$$\Delta u(y) \geqslant \fint_{B_r(y)} \Delta u(x)\,dx = \phi(y) \geqslant -\frac{\|\Delta u\|_{L^1(\Omega)}}{|B_r|}.$$ □

For the sake of completeness, we observe that the statement of Corollary 4.2 can be strengthen by showing, under additional regularity assumptions, that minimizers are super-harmonic, according to:

Proposition 4.3. *Let u be a minimizer of J. Assume that*

$$u \in C(\overline{\Omega}). \tag{4-6}$$

Assume also that

$$\Delta u \text{ is } C^1 \text{ in a neighborhood of } \partial\Omega, \tag{4-7}$$

and that

$$\partial\Omega \cap \{|u| > 0\} \text{ is dense in } \partial\Omega. \tag{4-8}$$

Then,

$$\Delta u \geqslant 0 \quad \text{a.e. in } \Omega. \tag{4-9}$$

We think that the result of Proposition 4.3 is helpful to understand the geometric structure of the minimizers: nevertheless, since it is not used in the rest of this paper, we deferred its proof to Appendix C.

In Example 4 of Section 5 (see page 903), we will further discuss the result of Proposition 4.3, also in view of the free boundary conditions provided by Theorem 1.3 and of the bi-harmonicity properties outside the free boundary discussed in Lemma 4.1.

Next we compute the first domain variation (for this, we use the notation in which subscripts denote differentiation and superscripts denote coordinates).

Lemma 4.4. *Let u be a minimizer or a one-phase minimizer of J. For any $\phi = (\phi^1, \dots, \phi^n) \in C_0^\infty(\Omega)$,*

$$2\int_\Omega \Delta u(x) \sum_{m=1}^n \big(2\nabla u_m(x)\cdot\nabla\phi^m(x)+u_m(x)\Delta\phi^m(x)\big)\,dx = \int_\Omega \big(|\Delta u(x)|^2+\chi_{\{u>0\}}(x)\big)\operatorname{div}\phi(x)\,dx. \tag{4-10}$$

Proof. Fix $\varepsilon \in \mathbb{R}$ (to be taken with $|\varepsilon|$ small in the sequel). Let

$$u_\varepsilon(x) := u(x+\varepsilon\phi(x)). \tag{4-11}$$

Notice that u_ε is an admissible competitor for u (in case we are dealing with the one-phase problem, observe that $u_\varepsilon \geqslant 0$ if $u \geqslant 0$).

For any $i \in \{1, \dots, n\}$, we have

$$\begin{aligned}
\partial_i u_\varepsilon &= \sum_{m=1}^n u_m(\delta_{mi}+\varepsilon\phi_i^m) \\
\partial_{ii} u_\varepsilon &= \sum_{m,l=1}^n u_{ml}(\delta_{li}+\varepsilon\phi_i^l)(\delta_{mi}+\varepsilon\phi_i^m) + \sum_{m=1}^n u_m\varepsilon\phi_{ii}^m \\
&= u_{ii} + \varepsilon\Big[\sum_{m,l=1}^n (u_{ml}\phi_i^l\delta_{mi} + u_{ml}\phi_i^m\delta_{li}) + \sum_{m=1}^n u_m\phi_{ii}^m\Big] + \varepsilon^2\sum_{m,l=1}^n u_{ml}\phi_i^l\phi_i^m \\
&= u_{ii} + \varepsilon\sum_{m=1}^n (2u_{mi}\phi_i^m + u_m\phi_{ii}^m) + \varepsilon^2\sum_{m,l=1}^n u_{ml}\phi_i^l\phi_i^m.
\end{aligned}$$

We use the change of variable $y := x+\varepsilon\phi(x)$. Noticing $\phi(x) = \phi(y-\varepsilon\phi(x)) = \phi(y)+O(\varepsilon)$, we get

$$\begin{aligned}
J[u_\varepsilon] &= \int_\Omega \Bigg\{\bigg|\sum_{i=1}^n\Big[u_{ii}(x+\varepsilon\phi(x)) + \varepsilon\sum_{m=1}^n\big(2u_{mi}(x+\varepsilon\phi(x))\phi_i^m(x) + u_m(x+\varepsilon\phi(x))\phi_{ii}^m(x)\big)\Big] \\
&\qquad\qquad + o(\varepsilon)\bigg|^2 + \chi_{\{u>0\}}(x+\varepsilon\phi(x))\Bigg\}\,dx \\
&= \int_\Omega \Bigg\{\bigg|\sum_{i=1}^n\Big[u_{ii}(y) + \varepsilon\sum_{m=1}^n\big(2u_{mi}(y)\phi_i^m(y) + u_m(y)\phi_{ii}^m(y)\big)\Big] + o(\varepsilon)\bigg|^2 + \chi_{\{u>0\}}(y)\Bigg\} \\
&\qquad\qquad \times (1-\varepsilon\operatorname{div}\phi(y)+o(\varepsilon))\,dy \\
&= \int_\Omega \Bigg\{\bigg|\sum_{i=1}^n u_{ii}(y) + \varepsilon\sum_{i,m=1}^n\big(2u_{mi}(y)\phi_i^m(y) + u_m(y)\phi_{ii}^m(y)\big)\bigg|^2 + \chi_{\{u>0\}}(y)\Bigg\}(1-\varepsilon\operatorname{div}\phi(y))\,dy + o(\varepsilon) \\
&= \int_\Omega \Bigg\{\sum_{i,j=1}^n u_{ii}(y)u_{jj}(y) + 2\varepsilon\sum_{i,j,m=1}^n \big(2u_{jj}(y)u_{mi}(y)\phi_i^m(y) + u_{jj}(y)u_m(y)\phi_{ii}^m(y)\big) + \chi_{\{u>0\}}(y)\Bigg\} \\
&\qquad\qquad \times (1-\varepsilon\operatorname{div}\phi(y))\,dy + o(\varepsilon) \\
&= J[u] - \varepsilon\int_\Omega \Bigg\{\big(|\Delta u(y)|^2 + \chi_{\{u>0\}}(y)\big)\operatorname{div}\phi(y) \\
&\qquad\qquad - 2\Delta u(y)\sum_{m=1}^n\big(2\nabla u_m(y)\cdot\nabla\phi^m(y) + u_m(y)\Delta\phi^m(y)\big)\Bigg\}\,dy + o(\varepsilon).
\end{aligned}$$

Thus, taking the derivative in ε and evaluating it at $\varepsilon = 0$, we obtain (4-10), as desired. □

As a consequence of Lemma 4.4, we obtain the free boundary condition of Theorem 1.3:

Proof of Theorem 1.3. We use the notation

$$g(x) := |\Delta u(x)|^2 + \chi_{\{u>0\}}(x), \quad G^m(x) := \Delta u(x)\nabla u_m(x), \quad \text{and} \quad H^m(x) := \Delta u(x) u_m(x)$$

for each $m \in \{1, \dots, n\}$.

We let $\phi \in C_0^\infty(\Omega)$, and we claim that

$$g \operatorname{div}\phi - 4\sum_{m=1}^{n} G^m \cdot \nabla\phi^m - 2\sum_{m=1}^{n} H^m \Delta\phi^m = 0 \quad \text{a.e. in } \Omega. \tag{4-12}$$

To check this, we recall:

$$\text{If } f \in W^{1,1}_{\text{loc}}(\Omega), \text{ then } \nabla f = 0 \text{ a.e. in } \{x \in \Omega : f = 0\}, \tag{4-13}$$

see, e.g., Theorem 6.19 in [Lieb and Loss 2001] (used here with $A := \{0\}$). Then, first of all, since $u \in W^{2,2}(\Omega)$, we deduce from (4-13) that

$$\nabla u(x) = 0 \quad \text{for all } x \in \{u = 0\} \setminus Z, \tag{4-14}$$

for a suitable Z of null measure. Furthermore, for every $j \in \{1, \dots, n\}$, we have that $\partial_j u \in W^{1,2}(\Omega)$. Accordingly, using (4-13) once again, we find

$$\nabla\partial_j u(x) = 0 \quad \text{for all } x \in \{\partial_j u = 0\} \setminus Z_j, \tag{4-15}$$

with Z_j of null measure.

We also remark that

$$\{\partial_j u = 0\} \supseteq \{u = 0\} \setminus Z,$$

thanks to (4-14), and therefore (4-15) yields

$$\nabla\partial_j u(x) = 0 \quad \text{for all } x \in \{u = 0\} \setminus (Z \cup Z_j). \tag{4-16}$$

Hence, defining $Z^\star := Z \cup Z_1 \cup \dots Z_n$, we have that $Z^\star$ has null measure and, by (4-14) and (4-16),

$$D^2 u(x) = 0 \quad \text{for every } x \in \{u = 0\} \setminus Z^\star. \tag{4-17}$$

Moreover, if $x \in \{u = 0\}$, then $\chi_{\{u>0\}}(x) = 0$. This and (4-17) give that $g = G^m = H^m = 0$ in $\{u = 0\} \setminus Z^\star$, which in turn yields (4-12), as desired.

As a consequence of (4-12) and of the Monotone Convergence Theorem, we deduce that

$$\int_\Omega \Big(g \operatorname{div}\phi - 4\sum_{m=1}^{n} G^m \cdot \nabla\phi^m - 2\sum_{m=1}^{n} H^m \Delta\phi^m \Big) = \lim_{\varepsilon\to 0} \int_{\Omega\cap\{|u|>\varepsilon\}} \Big(g \operatorname{div}\phi - 4\sum_{m=1}^{n} G^m \cdot \nabla\phi^m - 2\sum_{m=1}^{n} H^m \Delta\phi^m \Big).$$

Therefore, recalling (4-10) and (1-7), we find that

$$\begin{aligned} 0 &= \int_\Omega \Big(g \ \operatorname{div} \phi - 4 \sum_{m=1}^{n} G^m \cdot \nabla \phi^m - 2 \sum_{m=1}^{n} H^m \Delta \phi^m \Big) \\ &= \lim_{\varepsilon \to 0} \int_{\Omega \cap \{|u| > \varepsilon\}} \Big(g \ \operatorname{div} \phi - 4 \sum_{m=1}^{n} G^m \cdot \nabla \phi^m - 2 \sum_{m=1}^{n} H^m \Delta \phi^m \Big) \\ &= \lim_{\varepsilon \to 0} \int_{\Omega \cap \{|u| > \varepsilon\}} \Big(\operatorname{div}(g\, \phi) - 4 \sum_{m=1}^{n} \operatorname{div}(\phi^m G^m) - 2 \sum_{m=1}^{n} \operatorname{div}(H^m \nabla \phi^m) \\ &\qquad\qquad + 4 \sum_{m=1}^{n} \phi^m \operatorname{div} G^m + 2 \sum_{m=1}^{n} \nabla H^m \cdot \nabla \phi^m - \nabla g \cdot \phi \Big). \end{aligned} \tag{4-18}$$

We remark that, in $\{|u| > \varepsilon\}$,

$$\begin{aligned} &4 \sum_{m=1}^{n} \phi^m \operatorname{div} G^m + 2 \sum_{m=1}^{n} \nabla H^m \cdot \nabla \phi^m - \nabla g \cdot \phi \\ &= \sum_{m=1}^{n} \big(4\phi^m (\nabla \Delta u \cdot \nabla u_m + \Delta u \Delta u_m) + 2(u_m \nabla \Delta u + \Delta u \nabla u_m) \cdot \nabla \phi^m - 2 \Delta u \Delta u_m \phi^m \big) \\ &= \sum_{m=1}^{n} \big(4 \nabla \Delta u \cdot \nabla u_m \phi^m + 2 \Delta u \Delta u_m \phi^m + 2(u_m \nabla \Delta u + \Delta u \nabla u_m) \cdot \nabla \phi^m \big) \\ &= \sum_{m=1}^{n} \big(4 \nabla \Delta u \cdot \nabla u_m \phi^m + 2 \Delta u \Delta u_m \phi^m + 2 \operatorname{div}(\phi^m (u_m \nabla \Delta u + \Delta u \nabla u_m)) - 2 \operatorname{div}(u_m \nabla \Delta u + \Delta u \nabla u_m) \phi^m \big) \\ &= 2 \sum_{m=1}^{n} \big(\operatorname{div}(\phi^m (u_m \nabla \Delta u + \Delta u \nabla u_m)) - u_m \Delta^2 u \phi^m \big) = 2 \sum_{m=1}^{n} \operatorname{div}(\phi^m (u_m \nabla \Delta u + \Delta u \nabla u_m)), \end{aligned}$$

by virtue of Lemma 4.1. As a consequence, we see that

$$\begin{aligned} \int_{\Omega \cap \{|u| > \varepsilon\}} \Big(4 \sum_{m=1}^{n} \phi^m \operatorname{div} G^m + 2 \sum_{m=1}^{n} \nabla H^m \cdot \nabla \phi^m - \nabla g \cdot \phi \Big) &= 2 \sum_{m=1}^{n} \int_{\Omega \cap \{|u| > \varepsilon\}} \operatorname{div}(\phi^m (u_m \nabla \Delta u + \Delta u \nabla u_m)) \\ &= 2 \sum_{m=1}^{n} \int_{\partial(\Omega \cap \{|u| > \varepsilon\})} \phi^m (u_m \nabla \Delta u + \Delta u \nabla u_m) \cdot \nu, \end{aligned}$$

where ν is the exterior normal to $\Omega \cap \{|u| > \varepsilon\}$. Hence, using this information in (4-18), we obtain

$$\begin{aligned} 0 &= \lim_{\varepsilon \to 0} \int_{\partial(\Omega \cap \{|u| > \varepsilon\})} \Big(g\, \phi \cdot \nu - \sum_{m=1}^{n} \big(4 \phi^m G^m \cdot \nu + 2 H^m \nabla \phi^m \cdot \nu - 2 \phi^m (u_m \nabla \Delta u + \Delta u \nabla u_m) \cdot \nu \big) \Big) \\ &= \lim_{\varepsilon \to 0} \int_{\partial(\Omega \cap \{|u| > \varepsilon\})} \Big(\big(|\Delta u|^2 + \chi_{\{u > 0\}} \big) \phi \cdot \nu - 2 \sum_{m=1}^{n} \big(\phi^m (\Delta u \nabla u_m - u_m \nabla \Delta u) \cdot \nu + \Delta u u_m \nabla \phi^m \cdot \nu \big) \Big). \end{aligned}$$

This gives (1-8). To obtain (1-9), use the two different scales of the test function ϕ^m and its derivative. □

Remark 4.5. We point out if $n = 1$, when the free boundary divides regions of positivity and nonpositivity of u (say, $u^{(1)} > 0$ and the interior of $u^{(2)} \leqslant 0$), formula (1-9) gives the free boundary conditions

$$\ddot{u}^{(1)}\dot{u}^{(1)} = \ddot{u}^{(2)}\dot{u}^{(2)} \tag{4-19}$$

$$2\dot{u}^{(1)}\dddot{u}^{(1)} - |\ddot{u}^{(1)}|^2 + 1 = 2\dot{u}^{(2)}\dddot{u}^{(2)} - |\ddot{u}^{(2)}|^2. \tag{4-20}$$

Also, since $u \in W^{2,2}(\Omega)$ and $n = 1$, by standard embedding results we already know that $u \in C^1(\Omega)$. This, in view of (4-19), implies that either $\dot{u} = 0$ at a free boundary point, or $\ddot{u}^{(1)} = \ddot{u}^{(2)}$. That is, either u has horizontal tangent at a free boundary point, or it is C^2 across the free boundary point. Hence, from (4-20), we have the following one-dimensional dichotomy for the free boundary points:

$$\text{either: } \dot{u} = 0 \text{ and } |\ddot{u}^{(1)}|^2 - |\ddot{u}^{(2)}|^2 = 1, \tag{4-21}$$

$$\text{or: } \dot{u} \neq 0,\, u \text{ is } C^2 \text{ across and } \dddot{u}^{(1)} = \dddot{u}^{(2)} - \frac{1}{2\dot{u}}\,. \tag{4-22}$$

5. Some examples in dimension 1

Example 5.1. To better understand Remark 4.5, we can sketch some one-dimensional computations. Namely, we let $n = 1$, consider an interval $\Omega := (0, A)$, with $A > 0$, and prescribe the Navier conditions $u(0) = \ddot{u}(0) = 0$, $u(A) = 1$ and $\ddot{u}(A) = 0$. We look for one-phase minimizers of J with such boundary conditions.

In this case, by the finiteness of the energy and Sobolev embedding, we know that the one-phase minimizer is $C^1(0, A)$; also the free boundary points are minimal point for u, and therefore

$$\dot{u} = 0 \text{ at any free boundary point.} \tag{5-1}$$

Accordingly, condition (4-21) prescribes that

$$\ddot{u}^+ = 1. \tag{5-2}$$

Let us see how such condition emerges from energy considerations. We suppose that the problem develops a free boundary and we denote by $a \in (0, A)$ the largest free boundary point, i.e., $u(a) = 0$ and $u > 0$ in (a, A). From Lemma 4.1, we know that $\ddddot{u} = 0$ in (a, A), and so u is a polynomial of degree 3 in (a, A). Consequently, we can write, for any $x \in (a, A)$,

$$u(x) = \alpha(x-a) + \beta(x-a)^2 + \gamma(x-a)^3.$$

Recalling (5-1), we conclude that $\alpha = 0$. Imposing the boundary conditions at the point $x = A$, we find

$$\beta = \frac{3}{2(A-a)^2} \quad \text{and} \quad \gamma = -\frac{1}{2(A-a)^3},$$

and therefore,

$$u(x) = \frac{3(x-a)^2}{2(A-a)^2} - \frac{(x-a)^3}{2(A-a)^3}. \tag{5-3}$$

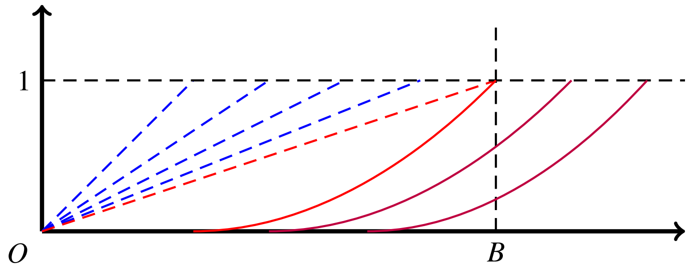

Figure 2. The one-phase minimizers of a one-dimensional problem, in dependence of the right endpoint. We stress that the ones with a nontrivial zero level sets are one-phase minimizers, but not minimizers (see Proposition B.1).

The goal is then to choose $a \in (0, A)$ in order to minimize the energy contribution of u in (a, A), namely we want to minimize the function

$$\begin{aligned}\Phi(a) &:= \int_a^A |\ddot{u}(x)|^2\,dx + (A-a)\\ &= \int_a^A \left|\frac{3}{(A-a)^2} - \frac{3(x-a)}{(A-a)^3}\right|^2 dx + (A-a)\\ &= 9\int_a^A \left|\frac{(A-a)-(x-a)}{(A-a)^3}\right|^2 dx + (A-a)\\ &= \frac{9}{(A-a)^6}\int_a^A |A-x|^2\,dx + (A-a) = \frac{3}{(A-a)^3} + (A-a),\end{aligned}$$

which attains its minimum for

$$a = A - \sqrt{3}. \tag{5-4}$$

That is, comparing with the linear function $\ell(x) := \dfrac{x}{A}$, we have that

$$A = J[\ell] \geqslant J[u] \geqslant \Phi(a) \geqslant \Phi(A-\sqrt{3}) = \frac{1}{\sqrt{3}} + \sqrt{3}.$$

This means that when $A < \frac{1}{\sqrt{3}} + \sqrt{3} =: B$, the problem does not develop any free boundary; when $A = B$ the problem has two minimizers, and when $A > B$ the minimizer in (5-3) becomes

$$u(x) = \frac{(x-a)^2}{2} - \frac{(x-a)^3}{2\cdot 3^{3/2}}, \tag{5-5}$$

for which $\ddot{u}(a^+) = 1$. This checks (5-2) in this case.

The description of the different one-phase minimizers in dependence of the endpoint A is sketched in Figure 2. It is also worth pointing out:

The one-phase minimizers described here are *not* super-biharmonic, (5-6) and this creates a major difference with respect to the case of minimizers, compare with Lemma 4.1: indeed, if $\varphi \in C_0^\infty((0,A),[0,+\infty))$ and $A > \frac{1}{\sqrt{3}} + \sqrt{3}$, from (5-4) and (5-5) we see that

$$\begin{aligned}\int_0^A \ddot{u}\ddot{\varphi} = \int_a^A \Big(1 - \frac{x-a}{\sqrt{3}}\Big)\ddot{\varphi} &= \Big(1-\frac{A-a}{\sqrt{3}}\Big)\dot{\varphi}(A) - \dot{\varphi}(a) - \int_a^A \frac{d}{dx}\Big(1-\frac{x-a}{\sqrt{3}}\Big)\dot{\varphi} \\ &= 0 - \dot{\varphi}(a) + \frac{1}{\sqrt{3}}\int_a^A \dot{\varphi} = -\dot{\varphi}(a) - \frac{\varphi(a)}{\sqrt{3}},\end{aligned}$$

which has no sign, thus proving (5-6).

Example 5.2. Having clarified condition (4-21) in a concrete example, we aim now at clarifying the role of condition (4-22). Such condition is, in a sense, more unusual, since it prescribes the matching of the second derivatives at the free boundary points with nontrivial slopes, with the bulk term of the energy producing a discontinuity on the third derivatives.

To understand this phenomenon in a concrete example, we fix a small parameter $\varepsilon > 0$ and minimize the energy functional

$$J[u] = \int_{-1}^{1} \big(|\ddot{u}(x)|^2 + \varepsilon\chi_{\{u>0\}}(x)\big)\,dx,$$

subject to the Navier conditions

$$u(-1) = -1, \quad \ddot{u}(-1) = 0, \quad u(1) = 1, \quad \ddot{u}(1) = 0. \tag{5-7}$$

If we call u_ε such minimizer, we can bound the energy of u_ε with that of the identity function. This produces a uniform bound for u_ε in $W^{2,2}((-1,1))$, which implies that u_ε converges in $C^1((-1,1))$ to the identity function as $\varepsilon \to 0$. Consequently, for a fixed and small $\varepsilon > 0$, we can find some $a \in (-1,1)$, which depends on ε, such that

$$u_\varepsilon(x) = \begin{cases} \underline{\alpha}(a-x) + \underline{\beta}(a-x)^2 + \underline{\gamma}(a-x)^3 & \text{if } x \in (-1,a), \\ \bar{\alpha}(x-a) + \bar{\beta}(x-a)^2 + \bar{\gamma}(x-a)^3 & \text{if } x \in [a,1). \end{cases}$$

The condition that $u_\varepsilon \in C^1((-1,1))$ (with derivative close to 1 when ε is small) implies that $-\underline{\alpha} = \bar{\alpha} = \alpha$, for some $\alpha > 0$ (which depends on ε and it is close to 1 when ε is small). Imposing the boundary conditions in (5-7), we find

$$\underline{\beta} = -\frac{3(1-\alpha(1+a))}{2(1+a)^2}, \quad \underline{\gamma} = \frac{1-\alpha(1+a)}{2(1+a)^3}, \quad \bar{\beta} = \frac{3(1-\alpha(1-a))}{2(1-a)^2}, \quad \bar{\gamma} = \frac{\alpha(1-a)-1}{2(1-a)^3}. \tag{5-8}$$

Therefore, the energy of u_ε corresponds to the function

$$\begin{aligned}\Psi(a,\alpha) := J[u_\varepsilon] &= \int_{-1}^{a} |2\underline{\beta} + 6\underline{\gamma}(a-x)|^2\,dx + \int_a^1 |2\bar{\beta} + 6\bar{\gamma}(x-a)|^2\,dx + \varepsilon(1-a) \\ &= \Big(\frac{3(1-\alpha(1+a))}{(1+a)^3}\Big)^2 \int_{-1}^{a} |1+x|^2\,dx + \Big(\frac{3(1-\alpha(1-a))}{(1-a)^3}\Big)^2 \int_a^1 |1-x|^2\,dx + \varepsilon(1-a) \\ &= \frac{3(1-\alpha(1+a))^2}{(1+a)^3} + \frac{3(1-\alpha(1-a))^2}{(1-a)^3} + \varepsilon(1-a).\end{aligned}$$

Thus, we have to minimize such function for $(a, \alpha) \in (-1, 1) \times (0, +\infty)$, and in fact we know that such minimum is localized at $(0, 1)$ when $\varepsilon = 0$. Therefore, to find the minima of Ψ, we solve the system

$$\begin{cases} 0 = \partial_a \Psi = \dfrac{12a(\alpha a^4(\alpha+2) + 2a^2(2\alpha - \alpha^2 + 3) + \alpha^2 - 6\alpha + 6)}{(1-a^2)^4} - \varepsilon, \\ 0 = \partial_\alpha \Psi = 12\, \dfrac{\alpha - 1 - a^2(1+\alpha)}{(1-a^2)^2}. \end{cases} \tag{5-9}$$

The latter equation produces

$$a^2 = \frac{\alpha - 1}{1+\alpha}. \tag{5-10}$$

We notice that, by (5-8),

$$\frac{2}{3}(\bar\beta - \underline{\beta}) = \frac{1-\alpha(1-a)}{(1-a)^2} + \frac{1-\alpha(1+a)}{(1+a)^2} = \frac{2((\alpha+1)a^2 - \alpha + 1)}{(1-a^2)^2}.$$

Hence, in view of (5-10),

$$\frac{2}{3}(\bar\beta - \underline{\beta}) = \frac{2((\alpha+1)\frac{\alpha-1}{1+\alpha} - \alpha + 1)}{(1-a^2)^2} = \frac{2(\alpha - 1 - \alpha + 1)}{(1-a^2)^2} = 0,$$

and so $\bar\beta = \underline{\beta}$. This says that the second derivatives match at the free boundary point, in agreement with the condition in (4-22).

In addition, by (5-8),

$$\begin{aligned} 4\alpha(\bar\gamma + \underline{\gamma}) &= 2\alpha\left(\frac{\alpha(1-a) - 1}{(1-a)^3} + \frac{1-\alpha(1+a)}{(1+a)^3}\right) \\ &= -\frac{4\alpha a\,(a^2(2\alpha+1) - 2\alpha + 3)}{(1-a^2)^3} = -\frac{4\alpha a\,(-2\alpha a^4 - a^4 + 4\alpha a^2 - 2a^2 - 2\alpha + 3)}{(1-a^2)^4}. \end{aligned} \tag{5-11}$$

On the other hand, the first equation in (5-9) says that

$$\frac{12a}{(1-a^2)^4} = \frac{\varepsilon}{\alpha a^4(\alpha+2) + 2a^2(2\alpha - \alpha^2 + 3) + \alpha^2 - 6\alpha + 6}.$$

Using this information in (5-11), we deduce that

$$12\alpha(\bar\gamma + \underline{\gamma}) = -\frac{\varepsilon\,\alpha\,(-2\alpha a^4 - a^4 + 4\alpha a^2 - 2a^2 - 2\alpha + 3)}{\alpha a^4(\alpha+2) + 2a^2(2\alpha - \alpha^2 + 3) + \alpha^2 - 6\alpha + 6}. \tag{5-12}$$

Moreover, in view of (5-10), we have

$$-2\alpha a^4 - a^4 + 4\alpha a^2 - 2a^2 - 2\alpha + 3 = \frac{4}{(1+\alpha)^2}, \quad \alpha a^4(\alpha+2) + 2a^2(2\alpha - \alpha^2 + 3) + \alpha^2 - 6\alpha + 6 = \frac{4\alpha}{(1+\alpha)^2}.$$

Hence, we insert these identities into (5-12) and we find that

$$2\dot u(a)\,(\,\ddot u(a^+) - \ddot u(a^-)) = 12\alpha(\bar\gamma + \underline{\gamma}) = -\frac{\varepsilon\alpha\dfrac{4}{(1+\alpha)^2}}{\dfrac{4\alpha}{(1+\alpha)^2}} = -\varepsilon,$$

in agreement with the third derivative prescription in (4-22).

Example 5.3. As a variation of Example 5.2, we point out that positive data can yield minimizers which change sign, thus providing an important difference with respect to the classical cases in which the energy is driven by the standard Dirichlet form. This example is interesting also because it shows that, in our framework, this "loss of Maximum Principle" can occur even when the domain is a ball (in fact, even in one dimension, when the domain is an interval) and even when the data is strictly positive.

In this sense, this example is instructive since it shows that, even in domains in which the Maximum Principle holds for biharmonic equations (such as the ball, as established in [Boggio 1905]), the Maximum Principle can be violated in our framework due to the important role played by the "bulk" term in the energy functional.

To construct our example, we take $A > 0$ and we look for minimizers in $(-A, A)$ with boundary conditions $u(A) = u(-A) = 1$ and $\ddot{u}(A) = \ddot{u}(-A) = 0$.

First of all, we observe that

$$J[u] \leqslant C, \tag{5-13}$$

for some $C > 0$ independent of A. To this end, we take $\phi \in C^\infty(\mathbb{R}, [0, +\infty))$ such that $\phi(x) = 0$ for all $x \leqslant 1$ and $\phi(x) = x - 2$ for all $x \geqslant \frac{5}{2}$. Then, assuming $A \geqslant 5$, we define

$$v(x) := \begin{cases} \phi(x+3-A) & \text{if } x \in (A-4, A], \\ 0 & \text{if } x \in [-A+4, A-4], \\ \phi(-x+3-A) & \text{if } x \in [-A, -A+4). \end{cases}$$

We observe $v(A) = \phi(3) = 3-2 = 1$ and $v(-A) = \phi(-x+3-A) = \phi(3) = 1$. Moreover $\ddot{v}(A) = \ddot{\phi}(3) = 0$ and $\ddot{v}(-A) = \ddot{\phi}(3) = 0$. Therefore,

$$\begin{aligned} J[u] \leqslant J[v] \leqslant \int_{-A}^{A} \big(|\ddot{v}|^2 + \chi_{\{v>0\}}\big) &= \int_{[-A,-A+4)\cup(A-4,A]} \big(|\ddot{v}|^2 + \chi_{\{v>0\}}\big) \\ &\leqslant \int_{[-A,-A+4)} |\ddot{\phi}(-x+3-A)|^2\,dx + \int_{(A-4,A]} |\ddot{\phi}(x+3-A)|^2\,dx \\ &= \int_{[-1,3)} |\ddot{\phi}(y)|^2\,dx + \int_{(-1,3]} |\ddot{\phi}(y)|^2\,dx + 8 \\ &\leqslant 8(\|\phi\|_{C^2([-1,3])} + 1), \end{aligned}$$

which proves (5-13).

Now we show that, if A is sufficiently large, then:

$$\text{The minimizer } u \text{ cannot be strictly positive in } (-A, A). \tag{5-14}$$

To check this, we argue by contradiction, supposing that $u > 0$ in $(-A, A)$. Therefore, $\ddot{\ddot{u}} = 0$, and hence u must be a polynomial of degree 3, namely

$$u(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3.$$

As a consequence,

$$0 = \ddot{u}(\pm A) = 2a_2 \pm 6a_3 A,$$

and hence

$$2a_2 + 6a_3 A = 0 = 2a_2 - 6a_3 A,$$

which yields $a_3 = 0$ and as a result $a_2 = 0$. Accordingly,

$$1 = u(\pm A) = a_0 \pm a_1 A,$$

giving that

$$a_0 + a_1 A = 1 = a_0 - a_1 A,$$

and therefore $a_1 = 0$, which also implies $a_0 = 1$. In this way, we found $u(x) = 1$ for all $x \in (-A, A)$, and consequently $J[u] = 2A$. This is in contradiction with (5-13) as long as A is sufficiently large, and so we have established (5-14).

We now strengthen (5-14) by proving:

$$\text{The set } \{u < 0\} \text{ is nonempty.} \tag{5-15}$$

For this, we first use (5-14) to find a point $\bar{x} \in (-A, A)$ such that $u(\bar{x}) \leqslant 0$. If $u(\bar{x}) < 0$ we are done, hence we can suppose $0 = u(\bar{x}) \leqslant u(x)$ for all $x \in (-A, A)$. By the finiteness of the energy and Sobolev embedding, we know the one-phase minimizer is $C^{1,\alpha}(0, A)$, for some $\alpha \in (0, 1)$. In particular, we can take $\bar{x}$ as large as possible in the zero set of u, finding that $u > 0$ in $(\bar{x}, A]$, and therefore we can write

$$0 < u(x) \leqslant C_0 |x - \bar{x}|^{1+\alpha} \quad \text{for all } x \in (\bar{x}, A],$$

for some $C_0 > 0$. Notice also that

$$1 = u(A) - u(\bar{x}) \leqslant \|u\|_{C^1((-A,A))}(A - \bar{x}),$$

and therefore, $A - \bar{x} \geqslant c_0$, for some $c_0 > 0$.

Now, given $\varepsilon > 0$, to be taken conveniently small in what follows, we define

$$\delta := \left(\frac{\varepsilon}{C_0}\right)^{1/(1+\alpha)}, \tag{5-16}$$

and in this way $\delta < c_0$ if ε is sufficiently small. Furthermore, we observe if $x \in (\bar{x}, \bar{x} + \delta] \subset (\bar{x}, A]$, then

$$0 < u(x) \leqslant C_0 \delta^{1+\alpha} = \varepsilon,$$

that is, $(\bar{x}, \bar{x} + \delta] \subseteq \{0 < u \leqslant \varepsilon\}$. For this reason,

$$\delta \leqslant |\{0 < u \leqslant \varepsilon\}| = |\{u > 0\}| - |\{u > \varepsilon\}|. \tag{5-17}$$

We now define

$$u_\varepsilon(x) := \frac{u(x) - \varepsilon}{1 - \varepsilon},$$

and we point out that

$$u_\varepsilon(\pm A) = \frac{u(\pm A) - \varepsilon}{1 - \varepsilon} = \frac{1 - \varepsilon}{1 - \varepsilon} = 1 \quad \text{and} \quad \ddot{u}_\varepsilon(\pm A) = \frac{\ddot{u}(\pm A)}{1 - \varepsilon} = 0.$$

This says that u_ε is a competitor for u, hence, recalling (5-13) and (5-17),

$$0 \leqslant J[u_\varepsilon] - J[u] = \int_{-A}^{A} \left(|\ddot{u}_\varepsilon|^2 - |\ddot{u}|^2 + \chi_{\{u_\varepsilon>0\}} - \chi_{\{u>0\}}\right) = \int_{-A}^{A} \left(\left|\frac{\ddot{u}}{1-\varepsilon}\right|^2 - |\ddot{u}|^2 + \chi_{\{u>\varepsilon\}} - \chi_{\{u>0\}}\right)$$
$$\leqslant \frac{2\varepsilon - \varepsilon^2}{(1-\varepsilon)^2} \int_{-A}^{A} |\ddot{u}|^2 + |\{u > \varepsilon\}| - |\{u > 0\}| \leqslant C_1 \varepsilon - \delta,$$

for some $C_1 > 0$.

From this and (5-16), it follows that

$$C_1 \geqslant \frac{\delta}{\varepsilon} = \frac{1}{\varepsilon}\left(\frac{\varepsilon}{C_0}\right)^{1/(1+\alpha)} = \frac{1}{C_0^{1/(1+\alpha)}\,\varepsilon^{\alpha/(1+\alpha)}},$$

which produces a contradiction when ε is sufficiently small and thus completes the proof of (5-15).

Example 5.4. A natural question arising from Proposition 4.3 (in view of of Lemma 4.1 and (4-21)) is whether a function $u \in C^{1,1}([-1, 1])$ satisfying

$$\begin{cases} \ddot{\ddot{u}} = 0 & \text{in } \{u > 0\} \cup \{u < 0\}, \\ \ddot{u}(-1) = \ddot{u}(1) = 0, \\ u > 0 \quad \text{in } (0, 1) & \text{and} \quad u < 0 \quad \text{in } (-1, 0), \\ \dot{u}(0) = 0 & \text{and} \quad |\ddot{u}(0^+)|^2 - |\ddot{u}(0^-)|^2 = 1. \end{cases} \tag{5-18}$$

needs necessarily to satisfy

$$\ddot{u} \geqslant 0 \quad \text{a.e. in } (-1, 1). \tag{5-19}$$

Were a statement like this true, the result of Proposition 4.3 could be strengthened (at least in dimension 1) by taking into account not only minimizers but solutions of Navier equations with prescribed free boundary conditions. The following example shows this is not the case, namely (5-18) does not imply (5-19): Let

$$u(x) := \begin{cases} \dfrac{\sqrt{2}\,x^2(3-x)}{6} & \text{if } x \in [0, 1], \\ -\dfrac{x^2(3+x)}{6} & \text{if } x \in [-1, 0). \end{cases}$$

We remark that

$$\ddot{u}(x) = \begin{cases} \sqrt{2}(1-x) & \text{if } x \in (0, 1], \\ -(1+x) & \text{if } x \in [-1, 0), \end{cases}$$

from which the system in (5-18) plainly follows.

Nevertheless, the claim in (5-19) does not hold, since $\ddot{u} < 0$ in $(-1, 0)$.

6. A dichotomy argument and proof of Theorem 1.7

We remark that if u is a minimizer of J in Ω in the admissible class in (1-2) and Ω' is a subdomain of Ω, then it is not necessarily true that u is a minimizer of J in Ω' in the admissible class in (1-2) with Ω replaced by Ω'. This is due to the fact that the admissible class in (1-2) with Ω replaced by Ω' does not prevent the Laplacian of $u - u_0$ to become singular at $\partial\Omega'$, and this provides an important difference with respect to the classical cases dealing with the standard Dirichlet energy. To circumvent this problem, we will consider local minimizers in subdomains:

Definition 6.1. Let Ω' be a subdomain of Ω with smooth boundary. We say that u is a local minimizer in Ω' if, in the notation of (1-1),

$$J[u,\Omega'] \leqslant J[v,\Omega']$$

for every $v \in W^{2,2}(\Omega')$ such that $v-u \in W_0^{2,2}(\Omega')$.

In this way, we have:

Lemma 6.2. *If u is a minimizer in Ω, then it is a local minimizer in every subdomain $\Omega' \subset\subset \Omega$ with smooth boundary.*

Proof. Let $v \in W^{2,2}(\Omega')$ such that $v-u \in W_0^{2,2}(\Omega')$. By the extension results in classical Sobolev spaces (see, e.g., Proposition IX.18 in [Brezis 1983]), we can extend v outside Ω' by setting $v(x) := u(x)$ for all $x \in \Omega \setminus \Omega'$, and we have that $v-u \in W_0^{2,2}(\Omega) \subseteq W_0^{1,2}(\Omega)$. In particular, recalling (1-2), we have that $v \in \mathcal{A}$, and thus,

$$0 \leqslant J[v,\Omega]-J[u,\Omega] = \int_{\Omega\setminus\Omega'} \big(|\Delta u|^2 + \chi_{\{u>0\}} - |\Delta v|^2 + \chi_{\{v>0\}}\big) + J[v,\Omega'] - J[u,\Omega'].$$

Since $u=v$ in $\Omega\setminus\Omega'$, this gives that $0 \leqslant J[v,\Omega'] - J[u,\Omega']$, as desired. □

Before proving Theorem 1.7, we show a result concerning the convergence of the blow-up sequence of a minimizer.

Lemma 6.3. *Let $D \subset\subset \Omega$. Let $u_k \in W^{2,2}(D)$, with $k \in \mathbb{N}$, be a sequence of local minimizers of*

$$\int_D \big(|\Delta u_k|^2 + M_k \chi_{\{u_k>0\}}\big), \tag{6-1}$$

with $M_k \in (0,1)$, such that $0 \in \partial\{u_k > 0\}$ and $|\nabla u_k(0)| = 0$.

Fix $R > 0$ such that $B_{5R} \subset\subset D$, and suppose that

$$\sup_{B_{4R}} u_k \leqslant C_0(R), \tag{6-2}$$

$$\|\Delta u_k\|_{L^1(B_{4R})} \leqslant \hat{C}_0(R), \tag{6-3}$$

for some $C_0(R)$, $\hat{C}_0(R) > 0$.

Then, there exists a positive constant $C(R)$, independent of k, such that

$$\|u_k\|_{W^{2,2}(B_R)} \leqslant C(R), \tag{6-4}$$

$$\|\Delta u_k\|_{BMO(B_R)} \leqslant C(R), \tag{6-5}$$

for any $k \in \mathbb{N}$.

Furthermore, if $u_k : \mathbb{R}^n \to \mathbb{R}$ and the minimization property in (6-1) holds true in any domain $D \subset \mathbb{R}^n$, and the corresponding assumptions in (6-2) and (6-3) are satisfied, then there exists $u_0 : \mathbb{R}^n \to \mathbb{R}$ such that, up to subsequences, as $k \to +\infty$, $u_k \to u_0$ in $W^{2,2}_{\mathrm{loc}}(\mathbb{R}^n) \cap C^{1,\alpha}_{\mathrm{loc}}(\mathbb{R}^n)$, for any $\alpha \in (0,1)$.

Proof. To check (6-4), we observe that, in virtue of Lemma 4.1,

$$\int_{B_{2R}} \Delta u_k \, \Delta\phi \leqslant 0, \tag{6-6}$$

for any $\phi \in W_0^{2,2}(B_{2R})$. Now, we take $\xi \in C_0^\infty(B_{2R}, [0, 1])$ such that

$$\xi = 1 \text{ in } B_R, \quad |\nabla\xi| \leqslant \frac{C}{R}, \quad \text{and} \quad |D^2\xi| \leqslant \frac{C}{R^2}, \tag{6-7}$$

for some $C > 0$. We set $m_k := \min_{B_{4R}} u_k$ and choose $\phi := (u_k - m_k)\xi^2 \geqslant 0$ in (6-6). In this way, setting

$$I_1 := 2\int_{B_{2R}} \Delta u_k \, \nabla u_k \cdot \nabla\xi^2 \quad \text{and} \quad I_2 := \int_{B_{2R}} (u_k - m_k)\, \Delta u_k \, \Delta\xi^2,$$

we have that

$$0 \geqslant \int_{B_{2R}} \Delta u_k \, \Delta\big((u_k - m_k)\xi^2\big) = \int_{B_{2R}} (\Delta u_k)^2\xi^2 + I_1 + I_2. \tag{6-8}$$

Thanks to Corollary 4.2, we can use the standard method to prove Caccioppoli's inequality, namely we take $\eta \in C_0^\infty(B_{4R}, [0, 1])$ such that $\eta = 1$ in B_{2R} and $|\nabla\eta| \leqslant \frac{C}{R}$ and we infer from Corollary 4.2 and (6-3)

$$\begin{aligned} \hat{C}\int_{B_{4R}} (u_k - m_k)\,\eta^2 &\geqslant -\int_{B_{4R}} \Delta u_k\,(u_k - m_k)\,\eta^2 \\ &= \int_{B_{4R}} |\nabla u_k|^2\eta^2 + \int_{B_{4R}} 2\eta\,(u_k - m_k)\,\nabla\eta \cdot \nabla u_k \\ &\geqslant \frac{1}{2}\int_{B_{4R}} |\nabla u_k|^2\eta^2 - C\int_{B_{4R}} (u_k - m_k)^2|\nabla\eta|^2. \end{aligned} \tag{6-9}$$

We remark that, in view of Corollary 4.2 and (6-3), we can choose here $\hat{C}$ proportional to $\tilde{C}(R)/R^n$. Hence, the result in (6-9) yields that

$$\int_{B_{2R}} |\nabla u_k|^2 \leqslant \frac{C}{R^2}\int_{B_{4R}} (u_k - m_k)^2 + C\int_{B_{4R}} (u_k - m_k) \tag{6-10}$$

for some $C > 0$, possibly varying from line to line.

Hence, by Young's inequality, (6-7) and (6-10), we get

$$\begin{aligned} |I_1| &\leqslant 2\bigg(\varepsilon\int_{B_{2R}} (\Delta u_k)^2\xi^2 + \frac{1}{\varepsilon}\int_{B_{2R}} |\nabla u_k|^2\,|\nabla\xi|^2\bigg) \\ &\leqslant 2\bigg(\varepsilon\int_{B_{2R}} (\Delta u_k)^2\xi^2 + \frac{C}{\varepsilon\,R^2}\int_{B_{2R}} |\nabla u_k|^2\bigg) \\ &\leqslant 2\bigg(\varepsilon\int_{B_{2R}} (\Delta u_k)^2\xi^2 + \frac{C}{\varepsilon\,R^4}\int_{B_{4R}} (u_k - m_k)^2 + \frac{C}{R^2}\int_{B_{4R}} (u_k - m_k)\bigg). \end{aligned} \tag{6-11}$$

Furthermore, noticing that $(u_k - m_k)\Delta u_k |\nabla\xi|^2 \geqslant -\hat{C}(u_k - m_k)|\nabla\xi|^2$, thanks to Corollary 4.2, and making again use of Young's inequality, we obtain that

$$\begin{aligned} I_2 &= \int_{B_{2R}} (u_k - m_k)\,\Delta u_k\,(2\xi\,\Delta\xi + |\nabla\xi|^2) \\ &\geqslant 2\int_{B_{2R}} (u_k - m_k)\,\Delta u_k\,\xi\,\Delta\xi - \hat{C}\int_{B_{2R}} (u_k - m_k)|\nabla\xi|^2 \\ &\geqslant -2\biggl(\varepsilon\int_{B_{2R}} (\Delta u_k)^2\xi^2 + \frac{1}{\varepsilon}\int_{B_{2R}} (u_k - m_k)^2(\Delta\xi)^2\biggr) - \hat{C}\int_{B_{2R}} (u_k - m_k)|\nabla\xi|^2 \\ &\geqslant -2\biggl(\varepsilon\int_{B_{2R}} (\Delta u_k)^2\xi^2 + \frac{C}{\varepsilon R^4}\int_{B_{2R}} (u_k - m_k)^2\biggr) - \frac{C}{R^2}\int_{B_{2R}} (u_k - m_k). \end{aligned}$$

From this, (6-8), and (6-11), we conclude

$$\begin{aligned} \int_{B_{2R}} (\Delta u_k)^2\xi^2 \leqslant 2\biggl(\varepsilon\int_{B_{2R}} (\Delta u_k)^2\xi^2 + \frac{C}{\varepsilon R^4}\int_{B_{2R}} (u_k - m_k)^2 + \frac{C}{R^2}\int_{B_{4R}} (u_k - m_k)\biggr) \\ +2\biggl(\varepsilon\int_{B_{2R}} (\Delta u_k)^2\xi^2 + \frac{C}{\varepsilon R^4}\int_{B_{2R}} (u_k - m_k)^2\biggr) + \frac{C}{R^2}\int_{B_{2R}} (u_k - m_k), \end{aligned}$$

which, in turn, implies that

$$(1-4\varepsilon)\int_{B_{2R}} (\Delta u_k)^2\xi^2 \leqslant \frac{C}{\varepsilon R^4}\int_{B_{2R}} (u_k - m_k)^2 + \frac{C}{R^2}\int_{B_{2R}} (u_k - m_k) \leqslant \frac{C}{\varepsilon} + C,$$

where the last step follows from (6-2). Choosing $\varepsilon = \frac{1}{8}$ and recalling (6-7), we obtain

$$\int_{B_R} (\Delta u_k)^2 \leqslant \int_{B_{2R}} (\Delta u_k)^2\xi^2 \leqslant C,$$

up to renaming $C > 0$, that does not depend on k. This implies the desired estimate in (6-4).

Moreover, the estimate in (6-5) follows from the BMO estimates in Section 3.

Finally, from the uniform estimate in (6-4), we can apply a customary compactness argument to conclude that there exists a function u_0 such that, up to a subsequence, $u_k \to u_0$ in $W^{2,2}_{\mathrm{loc}}(\mathbb{R}^n) \cap C^{1,\alpha}_{\mathrm{loc}}(\mathbb{R}^n)$, for any $\alpha \in (0, 1)$, as $k \to +\infty$. This completes the proof of Lemma 6.3. □

With this, we are now in the position of completing the proof of Theorem 1.7.

Proof of Theorem 1.7. We suppose that $B_1(x_0) \subset\subset D$, with x_0 as in the statement of Theorem 1.7. We claim that there exist an integer $k_0 > 0$ and a structural constant $C > 0$, depending only on δ, n, and $\mathrm{dist}(D, \Omega)$, such that the following inequality holds:

$$\sup_{B_{2^{-k-1}}(x_0)} |u| \leqslant \max\biggl\{\frac{C}{2^{2k}}, \frac{\sup_{B_{2^{-k}}(x_0)}|u|}{2^2}, \dots, \frac{\sup_{B_{2^{-k+m}}(x_0)}|u|}{2^{2(m+1)}}, \dots, \frac{\sup_{B_1(x_0)}|u|}{2^{2(k+1)}}\biggr\}, \tag{6-12}$$

for any $k \geqslant k_0$.

Indeed, if (6-12) fails, then, for any $j \in \mathbb{N}$, there exist singular free boundary points $x_j \in D$, integers k_j, and minimizers u_j (with $\|u_j\|_{W^{2,2}(\Omega)} = \|u\|_{W^{2,2}(\Omega)}$ be given) such that

$$\sup_{B_{2^{-k_j-1}}(x_j)} |u_j| > \max\left\{ \frac{j}{2^{2k_j}}, \frac{\sup_{B_{2^{-k_j}}(x_j)} |u_j|}{2^2}, \dots, \frac{\sup_{B_{2^{-k_j+m}}(x_j)} |u_j|}{2^{2(m+1)}}, \dots, \frac{\sup_{B_1(x_j)} |u_j|}{2^{2(k_j+1)}} \right\}. \tag{6-13}$$

We denote by $S_j := \sup_{B_{2^{-k_j-1}}}(x_j)|u_j|$, and we consider the scaled functions

$$v_j(x) := \frac{u_j(x_j + 2^{-k_j} x)}{S_j}.$$

In this way, (6-13) gives that

$$1 > \max\left\{ \frac{j}{2^{2k_j} S_j}, \frac{\sup_{B_1} |v_j|}{2^2}, \dots, \frac{\sup_{B_{2^m}} |v_j|}{2^{2(m+1)}}, \dots, \frac{\sup_{B_{2^{k_j}}} |v_j|}{2^{2(k_j+1)}} \right\}. \tag{6-14}$$

From this, we have that the functions v_j satisfy the following properties:

$$\sup_{B_{1/2}} v_j = 1, \quad v_j(0) = |\nabla v_j(0)| = 0, \quad \sup_{B_{2^m}} |v_j| \leqslant 4 \cdot 2^{2m} \text{ for any } m < k_j, \quad \sigma_j := \frac{1}{2^{2k_j}\, S_j} < \frac{1}{j}. \tag{6-15}$$

We also remark that, from the scaling properties of the functional J, we have

$$\int_{B_R} \big(|\Delta v_j|^2 + \sigma_j^2 \chi_{\{v_j>0\}}\big) = 2^{k_j n} \sigma_j^2 \int_{B_{R2^{-k_j}}(x_j)} \big(|\Delta u_j|^2 + \chi_{\{u_j>0\}}\big), \tag{6-16}$$

for every fixed $R < 2^{k_j}$.

We claim that

$$v_j \text{ is a local minimizer in } B_R. \tag{6-17}$$

Indeed, by Lemma 6.2, we know that u is a local minimizer in $B_{R2^{-k_j}}(x_j)$. Hence, if w_j is such that $w_j - v_j \in W_0^{2,2}(B_R)$, we define, for all $y \in B_{R2^{-k_j}}(x_j)$,

$$W_j(y) := S_j\, w_j(2^{k_j}(y - x_j)).$$

In this way, we have that $W_j \in W_0^{2,2}(B_{R2^{-k_j}}(x_j))$, thus yielding, in light of (6-16), that

$$\begin{aligned} 0 &\geqslant 2^{k_j n} \sigma_j^2 \bigg(\int_{B_{R2^{-k_j}}(x_j)} \big(|\Delta u_j|^2 + \chi_{\{u_j>0\}}\big) - \int_{B_{R2^{-k_j}}(x_j)} \big(|\Delta W_j|^2 + \chi_{\{W_j>0\}}\big) \bigg) \\ &= \int_{B_R} \big(|\Delta v_j|^2 + \sigma_j^2 \chi_{\{v_j>0\}}\big) - \int_{B_R} \big(|\Delta w_j|^2 + \sigma_j^2 \chi_{\{w_j>0\}}\big). \end{aligned}$$

This completes the proof of (6-17).

Now, by assumption, u_j is not δ-rank-2 flat at each level $r = 2^{-k}$, for any $k \geqslant 1$, at x_j. As a consequence, v_j is not δ-rank-2 flat in B_1. So, recalling (1-14) and Definition 1.6, this means that

$$h(1, 0) = \inf_{p \in P_2} h_{\min}(1, x_0, p) \geqslant \delta. \tag{6-18}$$

Also, we have that condition (6-2) is guaranteed in this case, in view of (6-15). In addition, we have that (6-3) holds true here, since, in view of (6-15), if $20R \in [2^{m-1}, 2^m]$,

$$v_j - \min_{B_{20R}} v_j \leqslant 2 \sup_{B_{20R}} |v_j| \leqslant 2 \sup_{B_{2^m}} |v_j| \leqslant 8 \cdot 2^{2m} \leqslant 8 \cdot (40R)^2 \leqslant CR^2,$$

and consequently, by Lemma A.1 and (6-14),

$$\begin{aligned}
&\int_{B_{5R}} |\Delta v_j(x)|\,dx \\
&= \int_{B_{5R}} \frac{2^{-2k_j}|\Delta u_j(x_j + 2^{-k_j}x)|}{S_j}\,dx = \frac{2^{(n-2)k_j}}{S_j} \int_{B_{5R2^{-k_j}}(x_j)} |\Delta u_j(y)|\,dy \\
&\leqslant \frac{2^{nk_j}}{2^{2k_j}S_j} \int_{B_{5R2^{-k_j}}(x_j)} |D^2 u_j(y)|\,dy = \frac{CR^n}{2^{2k_j}S_j} ⨍_{B_{5R2^{-k_j}}(x_j)} |D^2 u_j(y)|\,dy \\
&\leqslant \frac{CR^n}{2^{2k_j}S_j} \sqrt{⨍_{B_{5R2^{-k_j}}(x_j)} |D^2 u_j(y)|^2\,dy} \\
&\leqslant \frac{CR^n}{2^{2k_j}S_j} \bigg(\frac{2^{4k_j}}{R^4} ⨍_{B_{20R2^{-k_j}}(x_j)} \big(u_j - \min_{B_{20R2^{-k_j}}(x_j)} u_j\big)^2 + \frac{2^{2k_j}}{R^2} ⨍_{B_{20R2^{-k_j}}(x_j)} \big(u_j - \min_{B_{20R2^{-k_j}}(x_j)} u_j\big) \bigg)^{1/2} \\
&= \frac{CR^n}{2^{2k_j}S_j} \bigg(\frac{2^{4k_j}S_j^2}{R^4} ⨍_{B_{20R}} \big(v_j - \min_{B_{20R}} v_j\big)^2 + \frac{2^{2k_j}S_j}{R^2} ⨍_{B_{20R}} \big(v_j - \min_{B_{20R}} v_j\big) \bigg)^{1/2} \\
&\leqslant \frac{CR^n}{2^{2k_j}S_j} \big(2^{4k_j}S_j^2 + 2^{2k_j}S_j\big)^{1/2} \leqslant CR^n + \frac{CR^n}{\sqrt{2^{2k_j}S_j}} \leqslant CR^n + \frac{CR^n}{\sqrt{j}} \leqslant CR^n.
\end{aligned}$$

Therefore, recalling (6-16), from Lemma 6.3, applied here with $M_j := \sigma_j^2$, we know that, up to a subsequence, still denoted by v_j, there exists a function v_∞ such that

$$v_j \to v_\infty \text{ in } W^{2,2}(B_R) \cap C^{1,\alpha}(B_R), \quad \text{for any } \alpha \in (0,1), \text{ as } j \to +\infty. \tag{6-19}$$

Moreover, we have that $\Delta v_j \in BMO(B_R)$ uniformly. Consequently $v_\infty \in W^{2,2}(B_R) \cap C^{1,\alpha}(B_R)$, for all $\alpha \in (0,1)$, and $\Delta v_\infty \in BMO(B_R)$. Furthermore,

$$\Delta^2 v_\infty = 0 \text{ in } \mathbb{R}^n, \quad \sup_{B_{1/2}} v_\infty = 1, \quad |v_\infty(x)| \leqslant 8|x|^2 \text{ for any } x \in \mathbb{R}^n, \quad v_\infty(0) = |\nabla v_\infty(0)| = 0. \tag{6-20}$$

Let now $f := \Delta v_\infty$, then we have that f is harmonic in $\mathbb{R}^n$. Moreover, by Lemma A.1 and the second line in (6-20), we see that, for any $r > 0$,

$$\frac{1}{r^n} \int_{B_r} |D^2 v_\infty|^2 \leqslant \frac{C}{r^{n+4}} \int_{B_r} (v_\infty - \min_{B_{4r}} v_\infty)^2 + \frac{C}{r^{n+2}} \int_{B_r} (v_\infty - \min_{B_{4r}} v_\infty) \leqslant C,$$

up to renaming $C > 0$. Thus, from the Liouville Theorem we infer that f must be constant, i.e., $\Delta v_\infty = C_0$, for some $C_0 \in \mathbb{R}$.

Consequently, $v_\infty - \frac{C_0}{2n}|x|^2$ is harmonic in $\mathbb{R}^n$ with quadratic growth. Hence, by using the Liouville Theorem once again, we have that $v_\infty(x) = g(x) + \frac{C_0}{2n}|x|^2$, where g is a second order polynomial. Moreover, since $\nabla v_\infty(0) = 0$, we deduce that $g = cp$, for some $c \in \mathbb{R}$ and $p \in P_2$ (recall (1-11)).

Therefore, we can write

$$v_\infty(x) = x \cdot Ax,$$

for some constant and symmetric matrix A. Consequently, recalling the notation in (1-12),

$$\partial\{v_\infty > 0\} = S(p, 0) \tag{6-21}$$

for some $p \in P_2$. On the other hand, from our construction in (6-18), we have

$$\mathrm{HD}\big(\partial\{v_j > 0\} \cap B_1, S(p, 0) \cap B_1\big) \geqslant \delta$$

(recall the definitions of HD and $h_{\min}$ in (1-10) and (1-13), respectively). As a consequence, there exist points $z_j \in \partial\{v_j > 0\} \cap B_1$ such that

$$\mathrm{dist}(z_j, S(p, 0)) \geqslant \delta. \tag{6-22}$$

Now we extract a converging sequence, still denoted z_j, such that $z_j \to z_0$ as $j \to +\infty$, and we see from the uniform convergence of v_j given in (6-19) that $v_\infty(z_0) = 0$, which implies that $z_0 \in S(p, 0)$, thanks to (6-21). On the other hand, we also have that $\mathrm{dist}(z_0, S(p, 0)) \geqslant \delta$, in virtue of (6-22). Therefore, we reach a contradiction, and so the proof of Theorem 1.7 is finished. □

7. Nondegeneracy and proof of Theorems 1.8 and 1.10

In this section we deal with weak and strong nondegeneracy properties of the minimizers. Due to the lack of Harnack inequalities for biharmonic functions, the strong nondegeneracy result does not follow immediately from the weak one, unless we impose some additional conditions on the set $\{u > 0\}$.

7A. ***Weak nondegeneracy and proof of Theorem 1.8.*** Here we prove the weak nondegeneracy for u^+, according to the statement in Theorem 1.8.

Proof of Theorem 1.8. We prove the claims in **1°** and **2°** together, distinguishing the different structures of the two cases when needed.

After rescaling u by defining $r^{-2}u(x_0 + rx)$, we may assume without loss of generality that $r = 1$ and $x_0 = 0$. Also, denote by

$$\gamma := \sup_{B_1} |u|. \tag{7-1}$$

We remark that in the setting of **2°**, we have

$$B_1 \subseteq \{u > 0\}, \tag{7-2}$$

and therefore,

$$\gamma := \sup_{B_1} u. \tag{7-3}$$

We also remark that, in the setting of **1**°, in light of (1-16), we have

$$|\{u>0\}\cap B_{1/16}| \geqslant \theta_* \, |B_{1/16}|. \tag{7-4}$$

As a matter of fact, in case **2**°, the statement in (7-4) is also true, with $\theta_* := 1$, as a consequence of (7-2). Hence, we will exploit (7-4) in both the cases **1**° and **2**°, with the convention that $\theta_* = 1$ in the latter case.

We also point out that, in $B_{1/8}$

$$u - \min_{B_{1/8}} u \leqslant 2\gamma. \tag{7-5}$$

Indeed, in case **1**°, the claim in (7-5) follows from (7-1). Instead, in case **2**°, we exploit (7-2) to write that

$$u - \min_{B_{1/8}} u \leqslant u \leqslant \gamma,$$

thus completing the proof of (7-5).

Now, let $\psi \in C^\infty(\mathbb{R}^n, [0,1])$ such that $\psi = 0$ in $B_{1/16}$, $\psi > 0$ in $\mathbb{R}^n \setminus \overline{B}_{1/16}$, and $\psi = 1$ in $\mathbb{R}^n \setminus B_{1/8}$. Set $v := \psi u$. Then $u - v \in W_0^{2,2}(B_{1/8})$, and so v is a competitor for u in $B_{1/8}$. Therefore, from the local minimality of u (as warranted by Lemma 6.2) we have that

$$\int_{B_{1/8}} \big(|\Delta u|^2 + \chi_{\{u>0\}}\big) \leqslant \int_D \big(|\Delta v|^2 + \chi_{\{v>0\}}\big),$$

where $D := B_{1/8} \setminus \overline{B}_{1/16}$. From this, and recalling the definitions of v and ψ, we obtain that

$$\begin{aligned}
|\{u>0\}\cap B_{1/16}| &\leqslant \int_{B_{1/16}} \big(|\Delta u|^2 + \chi_{\{u>0\}}\big) \\
&\leqslant \int_D \big(|\Delta v|^2 + \chi_{\{v>0\}}\big) - \int_D \big(|\Delta u|^2 + \chi_{\{u>0\}}\big) = \int_D \big(|\Delta v|^2 - |\Delta u|^2\big) \\
&\leqslant \int_D |\Delta v|^2.
\end{aligned}$$

Hence, using Lemma A.1 and (7-5), it follows that

$$\begin{aligned}
|\{u>0\}\cap B_{1/16}| &\leqslant \int_D (u\Delta\psi + 2\nabla u \nabla\psi + \psi\Delta u)^2 \\
&\leqslant 2\|\psi\|_{C^2(B_{1/8})} \int_{B_{1/8}} u^2 + 4|\nabla u|^2 + |D^2 u|^2 \\
&\leqslant C\|\psi\|_{C^2(B_{1/8})} \int_{B_{1/8}} \Big(\big(u - \min_{B_{1/8}} u\big)^2 + \big(u - \min_{B_{1/8}} u\big)\Big) \\
&\leqslant C\|\psi\|_{C^2(B_{1/8})}\, \gamma(1+\gamma),
\end{aligned} \tag{7-6}$$

for some $C > 0$, possibly varying from line to line.

Combining this with (7-4) and (7-6), we conclude that

$$\gamma(1+\gamma) \geqslant \frac{|\{u>0\}\cap B_{1/16}|}{C\|\psi\|_{C^2(B_{1/8})}} \geqslant \frac{\theta_* \, |B_{1/16}|}{\|\psi\|_{C^2(B_{1/8})}},$$

which gives the desired result (using (7-1) in case **1**° and (7-3) in case **2**°). □

7B. ***Whitney's covering.*** Here we recall the Whitney's decomposition method, to obtain suitable conditions which allow us to use Theorem 1.8 (in our setting, the structural assumptions of Theorem 1.8 will be provided by formula (7-7)). Suppose that $E \subset \mathbb{R}^n$ is a nonempty compact set, then $\mathbb{R}^n \setminus E$ can be represented as a union of closed dyadic cubes Q_j^k with mutually disjoint interiors

$$\mathbb{R}^n \setminus E = \bigcup_{k\in\mathbb{Z}} \bigcup_{j=1}^{N_k} Q_j^k$$

such that

$$c_1 \leqslant \frac{\operatorname{dist}(Q_j^k, E)}{\operatorname{diam} Q_j^k} \leqslant c_2$$

for two universal constants $c_1, c_2 > 0$. Here Q_j^k is a cube with side length equal to 2^{-k}.

Let now $E := \{u \leqslant 0\} \cap \overline{Q_1(x_0)}$, where $Q_1(x_0)$ is the unit cube centered at $x_0 \in \partial\{u > 0\}$, and consider the Whitney's decomposition for $\mathbb{R}^n \setminus E$. Let $k_0 \in \mathbb{N}$ be fixed, and suppose that for every $k \geqslant k_0$ there exists $c > 0$ such that, for some Q_j^k, we have

$$\operatorname{dist}(x_0, Q_j^k) \leqslant c2^{-k}. \tag{7-7}$$

Then u^+ is strongly nondegenerate at x_0. To see this, for every large k let us take a cube Q_j^k such that (7-7) holds. Then, if x_1 is the center of Q_j^k, we have that $u(x_1) > 0$ and $\operatorname{dist}(x_1, \partial\{u > 0\}) \geqslant 2^{-k-1}$, Hence, in view of claim **2**° of Theorem 1.8, we find that

$$\sup_{B_{2^{-k-1}}(x_1)} u^+ \geqslant \bar{c}(2^{-k-1})^2 = \frac{\bar{c}}{4} 2^{-2k}. \tag{7-8}$$

On the other hand, by (7-7), we see that

$$|x_0 - x_1| \leqslant c2^{-k} + \sqrt{n}2^{-k} = (c + \sqrt{n})2^{-k},$$

and accordingly $B_{c^* 2^{-k}}(x_0) \supseteq B_{2^{-k-1}}(x_1)$, with $c^* := c + \sqrt{n} + \frac{1}{2}$. Therefore, by (7-8),

$$\sup_{B_{c^* 2^{-k}}(x_0)} u^+ \geqslant \frac{\bar{c}}{4} 2^{-2k}.$$

Definition 7.1. If (7-7) holds, then we say $\partial\{u > 0\}$ satisfies a weak c-covering condition at $x_0 \in \partial\{u > 0\}$.

We remark that the standard c-covering condition, introduced in [Martio and Vuorinen 1987], is stronger than (7-7) and indeed it requires that

$$\operatorname{dist}\left(x_0, \bigcup_{j=1}^{N_k} Q_j^k\right) \leqslant c2^{-k}.$$

Moreover, it is known that the weak c-covering condition of Definition 7.1 is satisfied by the John domains, see [Martio and Vuorinen 1987].

In order to recall the definition of a John domain, we let $0 < \alpha \leqslant \beta < \infty$. A domain $D \subset \mathbb{R}^n$ is called an (α, β)-John domain, denoted by $D \in \mathcal{J}(\alpha, \beta)$, if there exists $x_0 \in D$ such that every $x \in D$ has a rectifiable path $\gamma : [0, d] \to D$ with arc length as parameter such that $\gamma(0) = x$, $\gamma(d) = x_0$, $d \leqslant \beta$ and

$$\operatorname{dist}(\gamma(t), \partial D) \geqslant \frac{\alpha}{d} t, \quad \text{for all } t \in [0, d].$$

The point x_0 is called a center of D. A domain D is called a John domain if $D \in \mathcal{J}(\alpha, \beta)$ for some α and β. The class of all John domains in $\mathbb{R}^n$ is denoted by $\mathcal{J}$. For more on such coverings and applications of Whitney's decompositions we refer to [Martio and Vuorinen 1987].

Alternative sufficient geometric conditions on $\{u > 0\}$ guaranteeing the strong nondegeneracy of u can be given. Note that in order to pass from weak to strong nondegeneracy at some $z \in \partial\{u > 0\}$, it is enough to have a small ball $B' \subset B_r(z) \cap \{u > 0\}$ and $c > 0$ such that diam $B' \geqslant cr$ for every small r, since this guarantees (1-16).

Definition 7.2. We say that $\partial\{u > 0\}$ satisfies a nonuniform interior cone condition if for every $x \in \partial\{u > 0\}$ there exist a positive number $r_x > 0$ and a cone K_x with vertex at x, such that $B_{r_x}(x) \cap K_x \subset \{u > 0\}$.

We also say that $\partial\{u > 0\}$ satisfies a uniform interior cone condition if there exist a positive number $r > 0$ and a cone K with vertex at 0, such that for every $x \in \partial\{u > 0\}$ we have $B_r(x) \cap (x + K) \subset \{u > 0\}$.

From our observation above and Theorem 1.8, we immediately obtain the following result:

Corollary 7.3. *Let u be a minimizer for J in Ω, and $x_0 \in \Omega$. Suppose that $\{u > 0\}$ satisfies the interior cone condition at $x_0 \in \partial\{u > 0\}$, then $|u|$ is nondegenerate at x_0. Moreover, if $\{u > 0\}$ satisfies the uniform interior cone condition and $B_1 \subset \Omega$, then*

$$\sup_{B_r(z)} u^+ \geqslant C_0 r^2,$$

for any $z \in \partial\{u > 0\} \cap B_1$, for some $C_0 > 0$.

7C. *The biharmonic measure and proof of Theorem 1.10.* In this subsection, we describe the main features of the measure induced by the bi-Laplacian of a minimizer. For this, we observe that, since, by Lemma 4.1, Δu is super-harmonic:

$$\text{There exists a nonnegative measure } \mathcal{M}_u \text{ such that } -\Delta^2 u = \mathcal{M}_u. \tag{7-9}$$

Hence, for any $\psi \in C_0^\infty(\Omega)$, we have that

$$\int_\Omega \mathcal{M}_u \psi = \int_\Omega (-\Delta u)\Delta\psi. \tag{7-10}$$

Recalling the notion of flatness introduced in Definition 1.6, we have the following:

Lemma 7.4. *Let u be a minimizer of the functional J defined in* (1-1), *let $\delta > 0$, and let $x_0 \in \partial\{u > 0\}$ such that $\nabla u(x_0) = 0$ and $\partial\{u > 0\}$ is not δ-rank-2 flat at x_0 at any level $r > 0$ with $B_r(x_0) \subset\subset \Omega$. Then,*

$$\mathcal{M}_u(B_r(x_0)) \leqslant C r^{n-2} \tag{7-11}$$

for any $r > 0$ as above, for some $C > 0$.

Proof. Without loss of generality, we take $x_0 = 0$. We consider a function $\psi_0 \in C_0^\infty(B_2, [0, 1])$, with $\psi_0 = 1$ in B_1, and we let $\psi(x) := \psi_0(x/r)$. In this way, $\psi = 1$ in B_r and $|D^2\psi| \leqslant C/r^2$ for some $C > 0$.

We now exploit (7-10) with such ψ. Then, by Corollary A.2, we have

$$\mathcal{M}_u(B_r) \leqslant \int_\Omega \mathcal{M}_u \psi = \int_\Omega (-\Delta u)\Delta\psi \leqslant \sqrt{\int_{B_{2r}} |\Delta u|^2}\sqrt{\int_{B_{2r}} |\Delta\psi|^2} \leqslant C r^{n/2} r^{(n-4)/2},$$

which implies the desired result, up to renaming $C > 0$. □

We remark that a full counterpart of Lemma 7.4 does not hold for the one-phase problem (in particular, $\mathcal{M}_u$ as defined in (7-9) and (7-10) does not need to have a sign, see (5-6)). Nevertheless, the following result holds:

Lemma 7.5. *Let u be a one-phase minimizer of J. Assume that $u \in C^{1,1}(\Omega)$ and $\partial\{u > 0\}$ has null Lebesgue measure. Let $\varphi \in C_0^\infty(B_1, [0, 1])$ with*

$$\int_{B_1} \varphi = 1.$$

For any $\delta > 0$, let

$$\varphi_\delta(x) := \frac{1}{\delta^n}\varphi\Big(\frac{x}{\delta}\Big),$$

and $u_\delta := u * \varphi_\delta$. Then, for any $\Omega' \subset\subset \Omega$, we have that

$$\lim_{\delta\to 0}\int_{\Omega'} \Delta^2 u_\delta\, u_\delta = 0.$$

Proof. Let

$$\Gamma_\delta := \bigcup_{p\in\partial\{u>0\}} B_\delta(p).$$

We claim:

$$\text{If } x \in \Omega \setminus \Gamma_\delta, \text{ then } \Delta^2 u(x) = 0. \tag{7-12}$$

To prove this, we argue by contradiction, and we suppose that there exists $x \in \Omega \setminus \Gamma_\delta$ such that

$$\Delta^2 u(x) \text{ is either not defined or not null.} \tag{7-13}$$

We observe that:

$$\text{There exists } \rho, a > 0 \text{ such that } u \geqslant a \text{ in } B_\rho(x). \tag{7-14}$$

Because, if not, for any $k \in \mathbb{N}$, there exists x_k such that $|x - x_k| + u(x_k) \leqslant 1/k$, and thus $u(x) = 0$. Since x lies outside Γ_δ, it cannot be a free boundary point, hence u must vanish in a neighborhood of x. Consequently, $\Delta^2 u$ vanishes in a neighborhood of x, and this is in contradiction with (7-13), thus proving (7-14).

Then, from (7-14) and Lemma 4.1, it follows that u is biharmonic in $B_\rho(x)$. Once again, this is in contradiction with (7-13), and thus the proof of (7-12) is complete.

Now, by taking δ sufficiently small, we suppose that the distance from Ω' to $\partial\Omega$ is larger than δ. Thus, from (7-12) we obtain that, if $x \in \Omega' \setminus \Gamma_{2\delta}$ and $y \in B_\delta$, then $x - y \in \Omega' \setminus \Gamma_\delta$, hence $\Delta^2 u(x-y) = 0$.

Consequently, for every $x \in \Omega' \setminus \Gamma_{2\delta}$,

$$\Delta^2 u_\delta(x) = \int_{B_\delta} \Delta^2 u(x-y)\, \varphi_\delta(y)\, dy = 0.$$

This implies that

$$\int_{\Omega'} \Delta^2 u_\delta\, u_\delta = \int_{\Omega' \cap \Gamma_{2\delta}} \Delta^2 u_\delta\, u_\delta. \tag{7-15}$$

We also remark that

$$\begin{aligned} |\Delta^2 u_\delta(x)| &\leqslant \int_{B_\delta} |u(x-y)|\, |\Delta^2 \varphi_\delta(y)|\, dy = \frac{1}{\delta^{n+4}} \int_{B_\delta} |u(x-y)| \left| \Delta^2 \varphi\Big(\frac{y}{\delta}\Big) \right| dy \\ &= \frac{1}{\delta^4} \int_{B_1} |u(x-\delta y)|\, |\Delta^2 \varphi(y)|\, dy \leqslant \frac{C}{\delta^4} \int_{B_1} u(x-\delta y)\, dy, \end{aligned} \tag{7-16}$$

for some $C > 0$. Now, if $x \in \Gamma_{2\delta}$ and $y \in B_1$, we have that there exists $p \in \partial\{u > 0\} \subseteq \{u = 0\}$ such that $|p - x| \leqslant 2\delta$ and accordingly $|(x - \delta y) - p| \leqslant |x - p| + \delta \leqslant 3\delta$. Then, in this setting, the regularity of u implies that

$$u(x - \delta y) \leqslant 9 \|u\|_{C^{1,1}(\Omega)} \delta^2. \tag{7-17}$$

In particular, recalling (7-16), we find that, if $x \in \Gamma_{2\delta}$,

$$|\Delta^2 u_\delta(x)| \leqslant \frac{C}{\delta^2}, \tag{7-18}$$

up to renaming $C > 0$, also depending on $\|u\|_{C^{1,1}(\Omega)}$.

From (7-17) we also deduce that, if $x \in \Gamma_{2\delta}$,

$$|u_\delta(x)| \leqslant \int_{B_1} u(x-\delta y)\, \varphi(y)\, dy \leqslant 9 \|u\|_{C^{1,1}(\Omega)} \delta^2.$$

Using this information and (7-18) we conclude that, if $x \in \Gamma_{2\delta}$,

$$|\Delta^2 u_\delta(x)\, u_\delta(x)| \leqslant C,$$

and therefore,

$$\left| \int_{\Omega' \cap \Gamma_{2\delta}} \Delta^2 u_\delta\, u_\delta \right| \leqslant C |\Omega' \cap \Gamma_{2\delta}|,$$

up to renaming $C > 0$ once again.

This and (7-15) provide

$$\left| \int_{\Omega'} \Delta^2 u_\delta\, u_\delta \right| \leqslant C |\Omega' \cap \Gamma_{2\delta}|.$$

Hence, taking the limit as $\delta \to 0$,

$$\lim_{\delta \to 0} \left| \int_{\Omega'} \Delta^2 u_\delta\, u_\delta \right| \leqslant |\Omega' \cap \partial\{u > 0\}|. \qquad \square$$

Now we prove a counterpart of (7-11) at nondegenerate points of the free boundary of the minimizers. For this, recalling the setting in formula (1-14), we let $\mathcal{N}_\delta$ be the set of free boundary points x with the property that there exists $r_x > 0$ small enough such that $h(r, x) \geqslant \delta r$ for every $r < r_x$. Moreover, in the spirit of Definition 1.4, we also denote by

$$\mathcal{N}_\delta^{\text{sing}} := \{x \in \mathcal{N}_\delta : \nabla u(x) = 0\}.$$

Lemma 7.6. *Let u be a minimizer of J. Let $D \subset \Omega$ and suppose that there exists $\bar{c} > 0$ such that*

$$\liminf_{r\to 0} \frac{\sup_{B_r(x)} |u|}{r^2} \geqslant \bar{c} \tag{7-19}$$

for every $x \in \partial\{u > 0\} \cap \overline{D}$. Then there exists $c_0(\delta) > 0$, depending on n, δ, $\bar{c}$, $\|u\|_{W^{2,2}(\Omega)}$, and $\operatorname{dist}(\overline{D}, \partial\Omega)$, such that

$$\liminf_{r\to 0} \frac{\mathcal{M}_u(B_r(x))}{r^{n-2}} \geqslant c_0(\delta), \quad \text{for any } x \in \mathcal{N}_\delta^{\text{sing}}. \tag{7-20}$$

Proof. We argue by contradiction. If (7-20) fails, then there exists a sequence $x_j \in \mathcal{N}_\delta^{\text{sing}}$ such that

$$\liminf_{r\to 0} \frac{\mathcal{M}_u(B_r(x_j))}{r^{n-2}} < \varepsilon_j, \tag{7-21}$$

with $\varepsilon_j \to 0$. Since $x_j \in \mathcal{N}_\delta^{\text{sing}}$, there exists a sequence $r_j \to 0$ such that

$$h(r_j, x_j) \geqslant \delta r_j. \tag{7-22}$$

Now we define

$$U_j(x) := \frac{u(x_j + r_j x)}{r_j^2}.$$

By construction, recalling (7-19), we have that $\{U_j\}$ is nondegenerate with quadratic growth, i.e., there exists $C > 0$ independent of j such that

$$\frac{1}{C} R^2 \leqslant \sup_{B_R} |U_j| \leqslant C R^2 \quad \text{for any } R < \frac{1}{r_j}. \tag{7-23}$$

Moreover, by (7-21) and (7-22), we see that

$$h(1, 0) \geqslant \delta \quad \text{and} \quad \mathcal{M}_{U_j}(B_R) \leqslant \varepsilon_j R^{n-2} \to 0 \tag{7-24}$$

for every fixed $R > 0$.

As a consequence, using a customary compactness argument, we can extract a converging subsequence, still denoted by U_j, such that $U_j \to U_0$ locally uniformly as $j \to +\infty$. Then (7-24) translates into

$$h(1, 0) \geqslant \delta \quad \text{and} \quad \mathcal{M}_{U_0}(B_R) = 0 \tag{7-25}$$

for every fixed $R > 0$. In other words, in view of (7-23), we have that U_0 is an entire nontrivial biharmonic function with quadratic growth.

On the other hand, applying Corollary A.2 we also have that

$$\int_{B_R} |D^2 u|^2 \leqslant C R^n.$$

This, together with the Liouville Theorem, implies that

$$U_0 \text{ is a quadratic polynomial.} \tag{7-26}$$

Accordingly, there exists $\alpha \in \mathbb{R}$ such that $p := \alpha U_0 \in P_2$ (recall the notation in (1-11)). From (7-25), we conclude that

$$\mathrm{HD}(S(p,0) \cap B_1, \partial\{U_0 > 0\} \cap B_1) \geqslant \delta,$$

which is a contradiction with (7-26). □

We are now in position to complete our analysis of the free boundary regularity results which follow from the study of the biharmonic measure by proving Theorem 1.10.

Proof of Theorem 1.10. We start by proving **1**°. For this, let $D \subset\subset \Omega$ and $x \in \mathcal{F}_\delta := (\partial\{u > 0\} \cap D) \setminus \mathcal{N}_\delta$, where $\mathcal{N}_\delta$ has been introduced before Lemma 7.6. Then there exists $r_x > 0$ such that

$$|\partial\{u > 0\} \cap B_{r_x}(x)| \leqslant C(n)\delta r_x^n,$$

where $C(n)$ is a dimensional constant. In this way, we can cover $\mathcal{F}_\delta$ with balls $B_{r_x}(x)$, and we can then extract a Besicovitch covering such that

$$|\mathcal{F}_\delta \cap D| \leqslant C(n)\delta\, |D|. \tag{7-27}$$

Then, sending $\delta \to 0$ the result in **1**° follows.

We now focus on **2**°. In this case, thanks to (1-18) we can use Lemma 7.6 and find a Besicovitch covering by balls $B_{r_x}(x)$ of $\mathcal{N}_\delta^{\mathrm{sing}}$ such that

$$c_0(\delta) \sum r_x^{n-2} \leqslant \mathcal{M}_u(D') < \infty, \tag{7-28}$$

where $D' \Supset D$ is a subdomain of Ω such that

$$\mathrm{dist}(D, \partial D') < \sup_{x \in \partial\{u>0\} \cap D} r_x := r_0.$$

Therefore, letting $r_0 \to 0$ in (7-28), we get that

$$\mathcal{H}^{n-2}(\mathcal{N}_\delta^{\mathrm{sing}} \cap D) < +\infty. \tag{7-29}$$

Furthermore, since the free boundary is C^1 near points in $\mathcal{N}_\delta \setminus \mathcal{N}_\delta^{\mathrm{sing}}$, we have that

$$\mathcal{H}^{n-2}((\mathcal{N}_\delta \setminus \mathcal{N}_\delta^{\mathrm{sing}}) \cap D) < +\infty,$$

which, together with (7-29), implies that

$$\mathcal{H}^{n-2}(\mathcal{N}_\delta \cap D) < +\infty. \tag{7-30}$$

This gives the second claim in **2°**. We now prove the first claim in **2°**. For this, we use (7-27) and (7-30) to obtain

$$|\partial\{u>0\}\cap D| \leqslant |\mathcal{F}_\delta \cap D| + |\mathcal{N}_\delta \cap D| = |\mathcal{F}_\delta \cap D| \leqslant C(n)\delta\,|D|.$$

Then, sending $\delta \to 0$, we complete the proof of **2°**. □

Remark 7.7. If $\{u>0\}$ is a John domain, then $|u|$ is nondegenerate by the discussion in Section 7B. Alternatively, as in Theorem 1.8, if $\{u>0\}$ has uniformly positive Lebesgue density then $|u|$ is nondegenerate.

8. Stratification of free boundary and proof of Theorem 1.11

In this section we reformulate some results obtained in Section 6 related to the dichotomy between the notion of rank-2 flatness and the quadratic growth of the minimizer.

For this, to describe an appropriate flatness rate of the minimizers, we recall Definition 1.4 and we also define a suitable class, in the following way:

Definition 8.1. Fix $r>0$. We say that $u \in \mathcal{P}_r$ if:

- $u \in W^{2,2}(B_r)$ is a minimizer of J in (1-1) in B_r, among functions $v \in W^{2,2}(B_r)$, and $v-u \in W_0^{1,2}(B_r)$,
- $0 \in \partial_{\mathrm{sing}}\{u>0\}$.

If, in addition, given $\delta>0$, the free boundary is not (δ, r)-rank-2 flat at 0, then we say that $u \in \mathcal{P}_r(\delta)$.

In the setting of Definition 8.1, Theorem 1.7 can be reformulated as follows:

Proposition 8.2. *Let $u \in \mathcal{P}_r(\delta)$. Then there exist $r_0>0$ and $C>0$, possibly depending on n, δ, r, and $\|u\|_{W^{2,2}(\Omega)}$, such that*

$$|u(x)| \leqslant C|x|^2, \quad \text{for any } x \in B_{r_0}.$$

Moreover, recalling the definition of $h(r, x_0)$ in (1-14), a refinement of Theorem 1.7 can be formulated as:

Theorem 8.3. *Let $u \in \mathcal{P}_1$. Let $\delta \in (0,1)$, $k>10$, and $r_k := 2^{-k}$. Then, either $h(0, r_k) < \delta r_k$, or there exists $C>0$, possibly depending on n, δ, and $\|u\|_{W^{2,2}(\Omega)}$, such that*

$$\sup_{B_{r_k/2}} |u| \leqslant C r_k^2.$$

We are now ready to complete the proof of Theorem 1.11.

Proof of Theorem 1.11. Notice that (1-19) and (1-20) follow as a consequence of Theorem 8.3. Therefore, to complete the proof of Theorem 1.11, it only remains to prove that u^+ is strongly nondegenerate at $z \in \mathcal{F}$. After rescaling $U_r(x) := r^{-2}u(z+rx)$, we see that it is enough to show that

$$\sup_{B_1} U_r^+ \geqslant \hat{C}, \tag{8-1}$$

for some $\hat{C}>0$ (which here can depend on n, $\operatorname{dist}(z, \partial\Omega)$ and the minimizer u itself).

To check this, we first prove:

$$\begin{aligned}&\text{If } p \text{ is a homogeneous polynomial of degree two,}\\ &\text{then } \{p=0\} \text{ is contained in the union of finitely many hypersurfaces.}\end{aligned} \tag{8-2}$$

Indeed, up to a linear transformation, and possibly exchanging the order of the variables, we can suppose

$$p(x)=\sum_{i=1}^{n} a_i x_i^2,$$

with $(a_1,\dots,a_m)\in\mathbb{R}\setminus\{0\}$ and $a_{m+1}=\dots=a_n=0$, for some $m\in\{1,\dots,n\}$. Therefore the zero set of p is obtained by the zero set of the polynomial

$$\mathbb{R}^m\ni x\mapsto \tilde p(x)=\sum_{i=1}^{m} a_i x_i^2,$$

up to a Cartesian product with an $(n-m)$-dimensional linear space. Also:

$$\text{If } x\in\{\tilde p=0\},\ \text{ then } tx\in\{\tilde p=0\} \text{ for all } t\in\mathbb{R}. \tag{8-3}$$

Therefore,

$$\{\tilde p=0\}=\big\{tx,\ x\in\{\tilde p=0\}\cap\mathbb{S}^{m-1}\big\}. \tag{8-4}$$

Furthermore,

$$\{\nabla\tilde p=0\}=\{(2a_1x_1,\dots,2a_mx_m)=0\}=\{0\}. \tag{8-5}$$

Therefore, by (8-5), in the vicinity of any $x\in\{\tilde p=0\}\cap\mathbb{S}^{m-1}$, the set $\{\tilde p=0\}$ is an $(m-1)$-dimensional surface, which, in view of (8-3), is transverse to $\mathbb{S}^{m-1}$. Consequently, we have $\{\tilde p=0\}\cap\mathbb{S}^{m-1}$ is the union of $(m-2)$-dimensional surfaces. In addition, from (8-5) we know that these surfaces cannot accumulate to each other, and so $\{\tilde p=0\}\cap\mathbb{S}^{m-1}$ is the union of finitely many $(m-2)$-dimensional surfaces.

This and (8-4) imply that $\{\tilde p=0\}$ is the union of finitely many $(m-1)$-dimensional surfaces. Accordingly, we have that $\{p=0\}$ is the union of finitely many surfaces of dimension $(m-1)+(n-m)=n-1$. This completes the proof of (8-2).

We also stress that, in light of (8-3), the intersection of the hypersurfaces described in (8-2) and $\mathbb{S}^{n-1}$ have codimension 1 inside $\mathbb{S}^{n-1}$. In particular, for every $p\in\mathbb{S}^{n-1}$ outside these hypersurfaces there exists $\rho(p)\in(0,\frac12)$ such that $B_{\rho(p)}(p)$ does not intersect these hypersurfaces.

Given $x\in B_1\setminus\{0\}$, we now use the notation $\hat x:=x/|x|$, and we claim:

$$\text{There exists } x_*\in B_{1/2}\setminus\{0\} \text{ such that } U_r(x_*)>0 \text{ and } \hat x_* \text{ lies outside the hypersurfaces (8-2).} \tag{8-6}$$

Indeed, we can assume that $|B_{1/2}\cap\{U_r>0\}|>0$ (otherwise $u\leqslant 0$, contradicting the assumption that $z\in\partial\{u>0\}$), and from this we obtain (8-6).

From (8-6), we deduce that $B_{\rho(\hat x_*)}(\hat x_*)$ does not intersect the hypersurfaces in (8-2). Hence, by (8-3), setting $r(x_*):=|x_*|\rho(\hat x_*)$, we see that $B_{r(x_*)}(x_*)$ does not intersect the hypersurfaces in (8-2). Then, from (1-19), it follows that if $r=r_k$ is sufficiently small, then $B_{r(x_*)/2}(x_*)$ does not intersect $\partial\{U_r>0\}$. For this reason, since $U_r(x_*)>0$, we conclude that $B_{r(x_*)/2}(x_*)\subseteq\{U_r>0\}$.

Consequently, we are in the position of using claim **2**° in Theorem 1.8, thus obtaining that

$$\sup_{B_{r(x_*)/2}(x_*)} U_r^+\geqslant \bar c\left(\frac{r(x_*)}{2}\right)^2=\frac{\bar c\,(r(x_*))^2}{4}=\frac{\bar c\,(\rho(\hat x_*))^2}{4}\,|x_*|^2 \quad \text{for some } \bar c>0. \tag{8-7}$$

Now we claim that

$$B_1 \supseteq B_{r(x_*)/2}(x_*). \tag{8-8}$$

Indeed, if $y \in B_{r(x_*)/2}(x_*)$, we have

$$|y| \leqslant |y - x_*| + |x_*| \leqslant \frac{r(x_*)}{2} + |x_*| = \frac{\rho(\hat{x}_*)\,|x_*|}{2} + |x_*| \leqslant \frac{|x_*|}{4} + |x_*| = \frac{5|x_*|}{4} \leqslant \frac{5}{8} < 1,$$

thus proving (8-8).

Then, from (8-7) and (8-8) we obtain

$$\sup_{B_1} U_r^+ \geqslant \frac{\bar{c}\,(\rho(\hat{x}_*))^2}{4}\,|x_*|^2 =: \hat{C},$$

and (8-1) follows, as desired. □

9. Monotonicity formula: proof of Theorem 1.12

This section is devoted to the proof of Theorem 1.12, which is based on a series of careful integration by parts aimed at spotting suitable integral cancellations. In addition, some "high order of differentiability" terms naturally appear in the computations, which need to be suitably removed in order to rigorously make sense of the formal manipulations. We start with some general computations valid in $\mathbb{R}^n$, then, from (9-24) on, we specialize to the case $n = 2$. In this part of the paper, for the sake of shortness, we suppose that the assumptions of Theorem 1.12 are always satisfied without further mentioning them. Without loss of generality, we also suppose that $B_2 \subset\subset \Omega$. Then, we have the following identity:

Lemma 9.1. *For every $r_1, r_2 \in (0, 3/2)$,*

$$4\int_{r_1}^{r_2} R(r)\,dr + 2T(r_2) - 2T(r_1) + D(r_2) - D(r_1) = 0, \tag{9-1}$$

where

$$R(r) := \frac{1}{r^{n+1}} \sum_{m=1}^{n} \int_{B_r} \Delta u\, \nabla u_m \cdot e_m - \sum_{m=1}^{n} \int_{\partial B_r} \Delta u \nabla u_m \cdot \frac{x^m\, x}{r^{n+2}} = \frac{1}{r^{n+1}} \int_{B_r} |\Delta u|^2 - \frac{1}{r^n} \int_{\partial B_r} \Delta u\, \partial_r^2 u,$$

$$T(r) := \sum_{m=1}^{n} \int_{\partial B_r} \Delta u\, u_m\, \frac{x^m}{r^{n+1}} = \frac{1}{r^n} \int_{\partial B_r} \Delta u\, \partial_r u,$$

$$D(r) := \frac{1}{r^n} \int_{B_r} \big(|\Delta u|^2 + \chi_{\{u>0\}}\big), \tag{9-2}$$

and the notation $\partial_r := (x/|x|) \cdot \nabla$ has been used.

Proof. Fix $r \in (0, 3/2)$. We let $\delta > 0$ (to be taken as small as we wish in what follows), and consider a smooth function $\eta = \eta_\delta$ supported in $B_{r+\delta}$. Fixed $\varepsilon > 0$, we also consider the mollifier $\rho_\varepsilon(x) := (1/\varepsilon^n)\rho\big(x/\varepsilon\big)$, for a given even function $\rho \in C_0^\infty(B_1)$. We also define $\phi = (\phi^1, \dots, \phi^n) : \mathbb{R}^n \to \mathbb{R}^n$ as

$$\mathbb{R}^n \ni x = (x^1, \dots, x^n) \longmapsto \phi^m(x) := (\psi^m * \rho_\varepsilon)(x), \quad \text{where } \psi^m(x) := x^m \eta(x).$$

Let also

$$F^m(x) := \Delta u(x)\, u_m(x). \tag{9-3}$$

In view of (4-1) and (4-2) (if u is a minimizer), or recalling that u is assumed to be in $C^{1,1}(\Omega)$ (if u is a one-phase minimizer), we know that

$$F^m \in L^p(B_1) \quad \text{for every } p \in (1, +\infty).$$

We observe that ψ^m is supported in $B_{r+\delta}$, and so ϕ^m is supported in $B_{r+\delta+\varepsilon} \subset B_1$, as long as δ and ε are sufficiently small. Consequently,

$$\begin{aligned}\int_\Omega \Delta u\, u_m\, \Delta\phi^m &= \int_{\mathbb{R}^n} \Delta u\, u_m\, \Delta\phi^m = \int_{\mathbb{R}^n} F^m(\Delta\psi^m * \rho_\varepsilon) = \iint_{\mathbb{R}^n\times B_\varepsilon(x)} F^m(x)\Delta\psi^m(y)\rho_\varepsilon(x-y)\,dx\,dy\\ &= \iint_{B_\varepsilon(x)\times\mathbb{R}^n} F^m(x)\Delta\psi^m(y)\rho_\varepsilon(y-x)\,dx\,dy = \iint_{\mathbb{R}^n} (F^m * \rho_\varepsilon)(y)\Delta\psi^m(y)\,dy\\ &= \int_\Omega F^m_\varepsilon\, \Delta\psi^m = -\int_\Omega \nabla F^m_\varepsilon \cdot \nabla\psi^m, \end{aligned} \tag{9-4}$$

with

$$F^m_\varepsilon := F^m * \rho_\varepsilon. \tag{9-5}$$

Similarly, we have

$$\int_\Omega \Delta u \nabla u_m \cdot \nabla\phi^m = \int_\Omega \Delta u \nabla u_m \cdot (\nabla\psi^m * \rho_\varepsilon) = \int_\Omega ((\Delta u \nabla u_m) * \rho_\varepsilon) \cdot \nabla\psi^m. \tag{9-6}$$

Also,

$$\begin{aligned}\int_\Omega \big(|\Delta u|^2 + \chi_{\{u>0\}}\big) \operatorname{div}\phi &= \sum_{m=1}^n \int_\Omega \big(|\Delta u|^2 + \chi_{\{u>0\}}\big)(\psi^m_m * \rho_\varepsilon)\\ &= \int_\Omega \Big(\big(|\Delta u|^2 + \chi_{\{u>0\}}\big) * \rho_\varepsilon\Big) \operatorname{div}\psi.\end{aligned}$$

Then, we plug this information, (9-4), and (9-6) into (4-10), and we see that

$$\begin{aligned} 0 &= 2\int_\Omega \Delta u \sum_{m=1}^n \big(2\nabla u_m \cdot \nabla\phi^m + u_m\Delta\phi^m\big) - \int_\Omega \big(|\Delta u|^2 + \chi_{\{u>0\}}\big) \operatorname{div}\phi\\ &= 4\sum_{m=1}^n \int_\Omega ((\Delta u\nabla u_m) * \rho_\varepsilon) \cdot \nabla\psi^m - 2\sum_{m=1}^n \int_\Omega \nabla F^m_\varepsilon \cdot \nabla\psi^m - \int_\Omega \Big(\big(|\Delta u|^2 + \chi_{\{u>0\}}\big) * \rho_\varepsilon\Big) \operatorname{div}\psi. \end{aligned} \tag{9-7}$$

Since the latter identity only involves the first derivatives of ψ^m, up to an approximation argument we can choose η to be the radial Lipschitz function defined by

$$\eta(x) := \begin{cases} 1 & \text{if } x \in B_r,\\ \dfrac{r+\delta-|x|}{\delta} & \text{if } x \in B_{r+\delta} \setminus B_r,\\ 0 & \text{if } x \in \mathbb{R}^n \setminus B_{r+\delta}. \end{cases}$$

In this way, we have

$$\nabla\eta(x) = -\frac{x}{\delta\,|x|}\,\chi_{B_{r+\delta}\setminus B_r}(x) \quad \text{and} \quad \nabla\psi^m(x) = e_m\eta(x) - \frac{x^m\,x}{\delta\,|x|}\,\chi_{B_{r+\delta}\setminus B_r}(x),$$

which also gives that

$$\operatorname{div}\psi(x) = n\eta(x) - \frac{|x|}{\delta}\,\chi_{B_{r+\delta}\setminus B_r}(x).$$

Therefore, we infer from (9-7) that

$$\begin{aligned}0 = 2\sum_{m=1}^{n}\int_{B_r}\big(2((\Delta u\nabla u_m)*\rho_\varepsilon) - \nabla F_\varepsilon^m\big)\cdot e_m - n\int_{B_r}\big((|\Delta u|^2+\chi_{\{u>0\}})*\rho_\varepsilon\big)\\ +2\sum_{m=1}^{n}\int_{B_{r+\delta}\setminus B_r}\big(2((\Delta u\nabla u_m)*\rho_\varepsilon) - \nabla F_\varepsilon^m\big)\cdot\bigg(e_m\eta(x) - \frac{x^m\,x}{\delta\,|x|}\bigg)\\ -\int_{B_{r+\delta}\setminus B_r}\big((|\Delta u|^2+\chi_{\{u>0\}})*\rho_\varepsilon\big)\bigg(n\eta(x) - \frac{|x|}{\delta}\bigg).\end{aligned}$$

Then, sending $\delta \to 0^+$, we deduce that

$$\begin{aligned}0 &= 2\sum_{m=1}^{n}\int_{B_r}\big(2((\Delta u\nabla u_m)*\rho_\varepsilon) - \nabla F_\varepsilon^m\big)\cdot e_m - n\int_{B_r}\big((|\Delta u|^2+\chi_{\{u>0\}})*\rho_\varepsilon\big)\\ &\qquad -2\sum_{m=1}^{n}\int_{\partial B_r}\big(2((\Delta u\nabla u_m)*\rho_\varepsilon) - \nabla F_\varepsilon^m\big)\cdot\frac{x^m\,x}{r} + r\int_{\partial B_r}\big((|\Delta u|^2+\chi_{\{u>0\}})*\rho_\varepsilon\big)\\ &= 2\sum_{m=1}^{n}\int_{B_r}G_\varepsilon^m\cdot e_m - n\int_{B_r}\big((|\Delta u|^2+\chi_{\{u>0\}})*\rho_\varepsilon\big)\\ &\qquad -2\sum_{m=1}^{n}\int_{\partial B_r}G_\varepsilon^m\cdot\frac{x^m\,x}{r} + r\int_{\partial B_r}\big((|\Delta u|^2+\chi_{\{u>0\}})*\rho_\varepsilon\big),\end{aligned}\tag{9-8}$$

where

$$G_\varepsilon^m := 2((\Delta u\nabla u_m)*\rho_\varepsilon) - \nabla F_\varepsilon^m.\tag{9-9}$$

Furthermore, letting

$$D_\varepsilon(r) := \frac{1}{r^n}\int_{B_r}\big((|\Delta u|^2+\chi_{\{u>0\}})*\rho_\varepsilon\big),\tag{9-10}$$

we have

$$D_\varepsilon'(r) = \frac{1}{r^n}\int_{\partial B_r}\big((|\Delta u|^2+\chi_{\{u>0\}})*\rho_\varepsilon\big) - \frac{n}{r^{n+1}}\int_{B_r}\big((|\Delta u|^2+\chi_{\{u>0\}})*\rho_\varepsilon\big).\tag{9-11}$$

Thus, we multiply (9-8) by $1/r^{n+1}$, and we exploit (9-11) to conclude that

$$0 = \frac{2}{r^{n+1}}\sum_{m=1}^{n}\int_{B_r}G_\varepsilon^m\cdot e_m - 2\sum_{m=1}^{n}\int_{\partial B_r}G_\varepsilon^m\cdot\frac{x^m\,x}{r^{n+2}} + D_\varepsilon'(r) = 2Z_\varepsilon(r) + D_\varepsilon'(r),\tag{9-12}$$

where

$$Z_\varepsilon(r) := \frac{1}{r^{n+1}} \sum_{m=1}^{n} \int_{B_r} G_\varepsilon^m \cdot e_m - \sum_{m=1}^{n} \int_{\partial B_r} G_\varepsilon^m \cdot \frac{x^m\, x}{r^{n+2}}. \tag{9-13}$$

Now, in light of (9-3), we observe that ∇F_m (and thus ∇F_m^ε) involves third derivatives, and therefore we aim at "lowering the order of derivative" of this term from (9-13) in view of (9-9) (and this goal will be accomplished via a suitable averaging procedure). To this end, we observe that

$$\int_{B_r} \nabla F_\varepsilon^m \cdot e_m = \int_{B_r} \operatorname{div}(F_\varepsilon^m e_m) = \int_{\partial B_r} F_\varepsilon^m e_m \cdot \frac{x}{r} = \int_{\partial B_r} F_\varepsilon^m \frac{x^m}{r}. \tag{9-14}$$

We notice that the last term in (9-14) does not contain any third order derivatives. As for the boundary term in (9-8) that involves the third derivative, we have that

$$\begin{aligned}
\int_{\partial B_r} \nabla F_\varepsilon^m \cdot \frac{x^m\, x}{r^{n+2}} &= \int_{\partial B_1} \nabla F_\varepsilon^m(rx) \cdot \frac{x^m\, x}{r} \\
&= \int_{\partial B_1} \partial_r (F_\varepsilon^m(rx)) \cdot \frac{x^m}{r} \\
&= \frac{d}{dr}\left\{ \int_{\partial B_1} F_\varepsilon^m(rx) \frac{x^m}{r} \right\} + \int_{\partial B_1} F_\varepsilon^m(rx) \frac{x^m}{r^2} \\
&= \frac{d}{dr}\left\{ \int_{\partial B_r} F_\varepsilon^m \frac{x^m}{r^{n+1}} \right\} + \int_{\partial B_r} F_\varepsilon^m \frac{x^m}{r^{n+2}}.
\end{aligned}$$

As a consequence, using the latter identity, (9-9) and (9-14), we find that

$$\int_{B_r} G_\varepsilon^m \cdot e_m = 2\int_{B_r} ((\Delta u \nabla u_m) * \rho_\varepsilon) \cdot e_m - \int_{B_r} \nabla F_\varepsilon^m \cdot e_m = 2\int_{B_r} ((\Delta u \nabla u_m) * \rho_\varepsilon) \cdot e_m - \int_{\partial B_r} F_\varepsilon^m \frac{x^m}{r}$$

$$\begin{aligned}
\int_{\partial B_r} G_\varepsilon^m \cdot \frac{x^m\, x}{r^{n+2}} &= 2\int_{\partial B_r} ((\Delta u \nabla u_m) * \rho_\varepsilon) \cdot \frac{x^m\, x}{r^{n+2}} - \int_{\partial B_r} \nabla F_\varepsilon^m \cdot \frac{x^m\, x}{r^{n+2}} \\
&= 2\int_{\partial B_r} ((\Delta u \nabla u_m) * \rho_\varepsilon) \cdot \frac{x^m\, x}{r^{n+2}} - \int_{\partial B_r} F_\varepsilon^m \frac{x^m}{r^{n+2}} - \frac{d}{dr}\left\{ \int_{\partial B_r} F_\varepsilon^m \frac{x^m}{r^{n+1}} \right\}.
\end{aligned}$$

From this and (9-13), we obtain

$$\begin{aligned}
Z_\varepsilon(r) &= \frac{2}{r^{n+1}} \sum_{m=1}^{n} \int_{B_r} ((\Delta u \nabla u_m) * \rho_\varepsilon) \cdot e_m - 2\sum_{m=1}^{n} \int_{\partial B_r} ((\Delta u \nabla u_m) * \rho_\varepsilon) \cdot \frac{x^m\, x}{r^{n+2}} + \sum_{m=1}^{n} \frac{d}{dr}\left\{ \int_{\partial B_r} F_\varepsilon^m \frac{x^m}{r^{n+1}} \right\} \\
&= 2R_\varepsilon(r) + T_\varepsilon'(r),
\end{aligned}$$

with

$$\begin{aligned}
R_\varepsilon(r) &:= \frac{1}{r^{n+1}} \sum_{m=1}^{n} \int_{B_r} ((\Delta u \nabla u_m) * \rho_\varepsilon) \cdot e_m - \sum_{m=1}^{n} \int_{\partial B_r} ((\Delta u \nabla u_m) * \rho_\varepsilon) \cdot \frac{x^m\, x}{r^{n+2}}, \\
T_\varepsilon(r) &:= \sum_{m=1}^{n} \left\{ \int_{\partial B_r} F_\varepsilon^m \frac{x^m}{r^{n+1}} \right\} = \sum_{m=1}^{n} \left\{ \int_{\partial B_r} (\Delta u\, u_m) * \rho_\varepsilon \frac{x^m}{r^{n+1}} \right\},
\end{aligned} \tag{9-15}$$

where we have also used (9-3) and (9-5).

Consequently, integrating (9-12),

$$0=2\int_{r_1}^{r_2} Z_\varepsilon(r)\,dr+D_\varepsilon(r_2)-D_\varepsilon(r_1)=4\int_{r_1}^{r_2} R_\varepsilon(r)\,dr+2T_\varepsilon(r_2)-2T_\varepsilon(r_1)+D_\varepsilon(r_2)-D_\varepsilon(r_1). \tag{9-16}$$

Comparing (9-2) with (9-15), we see that $R_\varepsilon \to R$ and $T_\varepsilon \to T$ as $\varepsilon \to 0$, thanks to (4-1) and (4-2).

We thereby obtain the desired claim in (9-1) by passing to the limit the identity in (9-16). □

We also point out the following useful calculation:

Lemma 9.2. *In the notation stated by* (9-2), *we have that*

$$4\int_{r_1}^{r_2}\Big(\frac{1}{r^n}\int_{\partial B_r}\Delta u\left(2\frac{u_r}{r}-\partial_r^2 u-2\frac{u}{r^2}\right)\Big)\,dr-4V(r_2)+4V(r_1)+2T(r_2)-2T(r_1)+D(r_2)-D(r_1)=0, \tag{9-17}$$

where

$$V(r):=\frac{1}{r^{n+1}}\int_{\partial B_r}\Delta u u. \tag{9-18}$$

Proof. For any smooth function v,

$$\begin{aligned}\int_{B_r}|\Delta v|^2&=\int_{B_r}(\operatorname{div}(\Delta v\nabla v)-\nabla\Delta v\cdot\nabla v)=\int_{\partial B_r}\Delta v\, v_r-\int_{B_r}\nabla\Delta v\cdot\nabla v\\&=\int_{\partial B_r}\Delta v\, v_r-\int_{B_r}\operatorname{div}(v\nabla\Delta v)+\int_{B_r}\Delta^2 v\, v=\int_{\partial B_r}\Delta v\, v_r-\int_{\partial B_r}v\,\Delta v_r+\int_{B_r}\Delta^2 v\, v.\end{aligned} \tag{9-19}$$

We also observe that

$$\begin{aligned}\frac{d}{dr}\left(\frac{1}{r^{n+1}}\int_{\partial B_r}\Delta v v\right)&=\frac{d}{dr}\left(\frac{1}{r^2}\int_{\partial B_1}\Delta v(r\theta)v(r\theta)\right)\\&=-\frac{2}{r^3}\int_{\partial B_1}\Delta v(r\theta)v(r\theta)+\frac{1}{r^2}\int_{\partial B_1}\Delta v_r(r\theta)v(r\theta)+\frac{1}{r^2}\int_{\partial B_1}\Delta v(r\theta)v_r(r\theta)\\&=-\frac{2}{r^{n+2}}\int_{\partial B_r}\Delta v\, v+\frac{1}{r^{n+1}}\int_{\partial B_r}\Delta v_r\, v+\frac{1}{r^{n+1}}\int_{\partial B_r}\Delta v\, v_r.\end{aligned}$$

From this and (9-19), we obtain that, for any smooth function v,

$$\begin{aligned}\frac{1}{r^{n+1}}\int_{B_r}|\Delta v|^2-\frac{1}{r^n}\int_{\partial B_r}\Delta v\partial_r^2 v&=\frac{1}{r^{n+1}}\int_{\partial B_r}\Delta v\, v_r-\frac{1}{r^{n+1}}\int_{\partial B_r}v\,\Delta v_r+\frac{1}{r^{n+1}}\int_{B_r}\Delta^2 v\, v-\frac{1}{r^n}\int_{\partial B_r}\Delta v\,\partial_r^2 v\\&=\frac{1}{r^n}\int_{\partial B_r}\Delta v\Big(2\frac{v_r}{r}-\partial_r^2 v-2\frac{v}{r^2}\Big)+\frac{1}{r^{n+1}}\int_{B_r}\Delta^2 v v-\frac{d}{dr}\left(\frac{1}{r^{n+1}}\int_{\partial B_r}\Delta v v\right).\end{aligned}$$

Integrating this identity and setting

$$V_v(r):=\frac{1}{r^{n+1}}\int_{\partial B_r}\Delta v v, \tag{9-20}$$

we thereby obtain that

$$\int_{r_1}^{r_2}\left(\frac{1}{r^{n+1}}\int_{B_r}|\Delta v|^2-\frac{1}{r^n}\int_{\partial B_r}\Delta v\,\partial_r^2 v\right)dr \\ =\int_{r_1}^{r_2}\left(\frac{1}{r^n}\int_{\partial B_r}\Delta v\left(2\frac{v_r}{r}-\partial_r^2 v-2\frac{v}{r^2}\right)+\frac{1}{r^{n+1}}\int_{B_r}\Delta^2 v\,v\right)dr-V_v(r_2)+V_v(r_1). \tag{9-21}$$

The idea is now to take v as a mollification of u and use either (7-9) (if u is a minimizer) or Lemma 7.5 (if u is a one-phase minimizer). In this way, the term $\int_{B_r}\Delta^2 v\,v$ approaches either $\int_{B_r} u\,\mathcal{M}_u$, in the notation of (7-9) (if u is a minimizer), or 0 (if u is a one-phase minimizer, due to Lemma 7.5).

To make the notation uniform, we therefore define $\mathcal{M}_u^*:=\mathcal{M}_u$ if u is a minimizer and $\mathcal{M}_u^*:=0$ if u is a one-phase minimizer: then, approximating u, passing to the limit (9-21), and comparing (9-20) with (9-18), we can write

$$\int_{r_1}^{r_2}\left(\frac{1}{r^{n+1}}\int_{B_r}|\Delta u|^2-\frac{1}{r^n}\int_{\partial B_r}\Delta u\,\partial_r^2 u\right)dr \\ =\int_{r_1}^{r_2}\left(\frac{1}{r^n}\int_{\partial B_r}\Delta u\left(2\frac{u_r}{r}-\partial_r^2 u-2\frac{u}{r^2}\right)-\frac{1}{r^{n+1}}\int_{B_r}u\,\mathcal{M}_u^*\right)dr-V(r_2)+V(r_1).$$

That is, recalling (9-2),

$$\int_{r_1}^{r_2}R(r)\,dr=\int_{r_1}^{r_2}\left(\frac{1}{r^n}\int_{\partial B_r}\Delta u\left(2\frac{u_r}{r}-\partial_r^2 u-2\frac{u}{r^2}\right)-\frac{1}{r^{n+1}}\int_{B_r}u\,\mathcal{M}_u^*\right)dr-V(r_2)+V(r_1).$$

From this and (9-1) we obtain that

$$2T(r_1)-2T(r_2)+D(r_1)-D(r_2) \\ =4\int_{r_1}^{r_2}\left(\frac{1}{r^n}\int_{\partial B_r}\Delta u\left(2\frac{u_r}{r}-\partial_r^2 u-2\frac{u}{r^2}\right)-\frac{1}{r^{n+1}}\int_{B_r}u\,\mathcal{M}_u^*\right)dr-4V(r_2)+4V(r_1). \tag{9-22}$$

Now we claim that

$$\int_{B_r}u\,\mathcal{M}_u^*=0. \tag{9-23}$$

For this, since $\mathcal{M}_u^*=0$ in the one-phase problem, we can suppose that u is a minimizer, in which case $\mathcal{M}_u^*=\mathcal{M}_u$. Then, let us fix $\delta\in(0,1)$. From Lemma 4.1, we know that

$$-\int_{B_r\cap\{|u|\geqslant\delta\}}u\,\mathcal{M}_u=\int_{B_r\cap\{u\geqslant\delta\}}u\,\Delta^2 u+\int_{B_r\cap\{u\leqslant-\delta\}}u\,\Delta^2 u=0.$$

Therefore, exploiting Lemma 7.4,

$$\left|\int_{B_r}u\,\mathcal{M}_u\right|=\left|\int_{B_r\cap\{|u|<\delta\}}u\,\mathcal{M}_u\right|\leqslant\delta\mathcal{M}_u(B_r)\leqslant C\delta r^{n-2},$$

for some $C>0$. Then, sending $\delta\to 0^+$, we obtain (9-23) as desired.

Then, the identities in (9-22) and (9-23) lead to (9-17). □

Now we restrict the previous calculations to the case $n=2$, and we complete the proof of (1-21).

Proof of (1-21). Using polar coordinates (r,θ), we compute

$$-\frac{1}{r^n}\int_{\partial B_r}\Delta u\left(2\frac{u_r}{r}-\partial_r^2 u-2\frac{u}{r^2}\right)=\int_{\partial B_1}\frac{1}{r}\Delta u\left(u_{rr}-2\frac{u_r}{r}+2\frac{u}{r^2}\right)$$
$$=\int_{\partial B_1}\frac{1}{r}\left(u_{rr}+\frac{u_r}{r}+\frac{u_{\theta\theta}}{r^2}\right)\left(u_{rr}-2\frac{u_r}{r}+2\frac{u}{r^2}\right)=A(r)+B(r), \quad (9\text{-}24)$$

where

$$A(r):=\int_{\partial B_1}\frac{1}{r^3}u_{\theta\theta}\left(u_{rr}-2\frac{u_r}{r}+2\frac{u}{r^2}\right)\quad\text{and}\quad B(r):=\int_{\partial B_1}\frac{1}{r}\left(u_{rr}+\frac{u_r}{r}\right)\left(u_{rr}-2\frac{u_r}{r}+2\frac{u}{r^2}\right). \quad (9\text{-}25)$$

Now, we perform several integrations by parts involving the terms related to $A(r)$. First of all, we see that

$$\frac{1}{r^3}\int_{\partial B_1}u_{\theta\theta}u_{rr}=-\frac{1}{r^3}\int_{\partial B_1}u_\theta u_{\theta rr}$$
$$=-\frac{d}{dr}\int_{\partial B_1}\frac{u_\theta u_{r\theta}}{r^3}+\int_{\partial B_1}\frac{u_{r\theta}^2}{r^3}-3\int_{\partial B_1}\frac{u_\theta u_{\theta r}}{r^4}. \quad (9\text{-}26)$$

Similarly, we have that

$$-2\int_{\partial B_1}\frac{1}{r^4}u_{\theta\theta}u_r=2\int_{\partial B_1}\frac{u_\theta u_{\theta r}}{r^4}=2\int_{\partial B_1}\frac{u_\theta u_{\theta r}}{r^4} \quad (9\text{-}27)$$

and

$$2\int_{\partial B_1}\frac{1}{r^5}u_{\theta\theta}u=-2\int_{\partial B_1}\frac{u_\theta^2}{r^5}. \quad (9\text{-}28)$$

Combining (9-26), (9-27), and (9-28), and recalling (9-25), we get

$$A(r)=-\frac{d}{dr}\left(\int_{\partial B_1}\frac{u_\theta u_{r\theta}}{r^3}\right)+\int_{\partial B_1}\frac{u_{r\theta}^2}{r^3}-3\int_{\partial B_1}\frac{u_\theta u_{\theta r}}{r^4}+2\int_{\partial B_1}\frac{u_\theta u_{\theta r}}{r^4}-2\int_{\partial B_1}\frac{u_\theta^2}{r^5}$$
$$=-\frac{d}{dr}\left(\int_{\partial B_1}\frac{u_\theta u_{r\theta}}{r^3}\right)+\int_{\partial B_1}\frac{u_{r\theta}^2}{r^3}-\int_{\partial B_1}\frac{u_\theta u_{\theta r}}{r^4}-2\int_{\partial B_1}\frac{u_\theta^2}{r^5}$$
$$=-\frac{d}{dr}\left(\int_{\partial B_1}\frac{u_\theta u_{r\theta}}{r^3}\right)+\int_{\partial B_1}\frac{1}{r^3}\left(u_{\theta r}-\frac{2u_\theta}{r}\right)^2+3\int_{\partial B_1}\frac{u_\theta u_{\theta r}}{r^4}-6\int_{\partial B_1}\frac{u_\theta^2}{r^5}$$
$$=-\frac{d}{dr}\left(\int_{\partial B_1}\frac{u_\theta u_{r\theta}}{r^3}+\frac{3}{2}\int_{\partial B_1}\frac{u_\theta^2}{r^4}\right)+\int_{\partial B_1}\frac{1}{r^3}\left(u_{\theta r}-\frac{2u_r}{r}\right)^2$$
$$=-\frac{d}{dr}\left(\int_{\partial B_r}\frac{u_\theta u_{r\theta}}{r^4}+\frac{3}{2}\int_{\partial B_r}\frac{u_\theta^2}{r^5}\right)+\int_{\partial B_r}\frac{1}{r^4}\left(u_{\theta r}-\frac{2u_r}{r}\right)^2. \quad (9\text{-}29)$$

From (9-25), we also compute that

$$
\begin{aligned}
B(r) &= \int_{\partial B_1} \frac{1}{r}\left(u_{rr}^2 - \frac{2u_{rr}u_r}{r} + \frac{2uu_{rr}}{r^2} + \frac{u_r u_{rr}}{r} - \frac{2u_r^2}{r^2} + \frac{2uu_r}{r^3}\right) \\
&= \int_{\partial B_1} \frac{1}{r}\left(u_{rr}^2 - \frac{u_{rr}u_r}{r} + \frac{2uu_{rr}}{r^2} - \frac{2u_r^2}{r^2} + \frac{2uu_r}{r^3}\right) \\
&= \int_{\partial B_1} \frac{1}{r}\left(u_{rr} - \frac{3u_r}{r} + 4\frac{u}{r^2}\right)^2 + \frac{1}{r}\left(\frac{5u_r u_{rr}}{r} - \frac{6uu_{rr}}{r^2} - \frac{11u_r^2}{r^2} + \frac{26uu_r}{r^3} - \frac{16u^2}{r^4}\right) \\
&= \int_{\partial B_1} \frac{1}{r}\left(u_{rr} - \frac{3u_r}{r} + 4\frac{u}{r^2}\right)^2 + \frac{d}{dr}\left(\int_{\partial B_1} \frac{5u_r^2}{2r^2} - \int_{\partial B_1} \frac{6uu_r}{r^3} + \int_{\partial B_1} \frac{4u^2}{r^4}\right) \\
&= \int_{\partial B_r} \frac{1}{r^2}\left(u_{rr} - \frac{3u_r}{r} + 4\frac{u}{r^2}\right)^2 + \frac{d}{dr}\left(\int_{\partial B_r} \frac{5u_r^2}{2r^3} - \int_{\partial B_r} \frac{6uu_r}{r^4} + \int_{\partial B_r} \frac{4u^2}{r^5}\right).
\end{aligned} \tag{9-30}
$$

Using (9-29) and (9-30), we conclude that

$$
A(r) + B(r) = \frac{1}{r^2}\int_{\partial B_r}\left[\left(\frac{u_{\theta r}}{r} - \frac{2u_r}{r^2}\right)^2 + \left(u_{rr} - \frac{3u_r}{r} + 4\frac{u}{r^2}\right)^2\right] + W'(r), \tag{9-31}
$$

where

$$
W(r) := \int_{\partial B_r}\left(\frac{5u_r^2}{2r^3} - \frac{6uu_r}{r^4} + \frac{4u^2}{r^5} - \frac{u_\theta u_{r\theta}}{r^4} - \frac{3u_\theta^2}{2r^5}\right). \tag{9-32}
$$

Now, from (9-17) and (9-24), we see that

$$
\begin{aligned}
-4V(r_2) + 4V(r_1) + 2T(r_2) - 2T(r_1) + D(r_2) - D(r_1) &= -4\int_{r_1}^{r_2}\left(\frac{1}{r^n}\int_{\partial B_r} \Delta u\left(2\frac{u_r}{r} - \partial_r^2 u - 2\frac{u}{r^2}\right)\right) dr \\
&= 4\int_{r_1}^{r_2} (A(r) + B(r))\, dr.
\end{aligned}
$$

This and (9-31) give that

$$
\begin{aligned}
-V(r_2) + V(r_1) + \frac{T(r_2) - T(r_1)}{2} + \frac{D(r_2) - D(r_1)}{4} - W(r_2) + W(r_1) \\
= \int_{r_1}^{r_2}\left\{\frac{1}{r^2}\int_{\partial B_r}\left[\left(\frac{u_{\theta r}}{r} - \frac{2u_r}{r^2}\right)^2 + \left(u_{rr} - \frac{3u_r}{r} + 4\frac{u}{r^2}\right)^2\right]\right\}.
\end{aligned} \tag{9-33}
$$

Recalling (1-22), (9-2), (9-18), and (9-32), we see that

$$
\begin{aligned}
&-V(r) + \frac{T(r)}{2} + \frac{D(r)}{4} - \int_{\partial B_r}\left(\frac{5u_r^2}{2r^3} - \frac{6uu_r}{r^4} + \frac{4u^2}{r^5} - \frac{u_\theta u_{r\theta}}{r^4} - \frac{3u_\theta^2}{2r^5}\right) \\
&= -\frac{1}{r^3}\int_{\partial B_r} \Delta u u + \frac{1}{2r^2}\int_{\partial B_r} \Delta u\, \partial_r u + \frac{1}{4r^2}\int_{B_r}\left(|\Delta u|^2 + \chi_{\{u>0\}}\right) - \int_{\partial B_r}\left(\frac{5u_r^2}{2r^3} - \frac{6uu_r}{r^4} + \frac{4u^2}{r^5} - \frac{u_\theta u_{r\theta}}{r^4} - \frac{3u_\theta^2}{2r^5}\right) \\
&= E(r).
\end{aligned}
$$

This and (9-33) establish (1-21), as desired. □

Now, since the proof of (1-21) has been completed, to finish the proof of Theorem 1.12, we only need to show that the function E defined in (1-22) is bounded and to check that if E is constant then u is a homogeneous function of degree two.

These goals will be accomplished by the following arguments:

Proof of the boundedness of E. To show that E is bounded, we claim that there exist $C > 0$ and a sequence $r_k \to 0^+$ such that

$$\int_{\partial B_{r_k}} \left(\frac{|\nabla u|^2}{r_k^3} + \frac{|D^2 u|^2}{r_k} \right) \leqslant C. \tag{9-34}$$

The proof of (9-34) needs to distinguish the case in which u is a minimizer from the case in which u is a one-phase minimizer. Suppose first that u is a one-phase minimizer. Then, since $u(0) = 0 \leqslant u(x)$ for any $x \in \Omega$ and u is assumed to be $C^{1,1}(\Omega)$, we can write $|\nabla u(x)| \leqslant C|x|$ and $|D^2 u(x)| \leqslant C$, for some $C > 0$, from which (9-34) plainly follows in this case.

Now, we prove (9-34) assuming that u is a minimizer. We argue by contradiction, supposing that (9-34) does not hold. Then, for any $\bar{C} > 0$ there exists $\bar{r} \in (0, 1)$ such that for any $r \in (0, \bar{r})$ we have

$$\int_{\partial B_r} \left(\frac{|\nabla u|^2}{r^3} + \frac{|D^2 u|^2}{r} \right) \geqslant \bar{C}.$$

This, Corollary A.2 (if u is a minimizer) or the fact that u is assumed to be in $C^{1,1}(\Omega)$ (if u is a one-phase minimizer) imply that, for a suitable $C > 0$,

$$\begin{aligned}
C &\geqslant \frac{1}{\bar{r}^4} \int_{B_{\bar{r}}} |\nabla u|^2 + \frac{1}{\bar{r}^2} \int_{B_{\bar{r}}} |D^2 u|^2 \\
&= \frac{1}{\bar{r}^4} \int_0^{\bar{r}} \left(\int_{\partial B_r} |\nabla u|^2 \right) dr + \frac{1}{\bar{r}^2} \int_0^{\bar{r}} \left(\int_{\partial B_r} |D^2 u|^2 \right) dr = \frac{1}{\bar{r}} \int_0^{\bar{r}} \left(\int_{\partial B_r} \frac{|\nabla u|^2}{\bar{r}^3} + \int_{\partial B_r} \frac{|D^2 u|^2}{\bar{r}} \right) dr \\
&\geqslant \frac{1}{\bar{r}} \int_{\bar{r}/2}^{\bar{r}} \left(\int_{\partial B_r} \frac{|\nabla u|^2}{\bar{r}^3} + \int_{\partial B_r} \frac{|D^2 u|^2}{\bar{r}} \right) dr \\
&\geqslant \frac{1}{8\bar{r}} \int_{\bar{r}/2}^{\bar{r}} \left(\int_{\partial B_r} \frac{|\nabla u|^2}{r^3} + \int_{\partial B_r} \frac{|D^2 u|^2}{r} \right) dr \\
&\geqslant \frac{\bar{C}}{16},
\end{aligned}$$

which is a contradiction if $\bar{C}$ is suitably large, and this establishes (9-34).

As a consequence, using the Cauchy–Schwarz inequality, Theorem 1.7, and (9-34),

$$\begin{aligned}
&\int_{\partial B_{r_k}} \left| \frac{\Delta u\, u_r}{2r_k^2} - \frac{5u_r^2}{2r_k^3} - \frac{\Delta u u}{r_k^3} + \frac{6uu_r}{r_k^4} + \frac{u_\theta u_{\theta r}}{r_k^4} - \frac{4u^2}{r_k^5} - \frac{3u_\theta^2}{2r_k^5} \right| \\
&\leqslant C \int_{\partial B_{r_k}} \left(\frac{|D^2 u|\,|\nabla u|}{r_k^{1/2}\, r_k^{3/2}} + \frac{|\nabla u|^2}{r_k^3} + \frac{|\Delta u|}{r_k^{1/2}\, r_k^{1/2}} + \frac{|\nabla u|}{r_k^{3/2}\, r_k^{1/2}} + \frac{1}{r_k} \right) \leqslant C \int_{\partial B_{r_k}} \left(\frac{|\nabla u|^2}{r_k^3} + \frac{|D^2 u|^2}{r_k} + \frac{1}{r_k} \right) \leqslant C,
\end{aligned}$$

for some $C > 0$, possibly varying from line to line.

Using this, (1-22), and Corollary A.2 (if u is a minimizer) or the assumption that $u \in C^{1,1}(\Omega)$ (if u is a one-phase minimizer), we deduce that

$$|E(r_k)| \leqslant \int_{\partial B_{r_k}} \left| \frac{\Delta u\, u_r}{2r_k^2} - \frac{5u_r^2}{2r_k^3} - \frac{\Delta u u}{r_k^3} + \frac{6uu_r}{r_k^4} + \frac{u_\theta u_{\theta r}}{r_k^4} - \frac{4u^2}{r_k^5} - \frac{3u_\theta^2}{2r_k^5} \right| + \frac{1}{4r_k^2} \int_{B_{r_k}} \big(|\Delta u|^2 + \chi_{\{u>0\}} \big)$$
$$\leqslant C + \frac{1}{4r_k^2} \int_{B_{r_k}} \chi_{\{u>0\}} \leqslant C, \tag{9-35}$$

up to renaming $C > 0$.

Now, fix $r \in (0, 1)$. Let $\bar{k}$ sufficiently large, such that $r_{\bar{k}} \in (0, r)$. From (1-21), we know that $E(r_{\bar{k}}) \leqslant E(r) \leqslant E(1)$. Hence, by (9-35),

$$-C \leqslant E(r) \leqslant E(1). \qquad \square$$

Having already checked the validity of the monotonicity formula in (1-21) and the fact that E is bounded, in order to complete the proof of Theorem 1.12, we only need to show that if E is constant in $(0, \tau)$, then u is a homogeneous function of degree two. This is now a simple consequence of (1-21). The detailed argument goes as follows:

Proof of the case of constant E. Suppose now that E is constant in $(0, \tau)$. Then, by (1-21),

$$-\frac{\partial}{\partial \theta}\left(-\frac{u_r}{r} + \frac{2u}{r^2} \right) = \frac{u_{r\theta}}{r^2} - \frac{2u_\theta}{r} = 0 \quad \text{and} \quad -r\frac{\partial}{\partial r}\left(-\frac{u_r}{r} + \frac{2u}{r^2} \right) = u_{rr} - \frac{3u_r}{r} + \frac{4u}{r^2} = 0,$$

which, in turn, gives that

$$\nabla\left(-\frac{u_r}{r} + 2\frac{u}{r^2} \right) = 0.$$

Consequently, the function $-\frac{u_r}{r} + \frac{2u}{r^2}$ is constant for $|x| \in (0, \tau)$, hence we write

$$-\frac{u_r}{r} + \frac{2u}{r^2} = c, \tag{9-36}$$

for some $c \in \mathbb{R}$.

Now we define

$$v(r, \theta) := u(r, \theta) + cr^2 \log r. \tag{9-37}$$

Using (9-36), we obtain

$$v_r = u_r + 2cr \log r + cr = \frac{2u}{r} + 2cr \log r = \frac{2v}{r}.$$

Integrating this equation, fixed $\bar{r} \in (0, \tau)$, we find that

$$v(r, \theta) = \frac{r^2\, v(\bar{r}, \theta)}{\bar{r}^2}.$$

This and (9-37) provide

$$u(r, \theta) = \frac{r^2\, v(\bar{r}, \theta)}{\bar{r}^2} - cr^2 \log r.$$

Therefore, exploiting Theorem 1.7 (if u is a minimizer) or the assumption that $u \in C^{1,1}(\Omega)$ (if u is a one-phase minimizer),

$$C \geqslant \frac{|u(r,\theta)|}{r^2} \geqslant |c|\,|\log r| - \frac{|v(\bar r,\theta)|}{\bar r^2},$$

for some $C > 0$, and therefore,

$$|c| \leqslant \lim_{r\to 0} \frac{|v(\bar r,\theta)|}{\bar r^2\,|\log r|} + \frac{C}{|\log r|} = 0.$$

Hence, we get that $c = 0$ and, as a consequence, we can write (9-36) as

$$-\frac{u_r}{r} + \frac{2u}{r^2} = 0$$

for any $x \in B_\tau$, and therefore $\nabla u(x)\cdot x = 2u(x)$ for any $x \in B_\tau$. Observing that this is the Euler equation for homogeneous functions of degree two, we thus obtain the homogeneity of u. The proof of Theorem 1.12 is thereby complete. □

We finish this section by an explicit computation of the energy, E, for the homogeneous functions of degree two on the plane. It will be used later in the proof of Theorem 1.14.

Lemma 9.3. *Let $\mathcal{C} \subseteq \mathbb{R}^2$ be a cone in $\mathbb{R}^2$, written in polar coordinates as*

$$\mathcal{C} = \{(r,\theta) \in (0,+\infty) \times (\theta_1,\theta_2)\},$$

for some $0 \leqslant \theta_1 < \theta_2 \leqslant 2\pi$.

Let $u : \mathcal{C} \to \mathbb{R}$ be a homogeneous function of the form $u(x) = r^2 g(\theta)$, with $g \in C^2([\theta_1,\theta_2])$, $g > 0$ in (θ_1,θ_2), and

$$g(\theta_1) = g(\theta_2) = 0 \quad \textit{and} \quad g'(\theta_1) = g'(\theta_2) = 0.$$

Assume also that Δu is constant in $\mathcal{C}$. Then, for any $r > 0$,

$$\int_{\mathcal{C}\cap\partial B_r} \Big(\frac{\Delta u\, u_r}{2r^2} - \frac{5u_r^2}{2r^3} - \frac{\Delta u u}{r^3} + \frac{6uu_r}{r^4} + \frac{u_\theta u_{\theta r}}{r^4} - \frac{4u^2}{r^5} - \frac{3u_\theta^2}{2r^5} \Big) + \frac{1}{4r^2} \int_{\mathcal{C}\cap B_r} \big(|\Delta u|^2 + \chi_{\{u>0\}} \big)$$
$$= \frac{\pi}{4} \frac{|\{u>0\}\cap B_r|}{|B_r|} = \frac{\theta_2-\theta_1}{8}. \tag{9-38}$$

Proof. By assumption, in $\mathcal{C}$ we have that

$$C_0 = \Delta u = 4g + g'', \tag{9-39}$$

for some $C_0 \in \mathbb{R}$, and

$$\frac{\Delta u\, u_r}{2r^2} - \frac{5u_r^2}{2r^3} - \frac{\Delta u u}{r^3} + \frac{6uu_r}{r^4} + \frac{u_\theta u_{\theta r}}{r^4} - \frac{4u^2}{r^5} - \frac{3u_\theta^2}{2r^5}$$
$$= \frac{(4g+g'')g}{r} - \frac{10g^2}{r} - \frac{(4g+g'')g}{r} + \frac{12g^2}{r} + \frac{2(g')^2}{r} - \frac{4g^2}{r} - \frac{3(g')^2}{2r} = -\frac{2g^2}{r} + \frac{(g')^2}{2r}.$$

Therefore, after an integration by parts, and recalling (9-39), we have that

$$\begin{aligned}\int_{\mathcal{C}\cap\partial B_r}\left(\frac{\Delta u\,u_r}{2r^2}-\frac{5u_r^2}{2r^3}-\frac{\Delta u u}{r^3}+\frac{6uu_r}{r^4}+\frac{u_\theta u_{\theta r}}{r^4}-\frac{4u^2}{r^5}-\frac{3u_\theta^2}{2r^5}\right)\\ =\int_{\theta_1}^{\theta_2}\left(-2g^2+\frac{(g')^2}{2}\right)=\int_{\theta_1}^{\theta_2}\left(-2g^2-\frac{g''g}{2}\right)=-\frac{1}{2}\int_{\theta_1}^{\theta_2}g(4g+g'')\\ =-\frac{C_0}{2}\int_{\theta_1}^{\theta_2}g=\frac{C_0}{8}\int_{\theta_1}^{\theta_2}(g''-C_0)=-\frac{C_0^2\,(\theta_2-\theta_1)}{8}.\end{aligned}\tag{9-40}$$

On the other hand,

$$\frac{1}{4r^2}\int_{\mathcal{C}\cap B_r}|\Delta u|^2=\frac{1}{8}\int_{\theta_1}^{\theta_2}(4g+g'')^2=\frac{C_0^2\,(\theta_2-\theta_1)}{8}.$$

This and (9-40) provide

$$\int_{\mathcal{C}\cap\partial B_r}\left(\frac{\Delta u\,u_r}{2r^2}-\frac{5u_r^2}{2r^3}-\frac{\Delta u u}{r^3}+\frac{6uu_r}{r^4}+\frac{u_\theta u_{\theta r}}{r^4}-\frac{4u^2}{r^5}-\frac{3u_\theta^2}{2r^5}\right)+\frac{1}{4r^2}\int_{\mathcal{C}\cap B_r}\left(|\Delta u|^2+\chi_{\{u>0\}}\right)=\frac{1}{4r^2}\int_{B_r}\chi_{\{u>0\}},$$

which proves (9-38). □

10. Monotonicity formula: homogeneity of the blow-up limits and proof of Theorem 1.13

In this section, we apply the results in Theorem 1.12 to study the homogeneity properties of the blow-up limits of the minimizers of J at free boundary points with vanishing gradient, thus proving Theorem 1.13.

Proof of Theorem 1.13. Suppose that u does not vanish identically. We let

$$Q(u,x):=Q(u,r,\theta)=\left(-\frac{u_{r\theta}}{r}+2\frac{u_\theta}{r^2}\right)^2+\left(u_{rr}-3\frac{u_r}{r}+4\frac{u}{r^2}\right)^2.\tag{10-1}$$

Note that Q is invariant with respect to quadratic scaling. Indeed, if we define, for any $s>0$,

$$u_s(x):=\frac{u(sx)}{s^2},$$

we have that

$$\begin{aligned}Q(u_s,x)&=\left(-\frac{(u_s)_{r\theta}}{r}+2\frac{(u_s)_\theta}{r^2}\right)^2+\left((u_s)_{rr}-3\frac{(u_s)_r}{r}+4\frac{u_s}{r^2}\right)^2\\ &=\left(-\frac{u_{r\theta}(sx)}{sr}+2\frac{u_\theta(sx)}{(sr)^2}\right)^2+\left(u_{rr}(sx)-3\frac{u_r(sx)}{sr}+4\frac{u(sx)}{(sr)^2}\right)^2=Q(u,sx).\end{aligned}\tag{10-2}$$

Now, in view of (1-21) and (10-1), we observe that

$$\begin{aligned}E(\tau_2)-E(\tau_1)&=\int_{\tau_1}^{\tau_2}\left\{\frac{1}{r^2}\int_{\partial B_r}\left[\left(\frac{u_{\theta r}}{r}-\frac{2u_\theta}{r^2}\right)^2+\left(u_{rr}-\frac{3u_r}{r}+\frac{4u}{r^2}\right)^2\right]\right\}dr\\ &=\int_{\tau_1}^{\tau_2}\left(\frac{1}{r^2}\int_{\partial B_r}Q(u,x)\,dx\right)dr.\end{aligned}\tag{10-3}$$

As a consequence, for any $s > 0$, using the changes of variables $\rho = r/s$ and $y = x/s$, and making use of (10-2), we see that

$$\begin{aligned} E(s\tau_2) - E(s\tau_1) &= \int_{s\tau_1}^{s\tau_2} \left(\frac{1}{r^2} \int_{\partial B_r} Q(u, x)\, dx \right) dr \\ &= \int_{\tau_1}^{\tau_2} \left(\frac{1}{\rho^2} \int_{\partial B_\rho} Q(u, sy)\, dy \right) d\rho \\ &= \int_{\tau_1}^{\tau_2} \left(\frac{1}{\rho^2} \int_{\partial B_\rho} Q(u_s, y)\, dy \right) d\rho. \end{aligned} \tag{10-4}$$

On the other hand, by Theorem 1.12, we know that E is monotone and bounded, and therefore the limit as $\vartheta \to 0^+$ of $E(\vartheta)$ exists and it is finite. Consequently, we have that

$$E(s\tau_2) - E(s\tau_1) \to 0, \quad \text{as } s \to 0.$$

Hence, recalling (10-4), we conclude that

$$\int_{\tau_1}^{\tau_2} \left(\frac{1}{\rho^2} \int_{\partial B_\rho} Q(u_s, y)\, dy \right) d\rho \to 0, \quad \text{as } s \to 0. \tag{10-5}$$

Also, by compactness (ensured here, if u is a minimizer, by (1-24), which in turns allows us to exploit Corollary A.2, and, if u is a one-phase minimizer by the assumption that $u \in C^{1,1}(\Omega)$), we have that u_s converges to some u_0, up to a subsequence. Therefore, by (10-5),

$$\int_{\tau_1}^{\tau_2} \left(\frac{1}{\rho^2} \int_{\partial B_\rho} Q(u_0, y)\, dy \right) d\rho = 0$$

for all $\tau_2 > \tau_1 > 0$. Thus, since $Q \geqslant 0$, due to (10-1), it follows that $Q(u_0, y) = 0$. Consequently, by (10-3), we have that the function E relative to the minimizer u_0 is identically constant. Therefore, in view of the last claim in Theorem 1.12, it follows that u_0 is a homogeneous function of degree two. □

11. Regularity of the free boundary in two dimensions: explicit computations, classification results in $2D$, and proof of Theorem 1.14

In this section we study the regularity of free boundary of minimizers in dimension 2. Some of the results presented rely on direct calculations, while others are obtained by the monotone quantity E that has been analyzed in Theorems 1.12 and 1.13. In this setting, we have the following classification result for one-phase minimizers:

Theorem 11.1. *Let $u \in C^1(\mathbb{R}^n)$ be a one-phase local minimizer in any ball of $\mathbb{R}^n$, with $0 \in \partial_{\text{sing}}\{u > 0\}$. Let $u = r^2 g(\theta)$, where (r, θ) denotes the polar coordinates. Then, the following dichotomy holds*:

- *either u is a homogeneous polynomial of degree two*,
- *or, up to a rotation, $u(x) = a(x_1^+)^2$ for some $a > 0$.*

Proof. A direct computation shows that

$$\Delta u = u_{rr} + \frac{u_r}{r} + \frac{1}{r^2}\,\Delta_{\mathbb{S}^1} u = 2g + 2g + g'' = g'' + 4g. \tag{11-1}$$

Accordingly, by Lemma 4.1, we have that, in the positivity set of u,

$$r^2 \Delta^2 u = \frac{d^2}{d\theta^2}(g'' + 4g) = 0.$$

From this, we deduce that

$$g''(\theta) + 4g(\theta) = c_1\theta + c_2, \quad \text{for all } \theta \in \{g \neq 0\}, \tag{11-2}$$

for some constants c_1 and c_2. We notice that (11-2) has explicit solution

$$g(\theta) = \frac{c_1\theta}{4} + \frac{c_2}{4} + c_3\cos(2\theta) + c_4\sin(2\theta) = \frac{c_1\theta}{4} + \frac{c_2}{4} + c_3(\cos^2\theta - \sin^2\theta) + 2c_4\sin\theta\cos\theta \tag{11-3}$$

for some constants c_3 and c_4.

Since 0 is a free boundary point for u, we have that g cannot vanish identically. Hence, we distinguish some cases, depending on the number of zeros of g. First of all, we consider the cases in which either $g > 0$ for all $\theta \in [0, 2\pi)$ or g vanishes only at one point. Then, in this case the free boundary is contained in a ray and, up to a rotation, we can assume that $g(\theta) > 0$ for all $\theta \in (0, 2\pi)$ and so (11-3) is valid for all $\theta \in (0, 2\pi)$. The periodicity of g then implies that

$$0 = \lim_{\theta\to 0^+} g(\theta) - \lim_{\theta \to 2\pi^-} g(\theta) = -\frac{c_1\pi}{2},$$

and so $c_1 = 0$. As a consequence, by (11-3),

$$u(r,\theta) = \frac{c_2 r^2}{4} + c_3 r^2(\cos^2\theta - \sin^2\theta) + 2r^2 c_4 \sin\theta\cos\theta = \frac{c_2(x_1^2 + x_2^2)}{4} + c_3(x_1^2 - x_2^2) + 2c_4 x_1 x_2,$$

which is a homogeneous polynomial of degree two, thus proving the desired claim in this case.

Now we suppose that g vanishes at least at two points, say, up to a rotation, θ_0 and $-\theta_0$, for some $\theta_0 \in (0, \pi)$, that is

$$g(\theta) > 0 \text{ for all } \theta \in (-\theta_0, \theta_0) \quad \text{and} \quad g(\theta_0) = g(-\theta_0) = 0. \tag{11-4}$$

Then, by (11-3),

$$0 = g(\pm\theta_0) = \pm\frac{c_1\theta_0}{4} + \frac{c_2}{4} + c_3\cos(2\theta_0) \pm c_4\sin(2\theta_0). \tag{11-5}$$

By the assumptions that $u \in C^1(\mathbb{R}^n)$ and $g \geqslant 0$, we also know that

$$0 = g'(\pm\theta_0) = \frac{c_1}{4} \mp 2c_3\sin(2\theta_0) + 2c_4\cos(2\theta_0). \tag{11-6}$$

Then, we obtain from (11-5) and (11-6) the system

$$\begin{cases} \dfrac{c_1\theta_0}{4} + c_4 \sin(2\theta_0) = 0, \\ \dfrac{c_2}{4} + c_3 \cos(2\theta_0) = 0, \\ c_3 \sin(2\theta_0) = 0, \\ \dfrac{c_1}{4} + 2c_4 \cos(2\theta_0) = 0. \end{cases} \tag{11-7}$$

Now, if

$$\theta_0 \neq \pi/2, \tag{11-8}$$

from (11-7), we have that necessarily $c_3 = 0$, and accordingly

$$\begin{cases} \dfrac{c_1\theta_0}{4} + c_4 \sin(2\theta_0) = 0, \\ \dfrac{c_2}{4} = 0, \\ \dfrac{c_1}{4} + 2c_4 \cos(2\theta_0) = 0. \end{cases}$$

This implies that $c_2 = 0$, and so (11-3) becomes

$$g(\theta) = \frac{c_1\theta}{4} + c_4 \sin(2\theta).$$

In particular $g(0) = 0$, which is in contradiction with (11-4).

This says that the case in (11-8) must be ruled out, and thus $\theta_0 = \pi/2$ (and the positivity sets of u are either one or two half-planes). In this way, the system in (11-7) reduces to

$$\begin{cases} \dfrac{c_1\pi}{8} = 0, \\ \dfrac{c_2}{4} - c_3 = 0, \\ \dfrac{c_1}{4} - 2c_4 = 0, \end{cases}$$

which leads to $c_1 = c_4 = 0$ and $c_2/4 = c_3$. Substituting these conditions into (11-3), we obtain that, for all $\theta \in (-\pi/2, \pi/2)$,

$$g(\theta) = c_3(1 + \cos(2\theta)) = c_3(1 + \cos^2\theta - \sin^2\theta),$$

and therefore, for all $x = (x_1, x_2) \in \mathbb{R}^2$ with $x_1 > 0$,

$$u(x) = 2c_3 x_1^2.$$

This gives that either u is a homogeneous polynomial of degree two, or $u(x) = a\,(x_1^+)^2$ for some $a > 0$, or

$$u(x) = \begin{cases} a x_1^2 & \text{if } x_1 \geqslant 0, \\ b x_1^2 & \text{if } x_1 < 0, \end{cases}$$

with $a, b \in (0, +\infty)$ and

$$a \neq b. \tag{11-9}$$

To complete the proof of the desired result, we need to exclude this case. To this end, we observe that

$$\big(|\Delta u(0^+,1)|^2+1\big)-2\big(\Delta u(0^+,1)u_{11}(0^+,1)-u_1(0^+,1)\Delta u(0^+,1)\big)=((2a)^2+1)-2((2a)^2+0)=1-4a^2,$$

and similarly,

$$\big(|\Delta u(0^-,1)|^2+1\big)-2\big(\Delta u(0^-,1)u_{11}(0^-,1)-u_1(0^-,1)\Delta u(0^-,1)\big)=1-4b^2.$$

These identities and the free boundary condition (1-9) computed at the point (0, 1), where according to the definition in (1-6) we have $\lambda^{(1)}=\lambda^{(2)}=1$, lead to

$$1-4a^2=1-4b^2,$$

which provides $a^2=b^2$, and thus $a=b$. This contradicts with (11-9), and the desired result follows. □

With this, we are now in the position of completing the proof of Theorem 1.14.

Proof of Theorem 1.14. Let E be as in Theorem 1.12, and let[4]

$$E(0):=\lim_{\rho\to 0^+}E(\rho). \tag{11-10}$$

Let $\bar{x}\in\partial\{u>0\}$. Suppose that $u_{0,\bar{x}}$ is a blow-up of u at $\bar{x}$. Notice that $u_{0,\bar{x}}$ cannot be identically equal to zero, due to (1-26). Then by Theorem 11.1 we know that, after some rotation of coordinates,

$$u_{0,\bar{x}} \text{ must be either } \quad \frac{a_1(x_1-\bar{x}_1)^2+a_2(x_2-\bar{x}_2)^2}{2}, \quad \frac{a(x_1-\bar{x}_1)^2}{2}, \quad \text{or} \quad \frac{a((x_1-\bar{x}_1)^+)^2}{2}, \tag{11-11}$$

with a_1, a_2, $a>0$ (say, possibly depending on $\bar{x}$, though the free boundary conditions in Theorem 1.3 have to be fulfilled).

In particular, from (11-11), we know that

$$\Delta u \text{ is constant in the positivity cone of } u. \tag{11-12}$$

Now, from (1-25), we know that, if

$$u_{k,\bar{x}}(x):=\frac{u(\bar{x}+\rho_k x)}{\rho_k^2}, \tag{11-13}$$

with $\rho_k\to 0^+$, then, up to a subsequence,

$$u_{k,\bar{x}}\to u_{0,\bar{x}} \text{ in } C^{1,\alpha}_{\rm loc}(\mathbb{R}^n), \tag{11-14}$$

as $k\to+\infty$, for any $\alpha\in(0,1)$.

We claim that

$$u_{0,0} \text{ must necessarily be } \frac{a(x_1^+)^2}{2}, \tag{11-15}$$

[4] We observe that the limit in (11-10) exist, due to the monotonicity of E, recall Theorem 1.12.

namely the first and the second possibilities in (11-11) are excluded at the origin. To prove (11-15), we argue by contradiction. If not, by (11-14) and (11-11), necessarily

$$\frac{u(\rho_k x)}{\rho_k^2} = u_{k,0}(x) \to \left\{ \text{either } \frac{a_1 x_1^2 + a_2 x_2^2}{2} \text{ or } \frac{a x_1^2}{2} \right\} =: u_{0,0}(x)$$

in $C^{1,\alpha}_{\mathrm{loc}}(\mathbb{R}^n)$. Therefore, using the change of variable $y := \rho_k x$,

$$\lim_{k\to+\infty} \frac{|B_{\rho_k} \cap \{u > 0\}|}{|B_{\rho_k}|} = \lim_{k\to+\infty} \frac{1}{|B_{\rho_k}|} \int_{B_{\rho_k}\cap\{u>0\}} dx = \lim_{k\to+\infty} \frac{1}{|B_1|} \int_{B_1\cap\{u_{k,0}>0\}} dy = \frac{1}{|B_1|} \int_{B_1\cap\{u_{0,0}>0\}} dy = 1.$$

This is a contradiction with (1-27), and so (11-15) is proved.

We let $E_{k,\bar{x}}$ be the monotone function in (1-22) for $u_{k,\bar{x}}$ (while $E_{\bar{x}}$ denotes the same type of function for u centered at the point $\bar{x}$). Let also $E_{0,\bar{x}}$ be the monotone function in (1-22) for $u_{0,\bar{x}}$. In view of (11-14), we have that

$$E_{0,\bar{x}}(r) = \lim_{k\to+\infty} E_{k,\bar{x}}(r). \tag{11-16}$$

We remark that (1-22) is compatible with the blow-up scaling, namely

$$E_{k,\bar{x}}(r) = E_{\bar{x}}(\rho_k r).$$

As a consequence, by (11-10) and (11-16),

$$E_{0,\bar{x}}(r) = \lim_{k\to+\infty} E_{\bar{x}}(\rho_k r) = E_{\bar{x}}(0). \tag{11-17}$$

We now classify the free boundary points according to the monotone function induced by their blow-up limits. For this, we introduce the following notation: recalling (11-11), we say that $\bar{x}$ is Type-1 if, up to a rotation,

$$u_{0,\bar{x}}(x) = \frac{a_1(x_1 - \bar{x}_1)^2 + a_2(x_2 - \bar{x}_2)^2}{2}.$$

Similarly, we say that $\bar{x}$ is Type-2 if

$$u_{0,\bar{x}}(x) = \frac{a(x_1 - \bar{x}_1)^2}{2},$$

and Type-3 if

$$u_{0,\bar{x}}(x) = \frac{a((x_1 - \bar{x}_1)^+)^2}{2}.$$

In this notation, (11-15) says that the origin is Type-3.

Now, in light of (1-22) and Lemma 9.3 (which can be utilized here thanks to (11-12)), we have that

$$E_{0,\bar{x}}(r) = \begin{cases} \dfrac{\pi}{4}, & \text{if } \bar{x} \text{ is either Type-1 or Type-2,} \\ \dfrac{\pi}{8}, & \text{if } \bar{x} \text{ is Type-3.} \end{cases} \tag{11-18}$$

In particular, the monotone function E is minimized for Type-3 free boundary points.

Moreover, we have the semicontinuity property: if $x_j \in \partial\{u > 0\}$ and $x_j \to x_0$ as $j \to +\infty$, then

$$\limsup_{j\to+\infty} E_{x_j}(0) \leqslant E_{x_0}(0). \tag{11-19}$$

Indeed, by the monotonicity of E in Theorem 1.12 and (1-22), for any $r \in (0, 1)$ we have that

$$\limsup_{j\to+\infty} E_{x_j}(0) \leqslant \limsup_{j\to+\infty} E_{x_j}(r) = E_{x_0}(r).$$

Then, we take the limit as $r \to 0^+$, and we obtain (11-19), as desired.

Now we claim that there exists $r_0 > 0$ such that:

$$\text{For any } \bar{x} \in \partial\{u > 0\} \cap B_{r_0}, \text{ we have that } E_{\bar{x}}(0) = E_0(0). \tag{11-20}$$

In other words, in B_{r_0} all free boundary points must be of Type-3. To prove this we argue by contradiction: If not, there exists a sequence of points $\bar{x}_j \in \partial\{u > 0\}$ such that $\bar{x}_j \to 0$ as $j \to +\infty$ and

$$E_{\bar{x}_j}(0) \neq E_0(0). \tag{11-21}$$

From (11-11), (11-15), (11-17), (11-18), and (11-21), we deduce that

$$\left\{\frac{\pi}{8}, \frac{\pi}{4}\right\} \ni E_{0,\bar{x}_j}(r) = E_{\bar{x}_j}(0) \neq E_0(0) = E_{0,0}(r) = \frac{\pi}{8},$$

and accordingly

$$E_{\bar{x}_j}(0) = E_{0,\bar{x}_j}(r) = \frac{\pi}{4} > \frac{\pi}{8} = E_{0,0}(r) = E_0(0).$$

This gives that

$$\lim_{j\to+\infty} E_{\bar{x}_j}(0) = \frac{\pi}{4} > \frac{\pi}{8} = E_0(0),$$

which is in contradiction with (11-19), and so the proof of (11-20) is complete.

Then, by (11-18) and (11-20), it follows that if $\bar{x} \in \partial\{u > 0\} \cap B_{r_0}$, then $\bar{x}$ must necessarily be Type-3, i.e., up to rotations, $u_{0,\bar{x}}(x) = a((x_1 - \bar{x}_1)^+)^2/2$, which is the desired result. □

Appendix A. Decay estimate for D^2u

Here we provide some decay estimates for the gradient and the Hessian of a local minimizer of the functional J in (1-1).

Lemma A.1. *Let $n \geqslant 2$, u be a minimizer for the functional J defined in* (1-1), *and $x_0 \in \partial\{u > 0\}$. Assume that $B_{\bar{R}} \subset\subset \Omega$. Then, there exist $R_0 \in (0, \bar{R})$ and $C > 0$, depending only on n, $\|u\|_{W^{2,2}(\Omega)}$ and* $\operatorname{dist}(B_{\bar{R}}, \partial\Omega)$, *such that*

$$\frac{1}{R^{n+2}} \int_{B_R(x_0)} |\nabla u|^2 + \frac{1}{R^n} \int_{B_R(x_0)} |D^2u|^2 \leqslant \frac{C}{R^{n+4}} \int_{B_{4R}(x_0)} (u-m)^2 + \frac{C}{R^{n+2}} \int_{B_{4R}} (u-m),$$

for any $R \in (0, R_0)$, where

$$m := \min_{B_{4R}(x_0)} u. \tag{A-1}$$

Proof. Without loss of generality we suppose that $x_0 = 0$. Recalling Lemma 4.1, we have that, for any $\phi \in W^{2,2}(\Omega) \cap W_0^{1,2}(\Omega)$, with $\phi \geqslant 0$, it holds that

$$0 \geqslant \int_\Omega \Delta u \, \Delta\phi. \tag{A-2}$$

Now, let $\phi \in C_0^\infty(\Omega)$, with $\phi \geqslant 0$, and define $\phi_\varepsilon := \phi * \rho_\varepsilon$, where $\rho_\varepsilon(x) := (1/\varepsilon^n)\rho(x/\varepsilon)$, for any $x \in \mathbb{R}^n$, is a mollifying kernel, for any $\varepsilon \in (0, 1)$. We also set $u_\varepsilon := u * \rho_\varepsilon$. Then, if $\operatorname{dist}(\operatorname{supp}\phi, \partial\Omega) \gg \varepsilon$, we can use (A-2) and make an integration by parts twice to obtain that

$$\begin{aligned}
0 \geqslant \int_\Omega \Delta u\, \Delta\phi_\varepsilon &= \int_\Omega \Delta u (\Delta\phi) * \rho_\varepsilon = \int_\Omega \Delta u(x)\biggl(\int_\Omega \rho_\varepsilon(x-y)\Delta\phi(y)dy\biggr)dx \\
&= \int_\Omega \Delta\phi(y)\biggl(\int_\Omega \rho_\varepsilon(x-y)\Delta u(x)dx\biggr)dy = \int_\Omega \Delta\phi\, \Delta u_\varepsilon \\
&= \sum_{i,j=1}^n \int_\Omega \phi_{ii}(u_\varepsilon)_{jj} = \sum_{i,j=1}^n \int_{\partial\Omega} \phi_i (u_\varepsilon)_{jj}\nu^i - \sum_{i,j=1}^n \int_\Omega \phi_i (u_\varepsilon)_{ijj} \\
&= \sum_{i,j=1}^n \int_{\partial\Omega} \phi_i (u_\varepsilon)_{jj}\nu^i - \sum_{i,j=1}^n \int_{\partial\Omega} \phi_i (u_\varepsilon)_{ij}\nu^j + \sum_{i,j=1}^n \int_\Omega \phi_{ij}(u_\varepsilon)_{ij} \\
&= \sum_{i,j=1}^n \int_\Omega \phi_{ij}(u_\varepsilon)_{ij}.
\end{aligned} \tag{A-3}$$

Moreover, we observe that

$$\lim_{\varepsilon\to 0} \int_\Omega \phi_{ij}(u_\varepsilon)_{ij} = \int_\Omega \phi_{ij} u_{ij}.$$

From this and (A-3), we have that

$$\sum_{i,j=1}^n \int_\Omega \phi_{ij} u_{ij} \leqslant 0. \tag{A-4}$$

Now, we choose $\phi := (u-m)\eta^2$, where m is as in (A-1), and η is a standard cut-off function supported in $B_{2R} \subset\subset \Omega$, such that $\eta = 1$ in B_R and $\eta = 0$ outside B_{2R}. Therefore, we see that $\phi \in W^{2,2}(\Omega) \cap W_0^{1,2}(\Omega)$ and $\phi \geqslant 0$. With this choice,

$$\phi_{ij} = u_{ij}\eta^2 + 2u_i\eta_j\eta + 2u_j\eta_i\eta + (u-m)(\eta^2)_{ij}.$$

If we plug this into (A-4), we have that

$$\sum_{i,j=1}^n \int_\Omega \bigl(u_{ij}\eta^2 + 4u_i\eta_j\eta + (u-m)(\eta^2)_{ij}\bigr)\, u_{ij} \leqslant 0.$$

That is, rearranging the terms and integrating by parts,

$$\begin{aligned}
\sum_{i,j=1}^n \int_\Omega u_{ij}^2\eta^2 &\leqslant -\sum_{i,j=1}^n \int_\Omega (4u_{ij}u_i\eta_j\eta + (u-m)u_{ij}(\eta^2)_{ij}) \\
&= -\sum_{i,j=1}^n \int_\Omega 4(u_{ij}\eta)u_i\eta_j + \sum_{i,j=1}^n \int_\Omega ((u-m)u_i(\eta^2)_{ijj} + u_iu_j(\eta^2)_{ij}) \\
&\leqslant 2\delta \sum_{i,j=1}^n \int_\Omega u_{ij}^2\eta^2 + \frac{8}{\delta}\sum_{i,j=1}^n \int_\Omega u_i^2\eta_j^2 + \sum_{i,j=1}^n \int_\Omega ((u-m)u_i(\eta^2)_{ijj} + u_iu_j(\eta^2)_{ij}),
\end{aligned} \tag{A-5}$$

where the last line follows from a suitable application of the Hölder inequality, for some $\delta > 0$.

Now, by direct computations we have

$$(\eta^2)_{ij} = 2\eta_i\eta_j + 2\eta\eta_{ij} \quad \text{and} \quad (\eta^2)_{ijj} = 2\eta_{ij}\eta_j + 2\eta_i\eta_{jj} + 2\eta_j\eta_{ij} + 2\eta\eta_{ijj},$$

and therefore,

$$|(\eta^2)_{ij}| \leqslant \frac{C}{R^2} \quad \text{and} \quad |(\eta^2)_{ijj}| \leqslant \frac{C}{R^3},$$

for some $C > 0$.

As a consequence, plugging this information into (A-5) and using the Hölder inequality, we obtain that

$$\begin{aligned}(1-2\delta)\sum_{i,j=1}^{n}\int_\Omega u_{ij}^2\eta^2 &\leqslant \frac{8}{\delta}\sum_{i,j=1}^{n}\int_\Omega u_i^2\eta_j^2 + \sum_{i,j=1}^{n}\int_\Omega \big((u-m)u_i(\eta^2)_{ijj} + u_iu_j(\eta^2)_{ij}\big)\\ &\leqslant \frac{C}{\delta R^2}\int_{B_{2R}}|\nabla u|^2 + \frac{C}{R^3}\int_{B_{2R}}(u-m)|\nabla u| + \frac{C}{R^2}\int_{B_{2R}}|\nabla u|^2\\ &\leqslant \Big(1+\frac{1}{\delta}\Big)\frac{C}{R^2}\int_{B_{2R}}|\nabla u|^2 + \frac{C}{R^4}\int_{B_{2R}}(u-m)^2, \end{aligned} \tag{A-6}$$

up to renaming C. Since $\Delta u \geqslant -C$ (up to renaming constants, recall Corollary 4.2), then from the Caccioppoli inequality (see, e.g., (6-10)) we get that

$$\int_{B_{2R}}|\nabla u|^2 \leqslant \frac{C}{R^2}\int_{B_{4R}}(u-m)^2 + C\int_{B_{4R}}(u-m),$$

which implies that

$$\frac{1}{R^{n+2}}\int_{B_{2R}}|\nabla u|^2 \leqslant \frac{C}{R^{n+4}}\int_{B_{4R}}(u-m)^2 + \frac{C}{R^{n+2}}\int_{B_{4R}}(u-m). \tag{A-7}$$

Moreover, from (A-6) and (A-7), we conclude that

$$\frac{1-2\delta}{R^n}\sum_{i,j=1}^{n}\int_{B_R}u_{ij}^2 \leqslant \frac{1-2\delta}{R^n}\sum_{i,j=1}^{n}\int_\Omega u_{ij}^2\eta^2 \leqslant \frac{C}{R^{n+4}}\int_{B_{4R}}(u-m)^2 + \frac{C}{R^{n+2}}\int_{B_{4R}}(u-m)$$

up to renaming $C > 0$. Putting together this and (A-7), we obtain the desired estimate. □

Corollary A.2. *Let $n \geqslant 2$, $\delta > 0$, and u be a minimizer of the functional J defined in* (1-1) *in Ω. Assume that $B_{\bar R} \subset\subset \Omega$. Let $x_0 \in \partial\{u > 0\}$ such that $\nabla u(x_0) = 0$ and $\partial\{u > 0\}$ is not δ-rank-2 flat at x_0 at any level $r > 0$ in the sense of Definition 1.6.*

Then, there exist $R_0 \in (0, \bar R)$ and $C > 0$, depending only on n, $\|u\|_{W^{2,2}(\Omega)}$, and $\operatorname{dist}(B_{\bar R}, \partial\Omega)$, *such that*

$$\frac{1}{R^{n+2}}\int_{B_R(x_0)}|\nabla u|^2 + \frac{1}{R^n}\int_{B_R(x_0)}|D^2u|^2 \leqslant C,$$

for any $R < R_0$.

Proof. The estimate follows from Lemma A.1 and the quadratic growth of u, as given by Theorem 1.7. □

Appendix B. a remark on the one-phase problem

here, we show that the one-phase problem, as presented in Definition 1.2, and the analysis of the minimizers which happen to be nonnegative are structurally very different questions. indeed, while a "typical" one-phase minimizer exhibits nontrivial open regions in which it vanishes, the free minimizers that are nonnegative do not show the same phenomena. as a prototype result for this, we point out the following observation:

Proposition B.1. *Suppose that* $0 \in \omega$, $u \in c^{1,1}(\omega)$ *is such that* $u > 0$ *in* $\omega \cap \{x_n > 0\}$ *and* $u = 0$ *in* $\omega \cap \{x_n \leqslant 0\}$. *then*, u *cannot be a local minimizer for the functional* j *in* ω *in the class of admissible functions* $\dashv$ *given in* (1-2).

Proof. without loss of generality, we can assume that $b_2 \subset\subset \omega$. let $\varphi \in c_0^\infty(b_2, [0, 1])$ be such that $\varphi = 1$ in b_1. let also $\varepsilon \in (0, 1)$ and $u_\varepsilon := u - \varepsilon\varphi$.

we observe that the regularity of u and the fact that $u(x', 0) = 0 \leqslant u(y)$ for any x' such that $(x', 0) \in b_2$ and any $y \in b_2$ give that, for every $x = (x', x_n) \in b_1$,

$$u(x) \leqslant k x_n^2,$$

for some $k > 0$. consequently, for every $x \in b_1$ with $|x_n| < \sqrt{\varepsilon/k}$ we have that

$$u_\varepsilon(x) \leqslant k x_n^2 - \varepsilon < 0.$$

this gives that, for any $x \in (-1/n, 1/n)^{n-1} \times (0, \sqrt{\varepsilon/K}) =: Q_\varepsilon$,

$$u_\varepsilon(x) < 0 < u(x),$$

as long as $\varepsilon > 0$ is sufficiently small.

Also note that $u_\varepsilon \leqslant u$ and so $\{u_\varepsilon > 0\} \subseteq \{u > 0\}$. Accordingly, computing the energy functional in B_2,

$$\begin{aligned} J[u_\varepsilon] - J[u] &= \int_{B_2} \big(|\Delta u_\varepsilon|^2 - |\Delta u|^2\big) + |B_2 \cap \{u_\varepsilon > 0\}| - |B_2 \cap \{u > 0\}| \\ &= \int_{B_2} \big(|\Delta u - \varepsilon \Delta\varphi|^2 - |\Delta u|^2\big) - |B_2 \cap \{u_\varepsilon \leqslant 0 < u\}| \\ &\leqslant \int_{B_2} \big(\varepsilon^2 |\Delta\varphi|^2 - 2\varepsilon \Delta u \Delta\varphi\big) - |Q_\varepsilon| \leqslant C\varepsilon - \Big(\frac{2}{n}\Big)^{n-1} \sqrt{\frac{\varepsilon}{K}} < 0, \end{aligned}$$

provided that ε is small enough. □

Appendix C. Proof of an auxiliary result

For completeness, in this appendix we provide the proof of Proposition 4.3.

Proof of Proposition 4.3. Given $\delta > 0$, let $p \in \partial\Omega$ with $|u(p)| > \delta$. By (4-6), we can find $\rho > 0$ such that

$$\overline{\Omega} \cap B_\rho(p) \subset \Big\{|u(p)| > \frac{\delta}{2}\Big\}. \tag{C-1}$$

Let $\phi \in C_0^\infty(B_\rho(p))$, with $\phi = 0$ along $\partial\Omega$. For each $\varepsilon \in \mathbb{R}$ with $|\varepsilon| < \dfrac{\delta}{4(1+\|\phi\|_{L^\infty(\mathbb{R}^n)})}$, we let $u_\varepsilon := u + \varepsilon\phi$. We observe that

$$\chi_{\{u_\varepsilon>0\}} = \chi_{\{u>0\}}, \quad \text{in } \Omega. \tag{C-2}$$

Indeed, if $x \in \Omega \setminus B_\rho(p)$, we have that $\phi(x) = 0$, and thus $u_\varepsilon(x) = u(x)$, proving (C-2) in this case. If instead $x \in \Omega \cap B_\rho(p)$, by (C-1) we can assume $u(x) > \delta/2$ (the case $u(x) < -\delta/2$ being similar). Then,

$$u_\varepsilon(x) \geqslant u(x) - \varepsilon\|\phi\|_{L^\infty} > \frac{\delta}{2} - \frac{\delta\,\|\phi\|_{L^\infty}}{4(1+\|\phi\|_{L^\infty(\mathbb{R}^n)})} > \frac{\delta}{4},$$

and hence

$$\chi_{\{u_\varepsilon>0\}}(x) = 1 = \chi_{\{u>0\}}(x),$$

completing the proof of (C-2).

As a byproduct of (C-2), we have that

$$0 \leqslant J[u_\varepsilon] - J[u] = \int_{\Omega\cap B_\rho(p)} \big(|\Delta u + \varepsilon\Delta\phi|^2 - |\Delta u|^2\big) = \int_{\Omega\cap B_\rho(p)} \big(2\varepsilon\Delta u\Delta\phi + \varepsilon^2|\Delta\phi|^2\big)$$

yielding that

$$\int_{\Omega\cap B_\rho(p)} \Delta u\Delta\phi = 0. \tag{C-3}$$

That is, defining $v := \Delta u$, we have that v is weakly harmonic in $\Omega\cap B_\rho(p)$, hence harmonic in $\Omega\cap B_\rho(p)$, and therefore, v is smooth in $\Omega\cap B_\rho(p)$, up to the boundary. Hence, we deduce from (4-7) and (C-3) that

$$0 = \int_{\Omega\cap B_\rho(p)} v\Delta\phi = \int_{\Omega\cap B_\rho(p)} (\operatorname{div}(v\nabla\phi) - \operatorname{div}(\phi\nabla v)) = \int_{(\partial\Omega)\cap B_\rho(p)} (v\partial_\nu\phi - \phi\partial_\nu v) = \int_{(\partial\Omega)\cap B_\rho(p)} v\partial_\nu\phi.$$

Therefore, since v is continuous on $(\partial\Omega)\cap B_\rho(p)$, thanks to (4-7), we find that $v(p) = 0$.

By taking δ arbitrary, we thus conclude that $v = 0$ on $(\partial\Omega)\cap\{|u| > 0\}$. This and (4-8) give that

$$v = 0 \quad \text{along } \partial\Omega. \tag{C-4}$$

Now we prove (4-9) by arguing by contradiction: We define $V := -v = -\Delta u$, and we suppose that

$$M := \sup_\Omega V > 0.$$

Now, we use (4-7), and we find some $\rho > 0$ such that V is continuous in a ρ-neighborhood of $\partial\Omega$ that we denote by $\mathcal{O}_\rho$. Thus, V is uniformly continuous in $\mathcal{O}_{\rho/2}$. In particular, there exists $\delta \in (0, \rho/2)$ such that if $x, y \in \mathcal{O}_\delta$ with $|x - y| \leqslant \delta$, then $|V(x) - V(y)| \leqslant \frac{M}{2}$.

Consequently, taking $y \in \partial\Omega$ and recalling (C-4), we find that

$$|V(x)| \leqslant \frac{M}{2} \quad \text{for every } x \in \mathcal{O}_\delta, \tag{C-5}$$

and, as a result,

$$0 < M = \sup_\Omega V = \sup_{\Omega\setminus\mathcal{O}_\delta} V. \tag{C-6}$$

Furthermore, in view of Lemma 4.1, for every $\phi \in C_0^\infty(\Omega, [0, +\infty))$,

$$\int_\Omega V\,\Delta\phi = -\int_\Omega \Delta u\,\Delta\phi \geqslant 0,$$

hence V is weakly subharmonic. From this, (C-6), and Theorem B in [Littman 1963], we deduce that $V = M$ a.e. in Ω. This is in contradiction with (C-5), hence the claim in (4-9) is established. □

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References

[Adams and Vandenhouten 2000] D. R. Adams and R. F. Vandenhouten, "Stability for polyharmonic obstacle problems with varying obstacles", *Comm. Partial Differential Equations* **25**:7-8 (2000), 1171–1200. MR Zbl

[Aleksanyan 2019] G. Aleksanyan, "Regularity of the free boundary in the biharmonic obstacle problem", *Calc. Var. Partial Differential Equations* **58**:6 (2019), art. id. 206. MR Zbl

[Alt and Caffarelli 1981] H. W. Alt and L. A. Caffarelli, "Existence and regularity for a minimum problem with free boundary", *J. Reine Angew. Math.* **325** (1981), 105–144. MR Zbl

[Boggio 1905] T. Boggio, "Sulle funzioni di Green d'ordine *m*", *Rend. Circ. Mat. Palermo* **20** (1905), 97–135. Zbl

[Brezis 1983] H. Brezis, *Analyse fonctionnelle: théorie et applications*, Masson, Paris, 1983. MR Zbl

[Caffarelli 1980] L. A. Caffarelli, "Compactness methods in free boundary problems", *Comm. Partial Differential Equations* **5**:4 (1980), 427–448. MR Zbl

[Caffarelli and Friedman 1979] L. A. Caffarelli and A. Friedman, "The obstacle problem for the biharmonic operator", *Ann. Scuola Norm. Sup. Pisa Cl. Sci.* (4) **6**:1 (1979), 151–184. MR Zbl

[Caffarelli et al. 1981] L. A. Caffarelli, A. Friedman, and A. Torelli, "The free boundary for a fourth order variational inequality", *Illinois J. Math.* **25**:3 (1981), 402–422. MR Zbl

[Caffarelli et al. 1982] L. A. Caffarelli, A. Friedman, and A. Torelli, "The two-obstacle problem for the biharmonic operator", *Pacific J. Math.* **103**:2 (1982), 325–335. MR Zbl

[Da Lio et al. 2020] F. Da Lio, F. Palmurella, and T. Rivière, "A resolution of the Poisson problem for elastic plates", *Arch. Ration. Mech. Anal.* **236**:3 (2020), 1593–1676. MR Zbl

[Dipierro and Karakhanyan 2018] S. Dipierro and A. L. Karakhanyan, "Stratification of free boundary points for a two-phase variational problem", *Adv. Math.* **328** (2018), 40–81. MR Zbl

[Dipierro et al. 2017] S. Dipierro, A. Karakhanyan, and E. Valdinoci, "A nonlinear free boundary problem with a self-driven Bernoulli condition", *J. Funct. Anal.* **273**:11 (2017), 3549–3615. MR Zbl

[Dipierro et al. 2019] S. Dipierro, A. L. Karakhanyan, and E. Valdinoci, "Limit behaviour of a singular perturbation problem for the biharmonic operator", *Appl. Math. Optim.* **80**:3 (2019), 679–713. MR Zbl

[Evans 1998] L. C. Evans, *Partial differential equations*, Grad. Stud. Math. **19**, Amer. Math. Soc., Providence, RI, 1998. MR Zbl

[Frehse 1973] J. Frehse, "On the regularity of the solution of the biharmonic variational inequality", *Manuscripta Math.* **9** (1973), 91–103. MR Zbl

[Ganguli 2017] R. Ganguli, *Finite element analysis of rotating beams: physics based interpolation*, Springer, 2017. MR Zbl

[Gazzola et al. 2010] F. Gazzola, H.-C. Grunau, and G. Sweers, *Polyharmonic boundary value problems*, Lect. Notes Math. **1991**, Springer, 2010. MR Zbl

[Giaquinta 1983] M. Giaquinta, *Multiple integrals in the calculus of variations and nonlinear elliptic systems*, Ann. of Math. Stud. **105**, Princeton Univ. Press, 1983. MR Zbl

[Lieb and Loss 2001] E. H. Lieb and M. Loss, *Analysis*, 2nd ed., Grad. Stud. Math. **14**, Amer. Math. Soc., Providence, RI, 2001. MR Zbl

[Littman 1963] W. Littman, "Generalized subharmonic functions: monotonic approximations and an improved maximum principle", *Ann. Scuola Norm. Sup. Pisa Cl. Sci.* (3) **17**:3 (1963), 207–222. MR Zbl

[Mardanov and Zaripov 2016] R. F. Mardanov and S. K. Zaripov, "Solution of Stokes flow problem using biharmonic equation formulation and multiquadrics method", *Lobachevskii J. Math.* **37**:3 (2016), 268–273. MR Zbl

[Martio and Vuorinen 1987] O. Martio and M. Vuorinen, "Whitney cubes, p-capacity, and Minkowski content", *Expo. Math.* **5**:1 (1987), 17–40. MR Zbl

[Mawi 2014] H. Mawi, "A free boundary problem for higher order elliptic operators", *Complex Var. Elliptic Equ.* **59**:7 (2014), 937–946. MR Zbl

[McKenna and Walter 1987] P. J. McKenna and W. Walter, "Nonlinear oscillations in a suspension bridge", *Arch. Ration. Mech. Anal.* **98**:2 (1987), 167–177. MR Zbl

[Miura 2016] T. Miura, "Singular perturbation by bending for an adhesive obstacle problem", *Calc. Var. Partial Differential Equations* **55**:1 (2016), art. id. 19. MR Zbl

[Miura 2017] T. Miura, "Overhanging of membranes and filaments adhering to periodic graph substrates", *Phys. D* **355** (2017), 34–44. MR Zbl

[Monneau and Weiss 2007] R. Monneau and G. S. Weiss, "An unstable elliptic free boundary problem arising in solid combustion", *Duke Math. J.* **136**:2 (2007), 321–341. MR Zbl

[Novaga and Okabe 2015] M. Novaga and S. Okabe, "Regularity of the obstacle problem for the parabolic biharmonic equation", *Math. Ann.* **363**:3-4 (2015), 1147–1186. MR Zbl

[Novaga and Okabe 2016] M. Novaga and S. Okabe, "The two-obstacle problem for the parabolic biharmonic equation", *Nonlinear Anal.* **136** (2016), 215–233. MR Zbl

[Petrosyan 2002] A. Petrosyan, "On existence and uniqueness in a free boundary problem from combustion", *Comm. Partial Differential Equations* **27**:3-4 (2002), 763–789. MR Zbl

[Pozzolini and Léger 2008] C. Pozzolini and A. Léger, "A stability result concerning the obstacle problem for a plate", *J. Math. Pures Appl.* (9) **90**:6 (2008), 505–519. MR Zbl

[Serrin 2011] J. Serrin, "Weakly subharmonic function", *Boll. Unione Mat. Ital.* (9) **4**:3 (2011), 347–361. MR Zbl

[Sweers 2009] G. Sweers, "A survey on boundary conditions for the biharmonic", *Complex Var. Elliptic Equ.* **54**:2 (2009), 79–93. MR Zbl

[Weiss 1998] G. S. Weiss, "Partial regularity for weak solutions of an elliptic free boundary problem", *Comm. Partial Differential Equations* **23**:3-4 (1998), 439–455. MR Zbl

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QUANTUM FLUCTUATIONS AND LARGE-DEVIATION PRINCIPLE FOR MICROSCOPIC CURRENTS OF FREE FERMIONS IN DISORDERED MEDIA

JEAN-BERNARD BRU, WALTER DE SIQUEIRA PEDRA AND ANTSA RATSIMANETRIMANANA

We extend the large-deviation results obtained by N. J. B. Aza and the present authors on atomic-scale conductivity theory of free lattice fermions in disordered media. Disorder is modeled by a random external potential, as in the celebrated Anderson model, and a nearest-neighbor hopping term with random complex-valued amplitudes. In accordance with experimental observations, via the large-deviation formalism, our previous paper showed in this case that quantum uncertainty of microscopic electric current densities around their (classical) macroscopic value is suppressed, exponentially fast with respect to the volume of the region of the lattice where an external electric field is applied. Here, the quantum fluctuations of linear response currents are shown to exist in the thermodynamic limit, and we mathematically prove that they are related to the rate function of the large-deviation principle associated with current densities. We also demonstrate that, in general, they do not vanish (in the thermodynamic limit), and the quantum uncertainty around the macroscopic current density disappears exponentially fast with an exponential rate proportional to the squared deviation of the current from its macroscopic value and the inverse current fluctuation, with respect to growing space (volume) scales.

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1. Introduction

Surprisingly (in view of [Ferry 2012]), experimental measurements [Weber et al. 2012] of electric resistance of silicon nanowires doped with phosphorus demonstrate that the macroscopic laws for charge transport are already accurate at length scales larger than a few nanometers, even at very low temperatures (4.2 K). As a consequence, microscopic (quantum) effects on charge transport can very rapidly disappear with respect to growing space scales. Understanding the breakdown of the classical (macroscopic) conductivity theory at microscopic scales is an important technological issue, because of the growing need for smaller electronic components.

From a mathematical perspective, the convergence of the expectations of microscopic current densities with respect to growing space scales is proved in [Bru et al. 2016; Bru and de Siqueira Pedra 2015a], but no information about the suppression of quantum uncertainty was obtained in the macroscopic limit. In [Aza et al. 2019], in accordance with experimental observations, it was proved for noninteracting lattice fermions with disorder that quantum uncertainty of microscopic electric current densities around their (classical) macroscopic value is suppressed exponentially fast with respect to the volume of the region of the lattice where an external electric field is applied. This is proved in [Aza et al. 2019] via the large-deviation formalism [Deuschel and Stroock 1989; Dembo and Zeitouni 1998], which has been used in quantum statistical mechanics since the 1980s [Aza et al. 2017, Section 7]. Given a fixed electromagnetic field $\mathcal{E}$, we derive in particular in [Aza et al. 2019] the (good) rate function $\mathrm{I}^{(\mathcal{E})}$ associated with microscopic (linear response) current densities[1] $x_L^{(\mathcal{E})} \in \mathbb{R}$, $L \in \mathbb{R}_0^+$, meaning in this case that, in a cubic box of volume L^d (d-dimensional lattice), for any $a, b \in \mathbb{R}$,

$$\mathrm{Prob}\big[x_L^{(\mathcal{E})} \in [a,b]\big] \sim \mathrm{e}^{-L^d \inf_{x\in[a,b]} \mathrm{I}^{(\mathcal{E})}(x)}, \quad \text{as } L \to \infty, \tag{1}$$

with $\mathrm{I}^{(\mathcal{E})} \geq 0$ and $\mathrm{I}^{(\mathcal{E})}(x) = 0$ if and only if x is the macroscopic (linear response) current density, $x^{(\mathcal{E})}$.

In this paper, we complement these studies by rigorously showing two new properties of charge transport of quasifree fermions in disordered media:

(a) The quantum fluctuations of linear response currents exist in the thermodynamic limit and are meanwhile explicitly related to the rate function $\mathrm{I}^{(\mathcal{E})}$, as expected.

(b) In general, the quantum fluctuations of currents do not vanish in the thermodynamic limit and the quantum uncertainty around the macroscopic current density disappears exponentially fast with an exponential rate proportional to $(x - x^{(\mathcal{E})})^2$ and the inverse current fluctuation, with respect to growing space (volume) scales.

Properties (a) and (b) refer to Theorems 3.1 and 3.3, which are the main results of this paper.

Our results show that the experimental measure of the rate function $\mathrm{I}^{(\mathcal{E})}$ (see (1)) leads to an experimental estimate on the corresponding quantum fluctuations. Conversely, an experimental estimate on these quantum fluctuations gives the behavior of the corresponding rate function $\mathrm{I}^{(\mathcal{E})}$ around the macroscopic current density $x^{(\mathcal{E})}$. This fact is certainly not restricted to fermionic currents.

[1] In some direction of $\mathbb{R}^d$.

Note that the existence of quantum fluctuations and associated mathematical structures has been extensively studied for quantum many-body systems. This refers, for instance, to the construction of so-called algebra of normal fluctuations for transport phenomena, which are related to quantum central limit theorems (see, e.g., [Bru et al. 2014; 2016; Goderis et al. 1989a; 1989b; 1989c; 1990a; 1990b; 1991], as well as [Verbeure 2011, Chapter 6]). The explicit relation (a) we derive between quantum fluctuations and the large-deviation formalism in quantum statistical mechanics [Aza et al. 2017, Section 7] is, however, a new general observation on quantum many-body systems.

We use the mathematical framework of [Aza et al. 2019; Bru and de Siqueira Pedra 2015a; 2017a] to study fermions on the lattice. For simplicity we take a cubic lattice $\mathbb{Z}^d$, even if other types of lattices can be considered with very similar methods. Disorder within the conductive material, due to impurities, crystal lattice defects, etc., is modeled by (i) a random external potential, as in the celebrated Anderson model, and (ii) a nearest-neighbor hopping term with random complex-valued amplitudes. In particular, random (electromagnetic) vector potentials can also be implemented. The celebrated tight-binding Anderson model is one particular example of the general case considered here.

In order to prove Property (a), i.e., Theorem 3.1, we use the large-deviation formalism and follow the argument lines of [Aza et al. 2019, Section 4] to show [Aza et al. 2019, Theorem 3.1] via the Akcoglu–Krengel ergodic theorem [Aza et al. 2019, Theorem 4.17], for one has to control the thermodynamical limit of (finite-volume) generating functions that are random. We perform, in particular, the same box decomposition of these random functions, which can be justified with the help of the Bogoliubov-type inequality [Aza et al. 2019, Lemma 4.2] and the "locality" (or space decay) of both the quasifree dynamics and space correlations of KMS states, which is a consequence of Combes–Thomas estimates [Aza et al. 2019, Appendix A] (see [Aza et al. 2019, Section 4.3]). In this paper, we only give the new arguments that are necessary to prove Property (a), like the existence of the thermodynamic limit of quantum fluctuations of currents and the continuity of the second derivative of the generating function. In particular, as in the proof of [Aza et al. 2019, Corollary 4.20], we use the (Arzelà–)Ascoli theorem [Rudin 1991, Theorem A5], which requires uniform bounds on the third-order derivatives of finite-volume generating functions. This proof is much more computational than the one of [Aza et al. 2019, Proposition 4.9], which only controls the first and second derivatives of the same function. Note that derivatives of the logarithm of the expectations of an exponential, like the generating function we consider here, are generally related to so-called "truncated" or "connected" correlations. We demonstrate that it is the case for the third-order derivative we refer to above, allowing the reader to follow the computation of that derivative in a systematic way. Considering the third-order case, the algorithm to compute the derivatives of the generating functions at any order becomes apparent, showing that the generating function is in fact *smooth*. We give below further remarks on that.

In order to prove Property (b), i.e., Theorem 3.3 (Theorem 3.1 being proved), we rewrite the second derivative of the generating function, which is the thermodynamic limit of the quantum fluctuations of currents (Theorem 3.1(i)), as a trace of some explicit positive operator in the one-particle Hilbert space. This quantity can be estimated from below by the Hilbert–Schmidt norm of a kind of current observable in the one-particle Hilbert space. Various computations and estimates then imply Theorem 3.3.

As discussed in [Aza et al. 2019], observe the existence of vast mathematical literature on charged transport properties of fermions in disordered media, see for instance [Schulz-Baldes and Bellissard 1998; Bellissard et al. 1994; Bouclet et al. 2005; Klein et al. 2007; Klein and Müller 2008; 2015; Dombrowski and Germinet 2008; Prodan 2013; Brynildsen and Cornean 2013]. However, it is not the purpose of this introduction to go into the details of the history of this specific research field. For a (nonexhaustive) historical perspective on linear conductivity (Ohm's law), see, e.g., [Bru and de Siqueira Pedra 2015b] or our previous papers [Bru et al. 2014; 2015a; 2015b; 2016; Bru and de Siqueira Pedra 2015a; 2016; 2017a].

To conclude, this paper is organized as follows:

- In Section 2, we describe the mathematical framework, which is the one from [Aza et al. 2019; Bru and de Siqueira Pedra 2015a; 2017a]. It refers to quasifree fermions on the lattice in disordered media. Although all of the problem can be formulated, in a mathematically equivalent way, in the one-particle (or Hilbert space) setting [Aza et al. 2019, Appendix C.3], since the underlying physical system is a many-body one, it is conceptually more appropriate to state our results within the algebraic formulation for lattice fermion systems, as in [Aza et al. 2019; Bru and de Siqueira Pedra 2015a; 2017a]. Short complementary discussions on response of quasifree fermion systems to electric fields can be found in [Aza et al. 2019, Appendix C].
- In Section 3, the main results are stated. In particular, Property (a) described above refers to Section 3.1, while Property (b) is explained in Section 3.2.
- Section 4 gathers all technical proofs. In particular, Sections 4.1–4.2 give preliminary definitions and observations, while Sections 4.3 and 4.4 refer to the proofs of Theorems 3.1(i) and 3.3, respectively.

Notation 1.1. A norm on a generic vector space $\mathcal{X}$ is denoted by $\|\cdot\|_{\mathcal{X}}$. The Banach space of all bounded linear operators on $(\mathcal{X}, \|\cdot\|_{\mathcal{X}})$ is denoted by $\mathcal{B}(\mathcal{X})$. The scalar product of any Hilbert space $\mathcal{X}$ is denoted by $\langle\cdot,\cdot\rangle_{\mathcal{X}}$. We use the convention $\mathbb{R}^+ \doteq \{x \in \mathbb{R} : x > 0\}$, while $\mathbb{R}_0^+ \doteq \mathbb{R}^+ \cup \{0\}$. For any random variable X, $\mathbb{E}[X]$ denotes its expectation and $\mathrm{Var}[X]$ its variance.

2. Setup of the problem

We use the mathematical framework of [Aza et al. 2019; Bru and de Siqueira Pedra 2015a; 2017a] in order to study fermions on the lattice.

2.1. ***Random tight-binding model .*** We consider conducting fermions in a cubic crystal represented by the d-dimensional cubic lattice $\mathbb{Z}^d$ ($d \in \mathbb{N}$). The corresponding one-particle Hilbert space is thus $\mathfrak{h} \doteq \ell^2(\mathbb{Z}^d;\mathbb{C})$. Its canonical orthonormal basis is denoted by $\{\mathfrak{e}_x\}_{x\in\mathbb{Z}^d}$, where $\mathfrak{e}_x(y) \doteq \delta_{x,y}$ for all $x, y \in \mathbb{Z}^d$. ($\delta_{x,y}$ is the Kronecker delta).

Disorder in the crystal is modeled via a probability space $(\Omega, \mathfrak{A}_\Omega, \mathfrak{a}_\Omega)$, defined as follows: Using the sets

$$\mathbb{D} \doteq \{z \in \mathbb{C} : |z| \leq 1\} \quad \text{and} \quad \mathfrak{b} \doteq \left\{\{x, x'\} \subseteq \mathbb{Z}^d : |x - x'| = 1\right\},$$

we define

$$\Omega \doteq [-1, 1]^{\mathbb{Z}^d} \times \mathbb{D}^{\mathfrak{b}} \quad \text{and} \quad \mathfrak{A}_\Omega \doteq \left(\otimes_{x\in\mathbb{Z}^d}\mathfrak{A}_x^{(1)}\right) \otimes \left(\otimes_{\mathbf{x}\in\mathfrak{b}}\mathfrak{A}_{\mathbf{x}}^{(2)}\right),$$

where $\mathfrak{A}_x^{(1)}$, $x \in \mathbb{Z}^d$, and $\mathfrak{A}_{\boldsymbol{x}}^{(2)}$, $\boldsymbol{x} \in \mathfrak{b}$, are the Borel σ-algebras of, respectively, the interval $[-1, 1]$ and the unit disc $\mathbb{D}$, both with respect to their usual metric topology. The distribution $\mathfrak{a}_\Omega$ is an *ergodic* probability measure on the measurable space $(\Omega, \mathfrak{A}_\Omega)$. See [Aza et al. 2019] for more details. Below, $\mathbb{E}[\,\cdot\,]$ and $\mathrm{Var}[\,\cdot\,]$ always refer to expectations and variances associated with $\mathfrak{a}_\Omega$.

Given $\vartheta \in \mathbb{R}_0^+$ and $\omega = (\omega_1, \omega_2) \in \Omega$, we define a bounded self-adjoint operator $\Delta_{\omega,\vartheta} \in \mathcal{B}(\mathfrak{h})$ encoding the hopping amplitudes of a single particle in the lattice:

$$[\Delta_{\omega,\vartheta}(\psi)](x) \doteq 2d\psi(x) - \sum_{j=1}^{d} \big((1+\vartheta\overline{\omega_2(\{x, x-e_j\})})\psi(x-e_j) + \psi(x+e_j)(1+\vartheta\omega_2(\{x, x+e_j\}))\big) \quad (2)$$

for any $x \in \mathbb{Z}^d$ and $\psi \in \mathfrak{h}$, where $\{e_k\}_{k=1}^d$ is the canonical basis of $\mathbb{R}^d$. If $\vartheta = 0$, $\Delta_{\omega,0}$ is (up to a minus sign) the usual d-dimensional discrete Laplacian. Random (electromagnetic) vector potentials can also be implemented in our model, since ω_2 takes values in the unit disc $\mathbb{D} \subseteq \mathbb{C}$. Then, the random tight-binding model is the one-particle Hamiltonian defined by

$$h^{(\omega)} \doteq \Delta_{\omega,\vartheta} + \lambda\omega_1, \quad \omega = (\omega_1, \omega_2) \in \Omega, \quad \lambda, \vartheta \in \mathbb{R}_0^+, \quad (3)$$

where the function $\omega_1 : \mathbb{Z}^d \to [-1, 1]$ is identified with the corresponding (self-adjoint) multiplication operator. The celebrated tight-binding Anderson model corresponds to the special case $\vartheta = 0$.

2.2. *C*-algebraic setting* . We denote by $\mathcal{U}$ the universal unital C^*-algebra generated by elements $\{a(\psi)\}_{\psi\in\mathfrak{h}}$ satisfying the canonical anticommutation relations (CAR): For all $\psi, \varphi \in \mathfrak{h}$,

$$a(\psi)a(\varphi) = -a(\varphi)a(\psi), \quad a(\psi)a(\varphi)^* + a(\varphi)^*a(\psi) = \langle\psi, \varphi\rangle_{\mathfrak{h}}\mathbb{1}. \quad (4)$$

As is usual, $a(\psi)$ and $a(\psi)^*$ refer to, respectively, annihilation and creation operators in the fermionic Fock space representation.

For all $\omega \in \Omega$ and $\lambda, \vartheta \in \mathbb{R}_0^+$, a dynamics on the C^*-algebra $\mathcal{U}$ is defined by the unique strongly continuous group $\tau^{(\omega)} \doteq (\tau_t^{(\omega)})_{t\in\mathbb{R}}$ of (Bogoliubov) $*$-automorphisms of $\mathcal{U}$ satisfying

$$\tau_t^{(\omega)}(a(\psi)) = a(\mathrm{e}^{ith^{(\omega)}}\psi), \quad t \in \mathbb{R}, \psi \in \mathfrak{h}. \quad (5)$$

See (3), as well as [Bratteli and Robinson 1997, Theorem 5.2.5], for more details on Bogoliubov automorphisms.

For any realization $\omega \in \Omega$ and disorder strengths $\lambda, \vartheta \in \mathbb{R}_0^+$, the thermal equilibrium state of the system at inverse temperature $\beta \in \mathbb{R}^+$ (i.e., $\beta > 0$) is by definition the unique $(\tau^{(\omega)}, \beta)$-KMS state $\varrho^{(\omega)}$, see [Bratteli and Robinson 1997, Example 5.3.2.] or [Pillet 2006, Theorem 5.9]. It is well known that such a state is stationary with respect to the dynamics $\tau^{(\omega)}$, that is,

$$\varrho^{(\omega)} \circ \tau_t^{(\omega)} = \varrho^{(\omega)}, \quad \omega \in \Omega, t \in \mathbb{R}.$$

The state $\varrho^{(\omega)}$ is also gauge-invariant, quasifree, and satisfies

$$\varrho^{(\omega)}(a^*(\varphi)a(\psi)) = \Big\langle\psi, \frac{1}{1+\mathrm{e}^{\beta h^{(\omega)}}}\varphi\Big\rangle_{\mathfrak{h}}, \quad \varphi, \psi \in \mathfrak{h}. \quad (6)$$

The gauge-invariant quasifree state with two-point correlation functions given by (6) for $\beta = 0$ is the tracial state (or chaotic state), denoted by $\mathrm{tr} \in \mathcal{U}^*$.

Recall that gauge-invariant quasifree states are positive linear functionals $\rho \in \mathcal{U}^*$ such that $\rho(\mathfrak{1}) = 1$ and, for all $N_1, N_2 \in \mathbb{N}$ and $\psi_1, \ldots, \psi_{N_1+N_2} \in \mathfrak{h}$,

$$\rho(a^*(\psi_1) \cdots a^*(\psi_{N_1}) a(\psi_{N_1+N_2}) \cdots a(\psi_{N_1+1})) = 0 \tag{7}$$

if $N_1 \neq N_2$, while in the case $N_1 = N_2 \equiv N$,

$$\rho(a^*(\psi_1) \cdots a^*(\psi_N) a(\psi_{2N}) \cdots a(\psi_{N+1})) = \det\big[\rho(a^*(\psi_k) a(\psi_{N+l}))\big]_{k,l=1}^N. \tag{8}$$

See, e.g., [Araki 1970/71, Definition 3.1], which refers to a more general notion of quasifree states. The gauge-invariant property corresponds to (7) whereas [Araki 1970/71, Definition 3.1, Condition (3.1)] only imposes the quasifree state to be even, which is a strictly weaker property than being gauge-invariant.

2.3. ***Linear response current density*** **.** (i) Paramagnetic currents: Fix $\omega \in \Omega$ and $\vartheta \in \mathbb{R}_0^+$. For any oriented edge $(x, y) \in (\mathbb{Z}^d)^2$, we define the paramagnetic[2] current observable by

$$I_{(x,y)}^{(\omega)} \doteq -2\Im\mathrm{m}\big(\langle \mathfrak{e}_x, \Delta_{\omega,\vartheta} \mathfrak{e}_y \rangle_{\mathfrak{h}}\, a(\mathfrak{e}_x)^* a(\mathfrak{e}_y)\big), \tag{9}$$

where, as is usual, the real and imaginary parts of any element $A \in \mathcal{U}$ are respectively defined by

$$\Re\mathrm{e}(A) \doteq \frac{1}{2}(A + A^*) \quad \text{and} \quad \Im\mathrm{m}(A) \doteq \frac{1}{2i}(A - A^*). \tag{10}$$

The self-adjoint elements $I_{(x,y)}^{(\omega)} \in \mathcal{U}$ are seen as current observables, because they satisfy a discrete continuity equation, as explained in [Aza et al. 2019, Appendix C]. This "second-quantized" definition of a current observable and the usual one in the one-particle setting, as in [Schulz-Baldes and Bellissard 1998; Bouclet et al. 2005; Klein et al. 2007], are perfectly equivalent, in the case of noninteracting fermions. See for instance [Aza et al. 2019, Appendix C.3].

(ii) Conductivity: As is usual, $[A, B] \doteq AB - BA \in \mathcal{U}$ denotes the commutator between the elements $A \in \mathcal{U}$ and $B \in \mathcal{U}$. For any finite subset $\Lambda \subsetneq \mathbb{Z}^d$, we define the space-averaged transport coefficient observable $\mathcal{C}_\Lambda^{(\omega)} \in C^1(\mathbb{R}; \mathcal{B}(\mathbb{R}^d; \mathcal{U}^d))$, with respect to the canonical basis $\{e_q\}_{q=1}^d$ of $\mathbb{R}^d$, by the corresponding matrix entries

$$\begin{aligned}\big\{\mathcal{C}_\Lambda^{(\omega)}(t)\big\}_{k,q} \doteq \frac{1}{|\Lambda|} \sum_{\substack{x,y \in \Lambda \\ x+e_k, y+e_q \in \Lambda}} \int_0^t i[\tau_{-\alpha}^{(\omega)}(I_{(y+e_q,y)}^{(\omega)}), I_{(x+e_k,x)}^{(\omega)}]\, d\alpha \\ + \frac{2\delta_{k,q}}{|\Lambda|} \sum_{x \in \Lambda} \Re\mathrm{e}(\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta} \mathfrak{e}_x \rangle a(\mathfrak{e}_{x+e_k})^* a(\mathfrak{e}_x))\end{aligned} \tag{11}$$

[2] Diamagnetic currents correspond to the ballistic movement of charged particles driven by electric fields. Their presence leads to the progressive appearance of paramagnetic currents which are responsible for heat production. For more details, see [Bru and de Siqueira Pedra 2015a; Bru et al. 2015b; Bru and de Siqueira Pedra 2016] as well as [Aza et al. 2019, Appendix C] on linear response currents.

for any $\omega \in \Omega$, $t \in \mathbb{R}$, $\lambda, \vartheta \in \mathbb{R}_0^+$, and $k, q \in \{1, \ldots, d\}$. It is the conductivity observable matrix associated with the lattice region Λ and time t. See [Aza et al. 2019, Appendix C]. In fact, the first term in the right-hand side of (11) corresponds to the paramagnetic coefficient, whereas the second one is the diamagnetic component. For more details, see [Bru and de Siqueira Pedra 2016, Theorem 3.7].

(iii) Linear response current density: Fix a direction $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$ and a (time-dependent) continuous, compactly supported, electric field $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, i.e., the external electric field is a continuous function $t \mapsto \mathcal{E}(t) \in \mathbb{R}^d$ of time $t \in \mathbb{R}$, with compact support. Then, as it is explained in [Aza et al. 2019, Appendix C] as well as in [Bru and de Siqueira Pedra 2015a; 2016] [3], the space-averaged linear response current observable in the lattice region Λ and at time $t = 0$ in the direction $\vec{w}$ is equal to

$$\mathbb{I}_{\Lambda}^{(\omega,\mathcal{E})} \doteq \sum_{k,q=1}^{d} w_k \int_{-\infty}^{0} \{\mathcal{E}(\alpha)\}_q \left\{\mathcal{C}_{\Lambda}^{(\omega)}(-\alpha)\right\}_{k,q} d\alpha. \tag{12}$$

By [Bru et al. 2016; Bru and de Siqueira Pedra 2015a], the macroscopic (linear response) current density produced by electric fields $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$ at time $t = 0$ in the direction $\vec{w}$ is consequently equal to

$$x^{(\mathcal{E})} \doteq \lim_{L\to\infty} \mathbb{E}\left[\varrho^{(\cdot)}\left(\mathbb{I}_{\Lambda_L}^{(\cdot,\mathcal{E})}\right)\right] \in \mathbb{R}, \tag{13}$$

where $\Lambda_L \doteq \{\mathbb{Z} \cap [-L, L]\}^d$ for any $L \in \mathbb{R}_0^+$. In order to obtain the current density at any time $t \in \mathbb{R}$ in the direction $\vec{w}$, it suffices to replace $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$ in the last two equations with

$$\mathcal{E}_t(\alpha) \doteq \mathcal{E}(\alpha + t), \quad \alpha \in \mathbb{R}. \tag{14}$$

For a short summary on response of quasifree fermion systems to electric fields, see [Aza et al. 2019, Appendix C].

2.4. ***Large deviations for microscopic current densities.*** Fix again a direction $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$ and a time-dependent electric field $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$. Recall that $\Lambda_L \doteq \{\mathbb{Z} \cap [-L, L]\}^d$ for any $L \in \mathbb{R}_0^+$. From [Bru et al. 2016; Bru and de Siqueira Pedra 2015a] combined with [Aza et al. 2019, Corollary 3.2], it follows that the distributions[4] of the microscopic current density observables $(\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})})_{L\in\mathbb{R}^+}$, in the state $\varrho^{(\omega)}$, weak* converge, for $\omega \in \Omega$ almost surely, to the delta distribution at the macroscopic value $x^{(\mathcal{E})}$, well-defined by (13). By [Aza et al. 2019, Corollary 3.5], the quantum uncertainty around the macroscopic value disappears *exponentially fast*, as $L \to \infty$.

To arrive at that conclusion, we use in [Aza et al. 2019] the large-deviation formalism for the microscopic (linear response) current density in the state $\varrho^{(\omega)}$. More precisely, we prove in [Aza et al. 2019, Corollary 3.2] that, almost surely[5] (or with probability one in Ω), for any Borel subset $\mathcal{G}$ of $\mathbb{R}$ with interior

[3] Strictly speaking, these papers use smooth electric fields, but the extension to the continuous case is straightforward.

[4] Here, as in [Aza et al. 2019], the distribution associated to a selfadjoint element A of a unital C^*-algebra $\mathfrak{A}$ and to a state on this algebra is the probability measure on the spectrum of A representing the restriction of the state to the unital C^*-subalgebra of $\mathfrak{A}$ generated by A. Recall that this measure exists and is unique, by the Riesz–Markov representation theorem.

[5] The measurable subset $\tilde{\Omega} \subseteq \Omega$ of full measure of [Aza et al. 2019, Corollary 3.2] does not depend on $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$.

and closure respectively denoted by $\mathcal{G}^\circ$ and $\bar{\mathcal{G}}$,

$$-\inf_{x\in\mathcal{G}^\circ} \mathrm{I}^{(\mathcal{E})}(x) \leq \liminf_{L\to\infty} \frac{1}{|\Lambda_L|} \ln \varrho^{(\omega)}\big(\mathbf{1}\big[\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})} \in \mathcal{G}\big]\big) \leq \limsup_{L\to\infty} \frac{1}{|\Lambda_L|} \ln \varrho^{(\omega)}\big(\mathbf{1}\big[\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})} \in \mathcal{G}\big]\big) \leq -\inf_{x\in\bar{\mathcal{G}}} \mathrm{I}^{(\mathcal{E})}(x).$$

By an abuse of notation[6], we applied above the (discontinuous) characteristic function $\mathbf{1}[x \in \mathcal{G}]$ to $\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}$. Here, by [Aza et al. 2019, Theorems 3.1, 3.4, and Corollary 3.2], the so-called good[7] rate function $\mathrm{I}^{(\mathcal{E})}$ is a deterministic, positive, lower-semicontinuous, convex function defined by

$$\mathrm{I}^{(\mathcal{E})}(x) \doteq \sup_{s\in\mathbb{R}}\big\{sx - \mathrm{J}^{(s\mathcal{E})}\big\} \geq 0, \quad x \in \mathbb{R}, \tag{15}$$

where

$$\mathrm{J}^{(\mathcal{E})} \doteq \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \mathbb{E}\big[\ln \varrho^{(\cdot)}\big(\mathrm{e}^{|\Lambda_L|\mathbb{I}_{\Lambda_L}^{(\cdot,\mathcal{E})}}\big)\big] \in \mathbb{R} \tag{16}$$

for all $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$. By [Aza et al. 2019, Theorem 3.4], $\mathrm{I}^{(\mathcal{E})}$ restricted to the interior of its domain is continuous and, as clearly expected, the rate function $\mathrm{I}^{(\mathcal{E})}$ vanishes on the macroscopic (linear response) current density $x^{(\mathcal{E})}$, i.e., $\mathrm{I}^{(\mathcal{E})}(x^{(\mathcal{E})}) = 0$, whereas $\mathrm{I}^{(\mathcal{E})}(x) > 0$ for all $x \neq x^{(\mathcal{E})}$.

For any $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, note that (15) means that $\mathrm{I}^{(\mathcal{E})}$ is the Legendre–Fenchel transform of the generating function $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ from $\mathbb{R}$ to itself, which is a well-defined, continuously differentiable, convex function, by [Aza et al. 2019, Theorem 3.1]. Moreover, by [Aza et al. 2019, Corollary 4.20 and Equation (54)], for any $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$, the macroscopic current density defined by (13) can be expressed in terms of the generating function

$$x^{(\mathcal{E})} = \partial_s \mathrm{J}^{(s\mathcal{E})}\big|_{s=0}. \tag{17}$$

3. Main results

In order to provide a rather complete study of conductivity at the atomic scale for free-fermions in a lattice, we analyse here the rate function defined by (15) in much more detail than in [Aza et al. 2019]. See [Aza et al. 2019, Corollary 3.2]. We focus on the behavior of the rate function near the macroscopic value of the current density (see (17)), because it establishes a very interesting connection between exponential suppression of quantum uncertainties at the atomic scale and the concept of *quantum fluctuations*, in the case of currents.

3.1. ***Quantum fluctuations of linear response currents and rate function*** **.** For any inverse temperature $\beta \in \mathbb{R}^+$, disorder strengths $\vartheta, \lambda \in \mathbb{R}_0^+$, disorder realization $\omega \in \Omega$, direction $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$, and time-dependent electric field $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, the quantum fluctuations of linear response currents in

[6]In fact, the object $\varrho^{(\omega)}\big(\mathbf{1}\big[\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})} \in \mathcal{G}\big]\big)$ can be easily given a precise mathematical sense by using the (up to unitary equivalence) unique cyclic representation of the C^*-algebra $\mathcal{U}$ associated to the state $\varrho^{(\omega)}$, noting that the bicommutant of a $*$-algebra in any representation is a von Neumann algebra, and thus admits a measurable calculus.

[7]It means, in this context, that $\{x \in \mathbb{R} \colon \mathrm{I}^{(\mathcal{E})}(x) \leq m\}$ is compact for any $m \geq 0$.

cubic boxes are defined to be

$$\boldsymbol{F}_L^{(\omega,\mathcal{E})} \doteq |\Lambda_L| \Big(\varrho^{(\omega)}\big((\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})})^2 \big) - \varrho^{(\omega)}\big(\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})} \big)^2 \Big) \geq 0, \quad L \in \mathbb{R}_0^+, \tag{18}$$

with $\Lambda_L \doteq \{\mathbb{Z} \cap [-L, L]\}^d$ and $\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}(t)$ being the space-averaged linear response current defined by (12). Observe that

$$|\Lambda_L| \, \varrho^{(\omega)}\big(\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}(t)\big), \quad L \in \mathbb{R}_0^+,$$

is the (total) current linear response (in the direction $\vec{w}$) to the electric field; and, consequently,

$$\boldsymbol{F}_L^{(\omega,\mathcal{E})} = \frac{1}{|\Lambda_L|} \big(\varrho^{(\omega)}\big((|\Lambda_L| \, \mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})})^2 \big) - \varrho^{(\omega)}\big(|\Lambda_L| \, \mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})} \big)^2 \big), \quad L \in \mathbb{R}_0^+, \tag{19}$$

are naturally seen as (normal) quantum fluctuations of the (total) linear response current. Note that these quantum fluctuations are not quite the same current fluctuations of [Bru et al. 2014; 2016], which correspond only to the paramagnetic component of the current, whereas $(\boldsymbol{F}_L^{(\omega,\mathcal{E})})$ also includes the diamagnetic one, and thus refers to the total current.

Recall that $x^{(\mathcal{E})}$ is the macroscopic (linear response) current density defined by (13), and $\mathrm{I}^{(\mathcal{E})}$ (see (15)) is the (good) rate function associated with the large deviation principle of the sequence $\{\mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}\}_{L \in \mathbb{R}^+}$ of microscopic current densities, in the KMS state $\varrho^{(\omega)}$ and with speed $|\Lambda_L|$. See, e.g., [Aza et al. 2019, Theorems 3.1, 3.4, and Corollary 3.2]. We are now in a position to connect the quantum fluctuations of (linear) currents with the generating and rate functions associated with the large-deviation principle for microscopic current densities.

Theorem 3.1 (Quantum fluctuations and rate function). *There is a measurable subset $\tilde{\Omega} \subseteq \Omega$ of full measure such that, for all $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \tilde{\Omega}$, $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$, the following properties hold true*:

(i) *The generating function $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ defined by* (16) *belongs to $C^\infty(\mathbb{R}; \mathbb{R})$ and satisfies*

$$\partial_s^2 \, \mathrm{J}^{(s\mathcal{E})}\big|_{s=0} = \lim_{L\to\infty} \mathbb{E}\big[\boldsymbol{F}_L^{(\cdot,\mathcal{E})}\big] = \lim_{L\to\infty} \boldsymbol{F}_L^{(\omega,\mathcal{E})} \geq 0. \tag{20}$$

(ii) *The rate function $I^{(\mathcal{E})}$ satisfies the asymptotics*

$$I^{(\mathcal{E})}(x) = \frac{1}{2\partial_s^2 \, \mathrm{J}^{(s\mathcal{E})}\,|_{s=0}} \big(x - x^{(\mathcal{E})}\big)^2 + o\big((x - x^{(\mathcal{E})})^2\big),$$

provided that $\partial_s^2 \, \mathrm{J}^{(s\mathcal{E})}\,|_{s=0} \neq 0$.

Proof. Fix all parameters of the theorem. By Corollary 4.2, the generating function $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ belongs to $C^2(\mathbb{R}; \mathbb{R})$ and satisfies (20). As explained after Corollary 4.2, under the assumptions of Theorem 3.1, one can straightforwardly extend our arguments to prove that the generating function $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ defined by (16) is infinitely differentiable. Assertion (i) thus holds true. It remains to prove Assertion (ii): Since the map $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ from $\mathbb{R}$ to itself is convex and belongs (at least) to $C^1(\mathbb{R}; \mathbb{R})$ (see, e.g., Assertion (i) or [Aza et al. 2019, Theorem 3.1]), all finite solutions $s(x) \in \mathbb{R}$ to the variational problem (15) for $x \in \mathbb{R}$, i.e.,

$$\mathrm{I}^{(\mathcal{E})}(x) = s(x)x - \mathrm{J}^{(s(x)\mathcal{E})}, \tag{21}$$

satisfy

$$x = f(s(x)), \tag{22}$$

with f being the real-valued function defined by

$$f(s) \doteq \partial_s \mathrm{J}^{(s\mathcal{E})}, \quad s \in \mathbb{R}. \tag{23}$$

Assume now that $\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} \neq 0$, which is equivalent in this case to

$$\partial_s f(0) = \partial_s^2 \mathrm{J}^{(s\mathcal{E})}\big|_{s=0} > 0, \tag{24}$$

by positivity of fluctuations (see (i)). Since, by Corollary 4.2, the mapping $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ from $\mathbb{R}$ to itself belongs (at least) to $C^2(\mathbb{R};\mathbb{R})$, by the inverse function theorem combined with (21)–(24) and (17), there is an open interval

$$\mathcal{I} \subseteq \{f(s) : s \in \mathbb{R} \text{ such that } \partial_s f(s) > 0\} \subseteq \mathbb{R}$$

containing $x^{(\mathcal{E})} = f(0)$ and a C^1-function $x \mapsto s(x)$ from $\mathcal{I}$ to $\mathbb{R}$ such that (21)–(23) hold true. In particular,

$$\partial_s f(s(x)) = \partial_s^2 \mathrm{J}^{(s\mathcal{E})}\big|_{s=s(x)} > 0, \quad x \in \mathcal{I}. \tag{25}$$

Clearly,

$$\partial_x s(x) = \frac{1}{\partial_s f(s(x))}, \quad x \in \mathcal{I}. \tag{26}$$

We thus infer from (21)–(23) and (26), together with (i), that

$$\partial_x \mathrm{I}^{(\mathcal{E})}(x) = s(x), \quad x \in \mathcal{I}.$$

Consequently, $\partial_x \mathrm{I}^{(\mathcal{E})}$ is differentiable on $\mathcal{I}$ with derivative given by

$$\partial_x^2 \mathrm{I}^{(\mathcal{E})}(x) = \partial_x s(x), \quad x \in \mathcal{I}.$$

As a consequence, $\mathrm{I}^{(\mathcal{E})}$ is twice differentiable on $\mathcal{I} \supseteq \{x^{(\mathcal{E})}\}$ and, using the Taylor theorem at the point $x^{(\mathcal{E})}$, one obtains that

$$\mathrm{I}^{(\mathcal{E})}(x) = s(x^{(\mathcal{E})})(x - x^{(\mathcal{E})}) + \frac{1}{2}\partial_x s(x^{(\mathcal{E})})(x - x^{(\mathcal{E})})^2 + o\big((x - x^{(\mathcal{E})})^2\big), \tag{27}$$

provided (24) holds true. Since, by (17), (23), and (26), $s(x^{(\mathcal{E})}) = 0$ and

$$\partial_x s(x^{(\mathcal{E})}) = \frac{1}{\partial_s f(0)} = \frac{1}{\partial_s^2 \mathrm{J}^{(s\mathcal{E})}}\Big|_{s=0},$$

one thus deduces (ii) from (27). □

This theorem is a very interesting observation on the physics of fermionic systems, because it shows that the experimental measure of the rate function of currents around the expected value leads to an experimental estimate on the corresponding quantum fluctuations. Conversely, by Theorem 3.1, an experimental estimate on these quantum fluctuations gives the behavior of the corresponding rate function around the expected value. This phenomenon is certainly not restricted to fermionic currents, and this is a new observation on transport properties of quantum many-body systems, to our knowledge.

Remark 3.2 (Extension of Theorem 3.1). The proof of Theorem 3.1 can be generalized to very general kinetic terms (i.e., it does not really depend on the special choice $\Delta_{\omega,\vartheta}$), provided the pivotal Combes–Thomas estimate holds true for the one-particle Hamiltonian. Note, however, that this would require a new, more complicated, definition of currents, which results from the commutator of the density operator at fixed lattice site with the kinetic term (cf. continuity equations on the CAR algebra [Bru and de Siqueira Pedra 2016, Equations (38)–(39)]). We did not implement this generalization here, because we think that, conceptually, the gain is too small as compared to the drawbacks concerning notations, definitions, and technical proofs. Instead, we aim at obtaining an extension of Theorem 3.1 to weakly interacting fermionic systems by using new constructive methods based on Grassmann–Berezin integrals, Brydges–Kennedy expansions, etc.

3.2. *Nonvanishing quantum fluctuations of linear response currents*. By Theorem 3.1, the behavior of the rate function within a neighborhood of the macroscopic current densities is directly related to the quantum fluctuations of the linear response current, provided these fluctuations do not vanish in the thermodynamic limit, i.e., if $\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} \neq 0$ (see Theorem 3.1(i)). We do not expect this situation to appear in presence of disorder. We discuss this issue in Section 4.4, where we give sufficient conditions ensuring nonvanishing quantum fluctuations of linear response currents in the thermodynamic limit. This study leads to the following theorem:

Theorem 3.3 (Sufficient conditions for nonzero quantum fluctuations). *Take $\vartheta, \lambda \in \mathbb{R}_0^+$, $T, \beta \in \mathbb{R}^+$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$ with support in $[-T, 0]$, and $\vec{w} \doteq (w_1, \ldots, w_d) \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$. Assume that the random variables $\{\omega_1(z)\}_{z\in\mathbb{Z}^d}$ are independently and identically distributed (i.i.d.). Then, for sufficiently small T and ϑ,*

$$\partial_s^2 \mathrm{J}^{(s\mathcal{E})}\big|_{s=0} \geq \frac{\lambda^2 \Upsilon^{(\mathcal{E},\vec{w})}}{\left(1+\mathrm{e}^{\beta(2d(2+\vartheta)+\lambda)}\right)^2} \operatorname{Var}[(\,\cdot\,)_1(0)],$$

with

$$\Upsilon^{(\mathcal{E},\vec{w})} \doteq \left(\int_{-\infty}^0 \langle w, \mathcal{E}(\alpha)\rangle_{\mathbb{R}^d} \alpha^2 \, d\alpha\right)^2 + \frac{1}{2}\sum_{k=1}^d \left(w_k \int_{-\infty}^0 (\mathcal{E}(\alpha))_k \alpha^2 \, d\alpha\right)^2.$$

In particular, $\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} \neq 0$ whenever $\Upsilon^{(\mathcal{E},\vec{w})} > 0$, $\omega_1(0)$ is not almost surely constant (and thus, $\operatorname{Var}[(\,\cdot\,)_1(0)] > 0$, by Chebyshev's inequality), and T, ϑ are sufficiently small.

Proof. This is a direct consequence of (66) and (68) in Section 4. □

By Theorems 3.1 and 3.3, we thus demonstrate that, in general, the quantum fluctuations of linear response currents do not vanish in the thermodynamic limit, and the quantum uncertainty around the macroscopic current density $x^{(\mathcal{E})}$ disappears exponentially fast, as the volume of the cubic box Λ_L grows, with a rate proportional to the squared deviation of the current from $x^{(\mathcal{E})}$ and the inverse current fluctuation. In particular, by combining Theorem 3.1(i) with Theorem 3.3 we can obtain an *explicit* upper bound on the rate function $\mathrm{I}^{(\mathcal{E})}$ around $x^{(\mathcal{E})}$.

The fact that the random variables $\{\omega_1(z)\}_{z\in\mathbb{Z}^d}$ are independently and identically distributed (i.i.d.) in Theorem 3.3 is not essential here: For any $\omega \in \Omega$, let $w^{(\omega)} \doteq (w_1^{(\omega)}, \dots, w_d^{(\omega)}) \in \mathbb{R}^d$ be the random vector defined by

$$w_k^{(\omega)} \doteq (2\omega_1(0) - \omega_1(e_k) - \omega_1(-e_k))w_k, \quad k \in \{1, \dots, d\},$$

with $\{e_k\}_{k=1}^d$ being the canonical basis of $\mathbb{R}^d$. By (64), (66), and (67), it suffices that

$$\mathbb{E}\left[\left|\int_{-\infty}^{0} \langle w^{(\cdot)}, \mathcal{E}(\alpha)\rangle_{\mathbb{R}^d} \alpha^2 \, d\alpha\right|^2\right] = \mathrm{Var}\left[\int_{-\infty}^{0} \langle w^{(\cdot)}, \mathcal{E}(\alpha)\rangle_{\mathbb{R}^d} \alpha^2 \, d\alpha\right] > 0$$

in order to ensure nonvanishing quantum fluctuations of linear response currents in the thermodynamic limit, i.e., $\partial_s^2 \mathrm{J}^{(s\mathcal{E})}|_{s=0} \neq 0$.

Theorem 3.3 can be applied to the celebrated tight-binding Anderson model, which corresponds to the special case $\vartheta = 0$. This is why we focus on this important example in this theorem. The remaining case of larger parameters $\vartheta, T \in \mathbb{R}_0^+$ can certainly be studied, even if this is not done here.

4. Technical proofs

4.1. ***Quasifree fermions in subregions of the lattice .*** Let $\mathcal{P}_{\mathrm{f}}(\mathbb{Z}^d) \subseteq 2^{\mathbb{Z}^d}$ be the set of all nonempty *finite* subsets of $\mathbb{Z}^d$. Like in [Aza et al. 2019, Section 2.1], we need the sets

$$\mathfrak{Z} \doteq \{\mathcal{Z} \subseteq 2^{\mathbb{Z}^d} : (\forall Z_1, Z_2 \in \mathcal{Z})\ Z_1 \neq Z_2 \Rightarrow Z_1 \cap Z_2 = \varnothing\},$$
$$\mathfrak{Z}_{\mathrm{f}} \doteq \mathfrak{Z} \cap \{\mathcal{Z} \subseteq \mathcal{P}_{\mathrm{f}}(\mathbb{Z}^d) : |\mathcal{Z}| < \infty\}.$$

This kind of decomposition over collections of disjoint subsets of the lattice is important to prove Theorem 3.1(i).

Recall that $\mathfrak{h} \doteq \ell^2(\mathbb{Z}^d; \mathbb{C})$, and $\mathcal{B}(\mathfrak{h})$ is the Banach space of all bounded linear operators acting on $\mathfrak{h}$. One can restrict the quasifree dynamics defined by (5) to collections $\mathcal{Z} \in \mathfrak{Z}$ of disjoint subsets of the lattice by using the orthogonal projections P_Λ, $\Lambda \subseteq \mathbb{Z}^d$, defined on the Hilbert space $\mathfrak{h}$ by

$$[P_\Lambda(\psi)](x) \doteq \begin{cases} \psi(x) & \text{if } x \in \Lambda, \\ 0 & \text{else}, \end{cases} \tag{28}$$

for any $\psi \in \mathfrak{h}$. Then, the one-particle Hamiltonian within $\mathcal{Z} \in \mathfrak{Z}$ is, by definition, equal to

$$h_{\mathcal{Z}}^{(\omega)} \doteq \sum_{Z \in \mathcal{Z}} P_Z h^{(\omega)} P_Z \in \mathcal{B}(\mathfrak{h}), \tag{29}$$

where $h^{(\omega)} \in \mathcal{B}(\mathfrak{h})$ is the random tight-binding model defined by (3) for any $\omega \in \Omega$ and $\lambda, \vartheta \in \mathbb{R}_0^+$. For any $\mathcal{Z} \in \mathfrak{Z}$, it leads to the unitary group $\{\mathrm{e}^{ith_{\mathcal{Z}}^{(\omega)}}\}_{t\in\mathbb{R}}$ acting on the Hilbert space $\mathfrak{h}$.

Similar to (5), for any $\mathcal{Z} \in \mathfrak{Z}$, we consequently define the strongly continuous group $\tau^{(\omega,\mathcal{Z})} \doteq \{\tau_t^{(\omega,\mathcal{Z})}\}_{t\in\mathbb{R}}$ of Bogoliubov $*$-automorphisms of $\mathcal{U}$ by

$$\tau_t^{(\omega,\mathcal{Z})}(a(\psi)) = a(\mathrm{e}^{ith_{\mathcal{Z}}^{(\omega)}} \psi), \quad t \in \mathbb{R}, \psi \in \mathfrak{h}.$$

This corresponds to replace $h^{(\omega)}$ in (5) with $h_{\mathcal{Z}}^{(\omega)}$. Similarly, for any $\mathcal{Z} \in \mathfrak{Z}$, we define the quasifree state $\varrho_{\mathcal{Z}}{}^{(\omega)}$ by replacing $h^{(\omega)}$ in (6) with the one-particle Hamiltonian $h_{\mathcal{Z}}{}^{(\omega)}$ within $\mathcal{Z}$.

If $\mathcal{Z} \in \mathfrak{Z}_{\mathrm{f}}$, then both $\tau^{(\omega,\mathcal{Z})}$ and $\varrho_{\mathcal{Z}}^{(\omega)}$ can be written in terms of bilinear elements[8], defined as follows: The bilinear element associated with an operator in $C \in \mathcal{B}(\mathfrak{h})$ whose range, ran(C), is finite dimensional is defined by

$$\langle \mathrm{A}, C\,\mathrm{A}\rangle \doteq \sum_{i,j\in I} \langle \psi_i, C\psi_j\rangle_{\mathfrak{h}}\, a(\psi_i)^* a(\psi_j), \tag{30}$$

where $\{\psi_i\}_{i\in I}$ is any orthonormal basis[9] of a finite dimensional subspace

$$\mathcal{H} \supseteq \mathrm{ran}(C) \cup \mathrm{ran}(C^*)$$

of the Hilbert space $\mathfrak{h}$. See [Aza et al. 2019, Definition 4.3]. For any $\omega \in \Omega$ and $\lambda, \vartheta \in \mathbb{R}_0^+$, the range of $h_{\mathcal{Z}}^{(\omega)} \in \mathcal{B}(\mathfrak{h})$ is finite dimensional whenever $\mathcal{Z} \in \mathfrak{Z}_{\mathrm{f}}$ and one checks that, for any time $t \in \mathbb{R}$, inverse temperature $\beta \in \mathbb{R}^+$, finite collections $\mathcal{Z} \in \mathfrak{Z}_{\mathrm{f}}$ and elements $B \in \mathcal{U}$,

$$\tau_t^{(\omega,\mathcal{Z})}(B) = \mathrm{e}^{it\langle \mathrm{A}, h_{\mathcal{Z}}^{(\omega)}\,\mathrm{A}\rangle}\, B\, \mathrm{e}^{-it\langle \mathrm{A}, h_{\mathcal{Z}}^{(\omega)}\,\mathrm{A}\rangle} \quad \text{and} \quad \varrho_{\mathcal{Z}}^{(\omega)}(B) = \frac{\mathrm{tr}\big(B\,\mathrm{e}^{-\beta\langle \mathrm{A}, h_{\mathcal{Z}}^{(\omega)}\,\mathrm{A}\rangle}\big)}{\mathrm{tr}\big(\mathrm{e}^{-\beta\langle \mathrm{A}, h_{\mathcal{Z}}^{(\omega)}\,\mathrm{A}\rangle}\big)},$$

where $\mathrm{tr} \in \mathcal{U}^*$ is the tracial state, i.e., the gauge-invariant quasifree state with two-point correlation functions given by (6) for $\beta = 0$. See [Aza et al. 2019, Equations (27)–(28)]. The dynamics corresponds in this case to the usual dynamics written in the Heisenberg picture of quantum mechanics, while the above quasifree state is the Gibbs state at inverse temperature $\beta \in \mathbb{R}^+$, both associated with the Hamiltonian $\langle \mathrm{A}, h_{\mathcal{Z}}^{(\omega)}\,\mathrm{A}\rangle \in \mathcal{U}$ for $\mathcal{Z} \in \mathfrak{Z}_{\mathrm{f}}$.

In order to define the thermodynamic limit, we use the cubic boxes $\Lambda_\ell \doteq \{\mathbb{Z} \cap [-\ell, \ell]\}^d$ for $\ell \in \mathbb{R}_0^+$. Then, as $\ell \to \infty$, for any $t \in \mathbb{R}$, $\tau_t^{(\omega,\{\Lambda_\ell\})}$ converges strongly to $\tau_t^{(\omega)} \equiv \tau_t^{(\omega,\{\mathbb{Z}^d\})}$, while $\varrho_{\{\Lambda_\ell\}}^{(\omega)}$ converges in the weak* topology to $\varrho^{(\omega)} \equiv \varrho_{\{\mathbb{Z}^d\}}^{(\omega)}$. For an explicit proof of these well-known facts, see for instance [Ratsimanetrimanana 2019, Propositions 3.2.9 and 3.2.13].

4.2. ***Current observables in subregions of the lattice .*** Fix once and for all $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$. By [Aza et al. 2019, Equation (29)], for any $\lambda, \vartheta \in \mathbb{R}_0^+$, $\omega \in \Omega$, $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, $\mathcal{Z} \in \mathfrak{Z}_{\mathrm{f}}$, and $\mathcal{Z}^{(\tau)} \in \mathfrak{Z}$, the linear response current observable is, by definition, equal to

$$\begin{aligned}\mathfrak{K}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})} \doteq \sum_{k,q=1}^{d} w_k \sum_{Z\in\mathcal{Z}} \sum_{\substack{x,y\in Z\\ x+e_k,y+e_q\in Z}} \int_{-\infty}^{0} \{\mathcal{E}(\alpha)\}_q\, d\alpha \int_0^{-\alpha} ds\; i[\tau_{-s}^{(\omega,\mathcal{Z}^{(\tau)})}(I_{(y+e_q,y)}^{(\omega)}), I_{(x+e_k,x)}^{(\omega)}] \\ +2\sum_{k=1}^{d} w_k \sum_{Z\in\mathcal{Z}} \sum_{x,x+e_k\in Z} \left(\int_{-\infty}^{0} \{\mathcal{E}(\alpha)\}_q\, d\alpha\right) \Re\mathrm{e}(\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle a(\mathfrak{e}_{x+e_k})^* a(\mathfrak{e}_x)),\end{aligned} \tag{31}$$

with $\{e_k\}_{k=1}^d$ being the canonical basis of $\mathbb{R}^d$. Recall that $\Re\mathrm{e}(A) \in \mathcal{U}$ is the real part of $A \in \mathcal{U}$, see (10). Note from (11)–(12) that

$$\mathfrak{K}_{\{\Lambda\},\{\mathbb{Z}^d\}}^{(\omega,\mathcal{E})} = |\Lambda|\, \mathbb{I}_{\Lambda}^{(\omega,\mathcal{E})}, \qquad \Lambda \in \mathcal{P}_{\mathrm{f}}(\mathbb{Z}^d), \tag{32}$$

are linear response current observables within finite subsets of the lattice.

[8]This refers to the well-known second-quantization of one-particle Hamiltonians in the Fock space representation.

[9]$\langle \mathrm{A}, C\,\mathrm{A}\rangle$ does not depend on the particular choice of $\mathcal{H}$ and its orthonormal basis.

The above current observables can obviously be rewritten as bilinear elements (30) associated with one-particle operators acting on the Hilbert space $\mathfrak{h}$. In order to give an explicit expression of these operators, we first define, for any $x \in \mathbb{Z}^d$, the shift operator $s_x \in \mathcal{B}(\mathfrak{h})$ by

$$(s_x \psi)(y) \doteq \psi(x + y), \quad y \in \mathbb{Z}^d, \psi \in \mathfrak{h}. \tag{33}$$

Note that $s_x^* = s_{-x} = s_x^{-1}$ for any $x \in \mathbb{Z}^d$. Then, for every $\omega \in \Omega$ and $\vartheta \in \mathbb{R}_0^+$, the single-hopping operators are

$$S_{x,y}^{(\omega)} \doteq \langle \mathfrak{e}_x, \Delta_{\omega,\vartheta} \mathfrak{e}_y \rangle_{\mathfrak{h}} \, P_{\{x\}} s_{x-y} P_{\{y\}}, \quad x, y \in \mathbb{Z}^d, \tag{34}$$

where $P_{\{u\}}$ is the orthogonal projection defined by (28) for $\Lambda = \{u\}$ and $u \in \mathbb{Z}^d$. Observe that

$$\langle \mathrm{A}, S_{x,y}^{(\omega)} \mathrm{A} \rangle = \langle \mathfrak{e}_x, \Delta_{\omega,\vartheta} \mathfrak{e}_y \rangle_{\mathfrak{h}} \, a(\mathfrak{e}_x)^* a(\mathfrak{e}_y), \quad x, y \in \mathbb{Z}^d.$$

Similarly, by the identity

$$\Im\mathrm{m}\{\langle \mathrm{A}, C \, \mathrm{A} \rangle\} = \langle \mathrm{A}, \Im\mathrm{m}\{C\} \, \mathrm{A} \rangle$$

for any $C \in \mathcal{B}(\mathfrak{h})$ whose range is finite dimensional, the paramagnetic current observables defined by (9) equals

$$I_{(x,y)}^{(\omega)} = -2 \langle \mathrm{A}, \Im\mathrm{m}\{S_{x,y}^{(\omega)}\} \, \mathrm{A} \rangle, \quad x, y \in \mathbb{Z}^d,$$

for each $\omega \in \Omega$ and $\vartheta \in \mathbb{R}_0^+$. For any $\lambda, \vartheta \in \mathbb{R}_0^+$, $\omega \in \Omega$, $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, $\mathcal{Z}^{(\tau)} \in \mathfrak{Z}$, and $\mathcal{Z} \in \mathfrak{Z}_{\mathrm{f}}$, the current observable (31) can then be rewritten as

$$\mathfrak{K}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})} = \langle \mathrm{A}, K_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})} \, \mathrm{A} \rangle = \sum_{x,y \in \mathbb{Z}^d} \langle \mathfrak{e}_x, K_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})} \mathfrak{e}_y \rangle_{\mathfrak{h}} \, a(\mathfrak{e}_x)^* a(\mathfrak{e}_y), \tag{35}$$

where $K_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})} \in \mathcal{B}(\mathfrak{h})$ is the operator acting on the one-particle Hilbert space $\mathfrak{h}$ defined by

$$\begin{aligned} K_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})} \doteq 4 \sum_{k,q=1}^{d} w_k \sum_{Z \in \mathcal{Z}} \sum_{\substack{x,y \in Z \\ x+e_k, y+e_q \in Z}} & \int_{-\infty}^{0} \{\mathcal{E}(\alpha)\}_q \, d\alpha \\ & \times \int_0^{-\alpha} ds \; i \big[\mathrm{e}^{-ish_{\mathcal{Z}^{(\tau)}}^{(\omega)}} \Im\mathrm{m}\{S_{y+e_q,y}^{(\omega)}\} \, \mathrm{e}^{ish_{\mathcal{Z}^{(\tau)}}^{(\omega)}}, \Im\mathrm{m}\{S_{x+e_k,x}^{(\omega)}\} \big] \\ & + 2 \sum_{k=1}^{d} w_k \sum_{Z \in \mathcal{Z}} \sum_{x, x+e_k \in Z} \left(\int_{-\infty}^{0} \{\mathcal{E}(\alpha)\}_q \, d\alpha \right) \Re\mathrm{e}\{S_{x+e_k,x}^{(\omega)}\}. \end{aligned} \tag{36}$$

Note that the range of this bounded and self-adjoint operator is finite dimensional whenever $\mathcal{Z} \in \mathfrak{Z}_{\mathrm{f}}$.

4.3. *Differentiability class of generating functions*. The aim of this section is to prove Theorem 3.1(i), in particular that the generating function $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ defined by (16) belongs to $C^2(\mathbb{R}; \mathbb{R})$. By [Aza et al. 2019, Theorem 3.1], we already know that it is a well-defined, continuously differentiable, convex function. So, one has to prove here that the second derivative of the generating function exists and is continuous. To arrive at this assertion, we follow the argument lines of [Aza et al. 2019, Section 4], showing [Aza et al.

2019, Theorem 3.1] via the control of the thermodynamic limit of finite-volume generating functions that are random.

Fix once and for all $\beta \in \mathbb{R}^+$, $\lambda, \vartheta \in \mathbb{R}_0^+$, and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$. For any $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, $\omega \in \Omega$, and three finite collections $\mathcal{Z}, \mathcal{Z}^{(\varrho)}, \mathcal{Z}^{(\tau)} \in \mathfrak{Z}_{\mathrm{f}}$, we define the finite-volume generating function

$$\mathrm{J}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})} \doteq g_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})} - g_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}^{(\omega,0)}, \tag{37}$$

where

$$g_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})} \doteq \frac{1}{|\cup \mathcal{Z}|} \ln \mathrm{tr}\big(\exp(-\beta \langle \mathrm{A}, h_{\mathcal{Z}^{(\varrho)}}^{(\omega)} \mathrm{A}\rangle) \exp(\mathfrak{K}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})})\big). \tag{38}$$

Recall that the tracial state $\mathrm{tr} \in \mathcal{U}^*$ is the gauge-invariant quasifree state with two-point correlation function given by (6) for $\beta = 0$, while $h_{\mathcal{Z}^{(\varrho)}}^{(\omega)}$ is the one-particle Hamiltonian defined by (29). See also (30) and (31). Compare (37)–(38) with the equalities

$$\begin{aligned} \mathrm{J}^{(\mathcal{E})} &\doteq \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \mathbb{E}\big[\ln \varrho^{(\cdot)}\big(\mathrm{e}^{|\Lambda_L| \mathbb{I}_{\Lambda_L}^{(\cdot,\mathcal{E})}}\big)\big] \\ &= \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \ln \varrho^{(\omega)}\big(\mathrm{e}^{|\Lambda_L| \mathbb{I}_{\Lambda_L}^{(\omega,\mathcal{E})}}\big) = \lim_{L\to\infty} \lim_{L_\varrho\to\infty} \lim_{L_\tau\to\infty} \mathrm{J}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\},\{\Lambda_{L_\tau}\}}^{(\omega,\mathcal{E})}, \end{aligned} \tag{39}$$

where the random variable ω is in a measurable subset of full measure [10], by [Aza et al. 2019, Theorem 3.1 and Equation (45)]. Recall that $\Lambda_\ell \doteq \{\mathbb{Z} \cap [-\ell, \ell]\}^d$ for $\ell \in \mathbb{R}_0^+$. See again (16) for the definition of the generating function. In fact, by [Aza et al. 2019, Proposition 4.10], the above local generating functions can be approximately decomposed into boxes of fixed volume, and we use the Akcoglu–Krengel (superadditive) ergodic theorem [Aza et al. 2019, Theorem 4.17] to deduce, via [Aza et al. 2019, Proposition 4.8], the existence of the generating functions as the thermodynamic limit of finite-volume generating functions, as given in (39).

In order to prove that the generating function is continuously differentiable, one uses in [Aza et al. 2019, Corollary 4.20] the (Arzelà–)Ascoli theorem [Rudin 1991, Theorem A5]. This approach requires uniform bounds on the first and second derivatives of the finite-volume generating functions

$$s \mapsto \mathrm{J}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}^{(\omega,s\mathcal{E})}, \quad \mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d),\ \omega \in \Omega,\ \mathcal{Z}, \mathcal{Z}^{(\varrho)}, \mathcal{Z}^{(\tau)} \in \mathfrak{Z}_{\mathrm{f}}. \tag{40}$$

This is done in [Aza et al. 2019, Proposition 4.9], which establishes the following: Fixing $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$ and $\beta_1, s_1, \vartheta_1, \lambda_1 \in \mathbb{R}^+$, one has

$$\sup_{\substack{\beta\in(0,\beta_1],\ \vartheta\in[0,\vartheta_1],\ \lambda\in[0,\lambda_1] \\ \omega\in\Omega,\ s\in[-s_1,s_1],\ \mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}\in\mathfrak{Z}_{\mathrm{f}}}} \Big\{\big|\partial_s \mathrm{J}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}^{(\omega,s\mathcal{E})}\big| + \big|\partial_s^2 \mathrm{J}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}^{(\omega,s\mathcal{E})}\big|\Big\} < \infty. \tag{41}$$

In order to get in the same way the existence and continuity of the second derivative of the generating function, we need to control the *third*-order derivative of the same finite-volume generating functions (40).

[10]The measurable subset $\tilde{\Omega} \subseteq \Omega$ of full measure of [Aza et al. 2019, Theorem 3.1] does not depend on $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$ and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$.

Equation (41) is proved by using the CAR (4) and the Combes–Thomas estimate [Aza et al. 2019, Appendix A], in particular the bound

$$\sup_{\lambda\in\mathbb{R}_0^+}\ \sup_{\mathcal{Z}\in\mathfrak{Z}}\ \sup_{\omega\in\Omega}\left|\langle\mathfrak{e}_x, \mathrm{e}^{ith_{\mathcal{Z}}^{(\omega)}}\mathfrak{e}_y\rangle_{\mathfrak{h}}\right| \leq 36\,\mathrm{e}^{|t\eta|-2\mu_\eta|x-y|}, \quad x, y\in\mathbb{Z}^d, \vartheta\in\mathbb{R}_0^+, t\in\mathbb{R}, \tag{42}$$

(see [Aza et al. 2019, Equation (7)]), where

$$\mu_\eta \doteq \mu\min\left\{\frac{1}{2}, \frac{\eta}{8d(1+\vartheta)\,\mathrm{e}^{\mu}}\right\}, \tag{43}$$

the parameters $\eta, \mu\in\mathbb{R}^+$ being two arbitrarily fixed (strictly positive) constants. For any $\mathcal{E}\in C_0^0(\mathbb{R};\mathbb{R}^d)$ and $\beta_1, s_1, \vartheta_1, \lambda_1\in\mathbb{R}^+$, the Combes–Thomas estimate leads also to the uniform estimates

$$\sup_{\substack{\beta\in(0,\beta_1],\ \vartheta\in[0,\vartheta_1],\ \lambda\in[0,\lambda_1]\\ \omega\in\Omega,\ s\in[-s_1,s_1],\ \mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}\in\mathfrak{Z}_{\mathrm{f}}}}\ \sup_{x\in\mathbb{Z}^d}\sum_{y\in\mathbb{Z}^d}\left|\left\langle\mathfrak{e}_y, \frac{1}{1+\mathrm{e}^{-\frac{s}{2}K_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})}}\,\mathrm{e}^{\beta h_{\mathcal{Z}^{(\varrho)}}^{(\omega)}}\,\mathrm{e}^{-\frac{s}{2}K_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})}}}\mathfrak{e}_x\right\rangle_{\mathfrak{h}}\right| < \infty \tag{44}$$

(see the end of the proof of [Aza et al. 2019, Proposition 4.9]), as well as

$$\sup_{\vartheta\in[0,\vartheta_1]}\ \sup_{\lambda\in\mathbb{R}_0^+}\ \sup_{\mathcal{Z},\mathcal{Z}^{(\tau)}\in\mathfrak{Z}_{\mathrm{f}}}\ \sup_{\omega\in\Omega}\frac{1}{|\cup\mathcal{Z}|}\sum_{x,y\in\mathbb{Z}^d}\left|\langle\mathfrak{e}_x, K_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})}\mathfrak{e}_y\rangle_{\mathfrak{h}}\right| < \infty \tag{45}$$

and

$$\sup_{\vartheta\in[0,\vartheta_1]}\ \sup_{\lambda\in\mathbb{R}_0^+}\ \sup_{\mathcal{Z},\mathcal{Z}^{(\tau)}\in\mathfrak{Z}_{\mathrm{f}}}\ \sup_{\omega\in\Omega}\left|\langle\mathfrak{e}_x, K_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})}\mathfrak{e}_y\rangle_{\mathfrak{h}}\right| \leq C_{x,y}^{(\mathcal{E},\vartheta_1)} < \infty \tag{46}$$

for $x, y\in\mathbb{Z}^d$, where $C_{x,y}^{(\mathcal{E},\vartheta_1)}\in\mathbb{R}^+$ are constants satisfying

$$\sup_{x,y\in\mathbb{Z}^d} C_{x,y}^{(\mathcal{E},\vartheta_1)} < \infty \quad\text{and}\quad \sup_{x\in\mathbb{Z}^d}\sum_{y\in\mathbb{Z}^d} C_{x,y}^{(\mathcal{E},\vartheta_1)} < \infty. \tag{47}$$

Recall that $K_{\mathcal{Z},\mathcal{Z}^{(\tau)}}^{(\omega,\mathcal{E})}\in\mathcal{B}(\mathfrak{h})$ is the operator defining linear response current observables, by (35)–(36).

In order to give a uniform estimate on the third-order derivative of the finite-volume generating functions (40), similar to the proof of (41), we use again the Combes–Thomas estimate, which yields (44)–(47). This proof bears, however, on more complex computations than the one of (41), which only controls the first and second derivatives of the same function.

Proposition 4.1 (Uniform boundedness of third derivatives). *Fix an electric field $\mathcal{E}\in C_0^0(\mathbb{R};\mathbb{R}^d)$, $\vec{w}\in\mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d}=1$, and the parameters $\beta_1, s_1, \vartheta_1, \lambda_1\in\mathbb{R}^+$. Then,*

$$\sup_{\substack{\beta\in(0,\beta_1],\ \vartheta\in[0,\vartheta_1],\ \lambda\in[0,\lambda_1]\\ \omega\in\Omega,\ s\in[-s_1,s_1],\ \mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}\in\mathfrak{Z}_{\mathrm{f}}}}\left|\partial_s^3\,\mathrm{J}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}^{(\omega,s\mathcal{E})}\right| < \infty.$$

Proof. For any $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$, and $\mathcal{Z}, \mathcal{Z}^{(\varrho)}, \mathcal{Z}^{(\tau)} \in \mathfrak{Z}_{\mathrm{f}}$, a straightforward computation yields that

$$\begin{aligned} \partial_s^3 \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} &= \frac{1}{|\cup \mathcal{Z}|} \varpi_s^T \big(\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} ; \mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} ; \mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} \big) \\ &= \frac{1}{|\cup \mathcal{Z}|} \Big(\varpi_s \big(\big(\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\big)^3 \big) - 3\varpi_s \big(\big(\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\big)^2 \big) \varpi_s \big(\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} \big) + 2\varpi_s \big(\mathfrak{K}^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} \big)^3 \Big), \end{aligned} \tag{48}$$

where ϖ_s is the (unique) gauge-invariant quasifree state satisfying

$$\varpi_s(a^*(\varphi)a(\psi)) = \left\langle \psi, \frac{1}{1 + \mathrm{e}^{-\frac{s}{2} K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}} \mathrm{e}^{\beta h^{(\omega)}_{\mathcal{Z}^{(\varrho)}}} \mathrm{e}^{-\frac{s}{2} K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}}} \varphi \right\rangle_{\mathfrak{h}}, \quad \varphi, \psi \in \mathfrak{h}. \tag{49}$$

In the first equality of (48), $\varpi_s^T(\,\cdot\,;\,\cdot\,;\,\cdot\,)$ denotes the so-called "truncated" or "connected" correlation function of third order, associated with the state ϖ_s. Recall that, for all $A_1, A_2, A_3 \in \mathcal{U}$, this function is defined by

$$\begin{aligned} \varpi_s^T(A_1; A_2; A_3) \doteq \varpi_s(A_1A_2A_3) - \varpi_s(A_1)\varpi_s(A_2A_3) - \varpi_s(A_2)\varpi_s(A_1A_3) \\ - \varpi_s(A_3)\varpi_s(A_1A_2) + 2\varpi_s(A_1)\varpi_s(A_2)\varpi_s(A_3). \end{aligned}$$

(This is similar to [Aza et al. 2019, Proof of Proposition 4.9, until Equation (48)].) Recall that $\{\mathfrak{e}_x\}_{x\in\mathbb{Z}^d}$ is the canonical orthonormal basis of $\mathfrak{h}$, which is defined by $\mathfrak{e}_x(y) \doteq \delta_{x,y}$ for all $x, y \in \mathbb{Z}^d$. By linearity and continuity in each argument of $\varpi_s^T(\,\cdot\,;\,\cdot\,;\,\cdot)$, one has

$$\begin{aligned} \partial_s^3 \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} = \frac{1}{|\cup \mathcal{Z}|} \sum_{\substack{x_i, y_i \in \mathbb{Z}^d \\ i \in \{1,2,3\}}} \langle \mathfrak{e}_{x_1}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} \mathfrak{e}_{y_1} \rangle_{\mathfrak{h}} \langle \mathfrak{e}_{x_2}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} \mathfrak{e}_{y_2} \rangle_{\mathfrak{h}} \langle \mathfrak{e}_{x_3}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} \mathfrak{e}_{y_3} \rangle_{\mathfrak{h}} \\ \times \varpi_s^T(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_1}); a^*(\mathfrak{e}_{x_2})a(\mathfrak{e}_{y_2}); a^*(\mathfrak{e}_{x_3})a(\mathfrak{e}_{y_3})). \end{aligned}$$

Note that, by (8) and the fact that ϖ_s is a gauge-invariant quasifree state,

$$\begin{aligned} &\varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_1})a^*(\mathfrak{e}_{x_2})a(\mathfrak{e}_{y_2})a^*(\mathfrak{e}_{x_3})a(\mathfrak{e}_{y_3})) \\ &\quad = \det \begin{pmatrix} \varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_1})) & \varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_2})) & \varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_3})) \\ -\varpi_s(a(\mathfrak{e}_{y_1})a^*(\mathfrak{e}_{x_2})) & \varpi_s(a^*(\mathfrak{e}_{x_2})a(\mathfrak{e}_{y_2})) & \varpi_s(a^*(\mathfrak{e}_{x_2})a(\mathfrak{e}_{y_3})) \\ -\varpi_s(a(\mathfrak{e}_{y_1})a^*(\mathfrak{e}_{x_3})) & -\varpi_s(a(\mathfrak{e}_{y_2})a^*(\mathfrak{e}_{x_3})) & \varpi_s(a^*(\mathfrak{e}_{x_3})a(\mathfrak{e}_{y_3})) \end{pmatrix} = \sum_{g\in\mathcal{G}_3} \xi_s^g(x_1, y_1, x_2, y_2, x_3, y_3) \end{aligned}$$

(use, for instance, [Bru and de Siqueira Pedra 2017b, Lemma 3.1] to get the above determinant), where

$$\begin{aligned} \mathcal{G}_3 \doteq \{\{(1,1),(2,2),(3,3)\}, \{(1,1),(2,3),(3,2)\}, \{(1,2),(2,1),(3,3)\}\} \\ \cup \{\{(1,2),(2,3),(3,1)\}, \{(1,3),(2,1),(3,2)\}, \{(1,3),(2,2),(3,1)\}\} \end{aligned}$$

is a set of oriented graphs with vertex set {1, 2, 3} and

$$\begin{aligned}
\xi_s^{\{(1,1),(2,2),(3,3)\}}(x_1, y_1, x_2, y_2, x_3, y_3) &\doteq \varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_1}))\varpi_s(a^*(\mathfrak{e}_{x_2})a(\mathfrak{e}_{y_2}))\varpi_s(a^*(\mathfrak{e}_{x_3})a(\mathfrak{e}_{y_3})),\\
\xi_s^{\{(1,1),(2,3),(3,2)\}}(x_1, y_1, x_2, y_2, x_3, y_3) &\doteq \varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_1}))\varpi_s(a^*(\mathfrak{e}_{x_2})a(\mathfrak{e}_{y_3}))\varpi_s(a(\mathfrak{e}_{y_2})a^*(\mathfrak{e}_{x_3})),\\
\xi_s^{\{(1,2),(2,1),(3,3)\}}(x_1, y_1, x_2, y_2, x_3, y_3) &\doteq \varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_2}))\varpi_s(a(\mathfrak{e}_{y_1})a^*(\mathfrak{e}_{x_2}))\varpi_s(a^*(\mathfrak{e}_{x_3})a(\mathfrak{e}_{y_3})),\\
\xi_s^{\{(1,2),(2,3),(3,1)\}}(x_1, y_1, x_2, y_2, x_3, y_3) &\doteq -\varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_2}))\varpi_s(a^*(\mathfrak{e}_{x_2})a(\mathfrak{e}_{y_3}))\varpi_s(a(\mathfrak{e}_{y_1})a^*(\mathfrak{e}_{x_3})),\\
\xi_s^{\{(1,3),(2,1),(3,2)\}}(x_1, y_1, x_2, y_2, x_3, y_3) &\doteq \varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_3}))\varpi_s(a(\mathfrak{e}_{y_1})a^*(\mathfrak{e}_{x_2}))\varpi_s(a(\mathfrak{e}_{y_2})a^*(\mathfrak{e}_{x_3})),\\
\xi_s^{\{(1,3),(2,2),(3,1)\}}(x_1, y_1, x_2, y_2, x_3, y_3) &\doteq \varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_3}))\varpi_s(a^*(\mathfrak{e}_{x_2})a(\mathfrak{e}_{y_2}))\varpi_s(a(\mathfrak{e}_{y_1})a^*(\mathfrak{e}_{x_3})).
\end{aligned}$$

By elementary computations, one sees that taking connected correlations corresponds here, as is usual, to only keep the terms associated with connected graphs. That is,

$$\begin{aligned}
&\varpi_s^T(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_1}); a^*(\mathfrak{e}_{x_2})a(\mathfrak{e}_{y_2}); a^*(\mathfrak{e}_{x_3})a(\mathfrak{e}_{y_3}))\\
&\qquad = \varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_3}))\varpi_s(a(\mathfrak{e}_{y_1})a^*(\mathfrak{e}_{x_2}))\varpi_s(a(\mathfrak{e}_{y_2})a^*(\mathfrak{e}_{x_3}))\\
&\qquad\qquad -\varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_2}))\varpi_s(a^*(\mathfrak{e}_{x_2})a(\mathfrak{e}_{y_3}))\varpi_s(a(\mathfrak{e}_{y_1})a^*(\mathfrak{e}_{x_3})).
\end{aligned}$$

Hence,

$$\partial_s^3 \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} = \boldsymbol{K}_1 - \boldsymbol{K}_2, \tag{50}$$

where

$$\begin{aligned}
\boldsymbol{K}_1 \doteq \frac{1}{|\cup\mathcal{Z}|}\sum_{\substack{x_i, y_i\in\mathbb{Z}^d\\ i\in\{1,2,3\}}} &\langle \mathfrak{e}_{x_1}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathfrak{e}_{y_1}\rangle_{\mathfrak{h}}\,\langle \mathfrak{e}_{x_2}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathfrak{e}_{y_2}\rangle_{\mathfrak{h}}\,\langle \mathfrak{e}_{x_3}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathfrak{e}_{y_3}\rangle_{\mathfrak{h}}\\
&\times\varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_3}))\varpi_s(a(\mathfrak{e}_{y_1})a^*(\mathfrak{e}_{x_2}))\varpi_s(a(\mathfrak{e}_{y_2})a^*(\mathfrak{e}_{x_3}))
\end{aligned}\tag{51}$$

and

$$\begin{aligned}
\boldsymbol{K}_2 \doteq \frac{1}{|\cup\mathcal{Z}|}\sum_{\substack{x_i, y_i\in\mathbb{Z}^d\\ i\in\{1,2,3\}}} &\langle \mathfrak{e}_{x_1}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathfrak{e}_{y_1}\rangle_{\mathfrak{h}}\,\langle \mathfrak{e}_{x_2}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathfrak{e}_{y_2}\rangle_{\mathfrak{h}}\,\langle \mathfrak{e}_{x_3}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathfrak{e}_{y_3}\rangle_{\mathfrak{h}}\\
&\varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_2}))\varpi_s(a(\mathfrak{e}_{y_1})a^*(\mathfrak{e}_{x_3}))\varpi_s(a^*(\mathfrak{e}_{x_2})a(\mathfrak{e}_{y_3})).
\end{aligned}\tag{52}$$

Applying the triangle inequality, we now obtain that

$$\begin{aligned}
|\boldsymbol{K}_1| \leq \frac{1}{|\cup\mathcal{Z}|}\sum_{\substack{x_i, y_i\in\mathbb{Z}^d\\ i\in\{1,2,3\}}} &|\langle \mathfrak{e}_{x_1}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathfrak{e}_{y_1}\rangle_{\mathfrak{h}}|\,|\langle \mathfrak{e}_{x_2}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathfrak{e}_{y_2}\rangle_{\mathfrak{h}}|\,|\langle \mathfrak{e}_{x_3}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathfrak{e}_{y_3}\rangle_{\mathfrak{h}}|\\
&|\varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_3}))|\,|\varpi_s(a(\mathfrak{e}_{y_1})a^*(\mathfrak{e}_{x_2}))|\,|\varpi_s(a(\mathfrak{e}_{y_2})a^*(\mathfrak{e}_{x_3}))|\\
\leq \sup_{x_3,y_3\in\mathbb{Z}^d}|\langle \mathfrak{e}_{x_3}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathfrak{e}_{y_3}\rangle_{\mathfrak{h}}|&\sup_{x_2\in\mathbb{Z}^d}\sum_{y_2\in\mathbb{Z}^d}|\langle \mathfrak{e}_{x_2}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathfrak{e}_{y_2}\rangle_{\mathfrak{h}}|\frac{1}{|\cup\mathcal{Z}|}\sum_{x_1,y_1\in\mathbb{Z}^d}|\langle \mathfrak{e}_{x_1}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}}\mathfrak{e}_{y_1}\rangle_{\mathfrak{h}}|\\
\sup_{x_1\in\mathbb{Z}^d}\sum_{y_3\in\mathbb{Z}^d}|\varpi_s(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_3}))|&\sup_{y_1\in\mathbb{Z}^d}\sum_{x_2\in\mathbb{Z}^d}|\varpi_s(a(\mathfrak{e}_{y_1})a^*(\mathfrak{e}_{x_2}))|\sup_{y_2\in\mathbb{Z}^d}\sum_{x_3\in\mathbb{Z}^d}|\varpi_s(a(\mathfrak{e}_{y_2})a^*(\mathfrak{e}_{x_3}))|.
\end{aligned}$$

We can finally use (44)–(47) and (49) to arrive from the last upper bound at

$$\sup_{\substack{\beta\in(0,\beta_1],\ \vartheta\in[0,\vartheta_1],\ \lambda\in[0,\lambda_1]\\ \omega\in\Omega,\ s\in[-s_1,s_1],\ \mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}\in\mathfrak{Z}_{\mathrm{f}}}} |\boldsymbol{K}_1| < \infty.$$

The absolute value $|\boldsymbol{K}_2|$ of the other term of $\partial_s^3\, \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}$ (see (50)–(52)) can be bounded exactly in the same way. By the triangle inequality applied to (50), this concludes the proof. □

We can now sharpen the result given in [Aza et al. 2019, Corollary 4.20], stating that the mapping $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ defined by (16) is continuously differentiable with

$$\partial_s\, \mathrm{J}^{(s\mathcal{E})} = \lim_{L\to\infty} \frac{\varrho^{(\omega)}\big(\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L}\, \mathrm{e}^{s|\Lambda_L|\,\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L}}\big)}{\varrho^{(\omega)}\big(\mathrm{e}^{s|\Lambda_L|\,\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L}}\big)}.$$

Thanks to (41) and Proposition 4.1, we now obtain the following assertion:

Corollary 4.2 (Differentiability of generating functions). *There is a measurable subset* $\tilde{\Omega} \subseteq \Omega$ *of full measure such that, for all* $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \tilde{\Omega}$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$, *and* $\vec{w} \in \mathbb{R}^d$ *with* $\|\vec{w}\|_{\mathbb{R}^d} = 1$, *the mapping* $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ *from* $\mathbb{R}$ *to itself belongs to* $C^2(\mathbb{R};\mathbb{R})$ *and*

$$\partial_s\, \mathrm{J}^{(s\mathcal{E})}\,|_{s=0} = x^{(\mathcal{E})} \doteq \lim_{L\to\infty} \mathbb{E}\big[\varrho^{(\cdot)}\big(\mathbb{I}^{(\cdot,\mathcal{E})}_{\Lambda_L}\big)\big] = \lim_{L\to\infty} \varrho^{(\omega)}\big(\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L}\big),$$
$$\partial_s^2\, \mathrm{J}^{(s\mathcal{E})}\,|_{s=0} = \lim_{L\to\infty} \mathbb{E}\big[\boldsymbol{F}^{(\cdot,\mathcal{E})}_L\big] = \lim_{L\to\infty} \boldsymbol{F}^{(\omega,\mathcal{E})}_L \geq 0,$$

where $\boldsymbol{F}^{(\omega,\mathcal{E})}_L$ *is the quantum fluctuation of the linear response current defined by* (18) *for any* $L \in \mathbb{R}_0^+$. *See also* (13) *for the definition of the macroscopic current density* $x^{(\mathcal{E})}$.

Proof. [Aza et al. 2019, Corollary 4.19] states, among other things, the existence of a measurable set $\tilde{\Omega}$ of full measure such that, for all $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \tilde{\Omega}$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$, $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$, and $s \in \mathbb{R}$,

$$\mathrm{J}^{(s\mathcal{E})} = \lim_{L_\tau \geq L_\varrho \geq L\to\infty} \mathrm{J}^{(\omega,s\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\},\{\Lambda_{L_\tau}\}}\,. \tag{53}$$

Fix from now on all parameters $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \tilde{\Omega}$, $\mathcal{E} \in C_0^0(\mathbb{R};\mathbb{R}^d)$, and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$. By combining (41) and Proposition 4.1 with the mean value theorem and the (Arzelà–)Ascoli theorem [Rudin 1991, Theorem A5], there are three sequences

$$\{L_\tau^{(n)}\}_{n\in\mathbb{N}},\ \{L_\varrho^{(n)}\}_{n\in\mathbb{N}},\ \{L^{(n)}\}_{n\in\mathbb{N}} \subseteq \mathbb{R}_0^+, \tag{54}$$

with $L_\tau^{(n)} \geq L_\varrho^{(n)} \geq L^{(n)}$, such that, as $n \to \infty$, the mappings

$$s \mapsto \mathrm{J}^{(\omega,s\mathcal{E})}_{\{\Lambda_{L^{(n)}}\},\{\Lambda_{L_\varrho^{(n)}}\},\{\Lambda_{L_\tau^{(n)}}\}},\quad s \mapsto \partial_s\, \mathrm{J}^{(\omega,s\mathcal{E})}_{\{\Lambda_{L^{(n)}}\},\{\Lambda_{L_\varrho^{(n)}}\},\{\Lambda_{L_\tau^{(n)}}\}},\quad \text{and}\quad s \mapsto \partial_s^2\, \mathrm{J}^{(\omega,s\mathcal{E})}_{\{\Lambda_{L^{(n)}}\},\{\Lambda_{L_\varrho^{(n)}}\},\{\Lambda_{L_\tau^{(n)}}\}}$$

from $\mathbb{R}$ to itself converge uniformly for s in any compact subset of $\mathbb{R}$. So, the mapping $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ from $\mathbb{R}$ to itself is a C^2-function with

$$\partial_s \mathrm{J}^{(s\mathcal{E})} = \lim_{L_\tau \geq L_\varrho \geq L \to \infty} \partial_s \mathrm{J}^{(\omega,s\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\},\{\Lambda_{L_\tau}\}} = \lim_{L\to\infty} \left(\frac{\varrho^{(\omega)}\big(\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L} \, \mathrm{e}^{s|\Lambda_L|\,\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L}}\big)}{\varrho^{(\omega)}\big(\mathrm{e}^{s|\Lambda_L|\,\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L}}\big)} \right)$$

and

$$\begin{aligned}\partial_s^2 \mathrm{J}^{(s\mathcal{E})} &= \lim_{L_\tau \geq L_\varrho \geq L \to \infty} \partial_s^2 \mathrm{J}^{(\omega,s\mathcal{E})}_{\{\Lambda_L\},\{\Lambda_{L_\varrho}\},\{\Lambda_{L_\tau}\}} \\ &= \lim_{L\to\infty} |\Lambda_L| \left(\frac{\varrho^{(\omega)}\big((\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L})^2 \, \mathrm{e}^{s|\Lambda_L|\,\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L}}\big)\varrho^{(\omega)}\big(\mathrm{e}^{s|\Lambda_L|\,\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L}}\big) - \big(\varrho^{(\omega)}\big(\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L} \, \mathrm{e}^{s|\Lambda_L|\,\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L}}\big)\big)^2}{\big(\varrho^{(\omega)}\big(\mathrm{e}^{s|\Lambda_L|\,\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L}}\big)\big)^2} \right).\end{aligned}$$

See (32). Note that the above limits for the first- and second-order derivatives do not need to be taken only along subsequences, by the (Arzelà–)Ascoli theorem [Rudin 1991, Theorem A5] and (53). In particular, for $s = 0$,

$$\partial_s \mathrm{J}^{(s\mathcal{E})}\,|_{s=0} = \lim_{L\to\infty} \mathbb{E}\big[\varrho^{(\cdot)}\big(\mathbb{I}^{(\cdot,\mathcal{E})}_{\Lambda_L}\big)\big] = \lim_{L\to\infty} \varrho^{(\omega)}\big(\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L}\big) \tag{55}$$

and

$$\begin{aligned}\partial_s^2 \mathrm{J}^{(s\mathcal{E})}\,|_{s=0} &= \lim_{L\to\infty} |\Lambda_L| \mathbb{E}\big[\varrho^{(\cdot)}\big((\mathbb{I}^{(\cdot,\mathcal{E})}_{\Lambda_L})^2\big) - \big(\varrho^{(\cdot)}(\mathbb{I}^{(\cdot,\mathcal{E})}_{\Lambda_L})\big)^2\big] \\ &= \lim_{L\to\infty} |\Lambda_L| \big(\varrho^{(\omega)}\big((\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L})^2\big) - \big(\varrho^{(\omega)}(\mathbb{I}^{(\omega,\mathcal{E})}_{\Lambda_L})\big)^2\big).\end{aligned} \tag{56}$$

By (18)–(19) and (56), $\partial_s^2 \mathrm{J}^{(s\mathcal{E})}\,|_{s=0}$ is the thermodynamic limit of the quantum fluctuations of linear response currents. □

From the proof of Proposition 4.1, it is apparent that the n-th derivative $\partial_s^n \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}$, $n \in \mathbb{N}$, has the following structure:

$$\begin{aligned}\partial_s^n \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}} &= \frac{1}{|\cup\mathcal{Z}|} \sum_{k=1}^{n} \sum_{x_k,y_k\in\mathbb{Z}^d} \langle \mathfrak{e}_{x_1}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} \mathfrak{e}_{y_1}\rangle_{\mathfrak{h}} \cdots \langle \mathfrak{e}_{x_k}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} \mathfrak{e}_{y_k}\rangle_{\mathfrak{h}} \\ &\qquad\qquad \times \varpi_s^T\big(a^*(\mathfrak{e}_{x_1})a(\mathfrak{e}_{y_1}); \cdots ; a^*(\mathfrak{e}_{x_n})a(\mathfrak{e}_{x_n})\big) \\ &= \frac{1}{|\cup\mathcal{Z}|} \sum_{g\in\mathcal{G}_n^c} \sum_{k=1}^{n} \sum_{x_k,y_k\in\mathbb{Z}^d} \mathrm{sign}(g) \langle \mathfrak{e}_{x_1}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} \mathfrak{e}_{y_1}\rangle_{\mathfrak{h}} \cdots \langle \mathfrak{e}_{x_k}, K^{(\omega,\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\tau)}} \mathfrak{e}_{y_k}\rangle_{\mathfrak{h}} \\ &\qquad\qquad \times \prod_{l\in g} k_s(l; x_1, y_1, \ldots, x_n, y_n),\end{aligned}$$

where $\mathcal{G}_n^c$ is the set of all connected oriented graphs g such that, for each vertex $v \in \{1, \ldots, n\}$ of $g \in \mathcal{G}_n^c$, there is exactly one line of the form $(v, \tilde{v}_1) \in g$ and exactly one line of the form $(\tilde{v}_2, v) \in g$, for some $\tilde{v}_1, \tilde{v}_2 \in \{1, \ldots, n\}$. The constants $k_s(l; x_1, y_1, \ldots, x_n, y_n)$, $l \in \{1, \ldots, n\}^2$, $x_1, y_1, \ldots, x_n, y_n \in \mathbb{Z}^d$, are defined by

$$k_s((i, j); x_1, y_1, \ldots, x_n, y_n) \doteq \begin{cases} \varpi_s(a^*(\mathfrak{e}_{x_i})a(\mathfrak{e}_{y_j})) & \text{if } i \leq j, \\ \varpi_s(a(\mathfrak{e}_{y_j})a^*(\mathfrak{e}_{x_i})) & \text{if } i > j. \end{cases}$$

The quantity $\mathrm{sign}(g) \in \{-1, 1\}$ is a sign only depending on the graph $g \in \mathcal{G}_n^c$. By using this expression, exactly as in the special case $n = 3$, for any fixed $n \in \mathbb{N}$ and electric field $\mathcal{E}$, one can bound the n-th derivative $\partial_s^n \mathrm{J}^{(\omega,s\mathcal{E})}_{\mathcal{Z},\mathcal{Z}^{(\varrho)},\mathcal{Z}^{(\tau)}}$ uniformly. This implies that the generating function $s \mapsto \mathrm{J}^{(s\mathcal{E})}$ defined by (16) is a *smooth* function of $s \in \mathbb{R}$, by the (Arzelà–)Ascoli theorem [Rudin 1991, Theorem A5] used as in the proof of Corollary 4.2. We refrain from working out the full arguments to prove this claim since absolutely no new conceptual ingredient would appear in this generalization.

4.4. ***Nonvanishing second derivative of generating functions at the origin .*** We discuss necessary conditions for

$$\partial_s^2 \mathrm{J}^{(s\mathcal{E})} |_{s=0} \neq 0, \tag{57}$$

which is a condition appearing in Theorem 3.1(ii). In other words, the aim of this section is to prove Theorem 3.3. To this end, it is convenient to write this quantity by means of the one-particle Hilbert space $\mathfrak{h}$.

Lemma 4.3 (Quantum fluctuations on the one-particle Hilbert space). *For all* $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, *and* $\vec{w} \in \mathbb{R}^d$ *with* $\|\vec{w}\|_{\mathbb{R}^d} = 1$,

$$\partial_s^2 \mathrm{J}^{(s\mathcal{E})} |_{s=0} = \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \mathbb{E}\Big[\mathrm{Tr}_{\mathfrak{h}}\Big(K^{(\,\cdot\,,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \frac{1}{1+\mathrm{e}^{-\beta h^{(\cdot)}}} K^{(\,\cdot\,,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \frac{1}{1+\mathrm{e}^{\beta h^{(\cdot)}}}\Big)\Big],$$

with $\mathrm{Tr}_{\mathfrak{h}}$ *being the trace on* $\mathfrak{h} \doteq \ell^2(\mathbb{Z}^d; \mathbb{C})$.

Proof. Fix all parameters of the lemma. Using (32) and (35) together with the quasifree property of $\varrho^{(\omega)}$, one obtains from (56) that

$$\partial_s^2 \mathrm{J}^{(s\mathcal{E})} |_{s=0} = \lim_{L\to\infty} \frac{1}{|\Lambda_L|} \sum_{x,y,u,v\in\mathbb{Z}^d} \langle \mathfrak{e}_x, K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \mathfrak{e}_y \rangle_{\mathfrak{h}} \langle \mathfrak{e}_u, K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \mathfrak{e}_v \rangle_{\mathfrak{h}} \times \varrho^{(\omega)}(a(\mathfrak{e}_y)a(\mathfrak{e}_u)^*)\varrho^{(\omega)}(a(\mathfrak{e}_x)^* a(\mathfrak{e}_v)),$$

because of the identity

$$\rho(a(\mathfrak{e}_x)^* a(\mathfrak{e}_y) a(\mathfrak{e}_u)^* a(\mathfrak{e}_v)) = \rho(a(\mathfrak{e}_x)^* a(\mathfrak{e}_y))\rho(a(\mathfrak{e}_u)^* a(\mathfrak{e}_v)) + \rho(a(\mathfrak{e}_y) a(\mathfrak{e}_u)^*)\rho(a(\mathfrak{e}_x)^* a(\mathfrak{e}_v))$$

for any $x, y, u, v \in \mathbb{Z}^d$ and quasifree state ρ on $\mathcal{U}$, see (4) and (8). By (6) and straightforward computations, the assertion follows. ☐

Therefore, (57) holds true if

$$\lim_{L\to\infty} \left\{ \frac{1}{|\Lambda_L|} \left| \mathrm{Tr}_{\mathfrak{h}}\Big(K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \frac{1}{1+\mathrm{e}^{-\beta h^{(\omega)}}} K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \frac{1}{1+\mathrm{e}^{\beta h^{(\omega)}}}\Big) \right| \right\} \geq \varepsilon > 0$$

for some strictly positive constant $\varepsilon \in \mathbb{R}^+$. To verify this bound, we start with an elementary observation:

Lemma 4.4 (Quantum fluctuations and the Hilbert–Schmidt norm of $K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}$). *For all* $\beta \in \mathbb{R}^+$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$, $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$, *and* $\vec{w} \in \mathbb{R}^d$ *with* $\|\vec{w}\|_{\mathbb{R}^d} = 1$,

$$\mathrm{Tr}_{\mathfrak{h}}\Big(K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \frac{1}{1+\mathrm{e}^{-\beta h^{(\omega)}}} K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \frac{1}{1+\mathrm{e}^{\beta h^{(\omega)}}}\Big) \geq \frac{1}{(1+\mathrm{e}^{\beta(2d(2+\vartheta)+\lambda)})^2} \mathrm{Tr}_{\mathfrak{h}}\big((K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}})^* K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\big).$$

Proof. Fix all parameters of the lemma. By the functional calculus, $(1+\mathrm{e}^{\pm\beta h^{(\omega)}})^{-1}$ are positive operators satisfying

$$\frac{1}{1+\mathrm{e}^{\pm\beta h^{(\omega)}}} \geq \frac{1}{1+\mathrm{e}^{\beta \sup_{\omega\in\Omega}\|h^{(\omega)}\|_{\mathcal{B}(\mathfrak{h})}}}\mathbf{1}_{\mathfrak{h}}\,,$$

while, for any $\omega=(\omega_1,\omega_2)\in\Omega$ and $\lambda,\vartheta\in\mathbb{R}_0^+$,

$$\|h^{(\omega)}\|_{\mathcal{B}(\mathfrak{h})} \leq \|\Delta_{\omega,\vartheta}\|_{\mathcal{B}(\mathfrak{h})}+\lambda\|\omega_1\|_{\mathcal{B}(\mathfrak{h})} \leq 2d(2+\vartheta)+\lambda, \tag{58}$$

see (2)–(3). Since $K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}$ is a self-adjoint operator (see (36) or (59) below), it thus suffices to use the cyclicity of the trace to prove the lemma. □

Recall that $K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}$ is defined by (36), that is in this case,

$$K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \doteq \sum_{k,q=1}^{d} w_k \int_{-\infty}^{0} \{\mathcal{E}(\alpha)\}_q \left(\delta_{k,q}\boldsymbol{M}_k^{(L,\omega)}+\int_0^{-\alpha}\boldsymbol{N}^{(L,\omega)}_{\gamma,q,k}\,d\gamma\right)d\alpha, \tag{59}$$

where, for any $k,q\in\{1,\dots,d\}$, $\gamma\in\mathbb{R}$, $\vartheta,\lambda\in\mathbb{R}_0^+$, $\omega\in\Omega$, and $L\in\mathbb{R}^+$,

$$\boldsymbol{M}_k^{(L,\omega)} \doteq \sum_{x,x+e_k\in\Lambda_L} 2\Re\mathrm{e}\{S^{(\omega)}_{x+e_k,x}\}, \tag{60}$$

$$\boldsymbol{N}^{(L,\omega)}_{\gamma,q,k} \doteq \sum_{\substack{x,y\in\Lambda_L\\ x+e_k,y+e_q\in\Lambda_L}} 4i\big[\mathrm{e}^{-i\gamma h^{(\omega)}}\,\Im\mathrm{m}\{S^{(\omega)}_{y+e_q,y}\}\,\mathrm{e}^{i\gamma h^{(\omega)}},\Im\mathrm{m}\{S^{(\omega)}_{x+e_k,x}\}\big], \tag{61}$$

with $S^{(\omega)}_{x,y}$ being the single-hopping operators defined by (33)–(34) for any $x,y\in\mathbb{Z}^d$.

The square of the Hilbert–Schmidt norm of $K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}$ is obviously equal to

$$\mathrm{Tr}_{\mathfrak{h}}\big(\big(K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\big)^*K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\big)=\sum_{z\in\mathbb{Z}^d}\big\|K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\mathfrak{e}_z\big\|^2_{\mathfrak{h}},$$

and, consequently, we derive an explicit expression for the vectors

$$K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\mathfrak{e}_z\in\mathfrak{h},\qquad z\in\mathbb{Z}^d.$$

This can be directly obtained from (59) together with the following assertion:

Lemma 4.5 (Explicit computations of $\boldsymbol{M}_k^{(L,\omega)}$ and $\boldsymbol{N}^{(L,\omega)}_{\gamma,q,k}$ in the canonical basis). *For all* $k,q\in\{1,\dots,d\}$, $\gamma\in\mathbb{R}$, $\vartheta,\lambda\in\mathbb{R}_0^+$, $\omega\in\Omega$, $\gamma\in\mathbb{R}$, $L\geq 2$, *and* $z\in\Lambda_{L/2}$,

$$\boldsymbol{M}_k^{(L,\omega)}\mathfrak{e}_z=\langle\mathfrak{e}_{z-e_k},\Delta_{\omega,\vartheta}\mathfrak{e}_z\rangle_{\mathfrak{h}}\,\mathfrak{e}_{z-e_k}+\langle\mathfrak{e}_{z+e_k},\Delta_{\omega,\vartheta}\mathfrak{e}_z\rangle_{\mathfrak{h}}\,\mathfrak{e}_{z+e_k},$$

and, in the limit $L\to\infty$,

$$\boldsymbol{N}^{(L,\omega)}_{\gamma,q,k}\mathfrak{e}_z=\sum_{x,y\in\mathbb{Z}^d}\zeta_{x,y,z}\mathfrak{e}_x+\boldsymbol{R}^{(L,\omega)}_{\gamma,q,k}\mathfrak{e}_z,\qquad \sum_{x,y\in\mathbb{Z}^d}|\zeta_{x,y,z}|^2<\infty,$$

with $\boldsymbol{R}^{(L,\omega)}_{\gamma,q,k}\in\mathcal{B}(\mathfrak{h})$ *satisfying*

$$\lim_{L\to\infty}\big\|\boldsymbol{R}^{(L,\omega)}_{\gamma,q,k}\big\|_{\mathcal{B}(\mathfrak{h})}=0, \tag{62}$$

uniformly with respect to $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, and ϑ, γ in compact subsets of $\mathbb{R}_0^+$ and $\mathbb{R}$, respectively, and where, for any $x, y, z \in \mathbb{Z}^d$,

$$\begin{aligned}
\zeta_{x,y,z} \doteq{}& i(1+\vartheta\omega_2(\{x-e_k,x\}))(1+\vartheta\omega_2(\{y,y+e_q\}))\langle \mathfrak{e}_{x-e_k}, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_y, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_z\rangle_{\mathfrak{h}} \\
&-i(1+\vartheta\omega_2(\{x-e_k,x\}))(1+\vartheta\overline{\omega_2(\{y+e_q,y\})})\langle \mathfrak{e}_{x-e_k}, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_z\rangle_{\mathfrak{h}} \\
&-i(1+\vartheta\overline{\omega_2(\{x+e_k,x\})})(1+\vartheta\omega_2(\{y,y+e_q\}))\langle \mathfrak{e}_{x+e_k}, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_y, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_z\rangle_{\mathfrak{h}} \\
&+i(1+\vartheta\overline{\omega_2(\{x+e_k,x\})})(1+\vartheta\overline{\omega_2(\{y+e_q,y\})})\langle \mathfrak{e}_{x+e_k}, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_z\rangle_{\mathfrak{h}} \\
&-i(1+\vartheta\omega_2(\{y,y+e_q\}))(1+\vartheta\omega_2(\{z,z+e_k\}))\langle \mathfrak{e}_{y}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_{z+e_k}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_x, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}} \\
&+i(1+\vartheta\omega_2(\{y,y+e_q\}))(1+\vartheta\overline{\omega_2(\{z,z-e_k\})})\langle \mathfrak{e}_{y}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_{z-e_k}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_x, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}} \\
&+i(1+\vartheta\overline{\omega_2(\{y+e_q,y\})})(1+\vartheta\omega_2(\{z,z+e_k\}))\langle \mathfrak{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_{z+e_k}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_x, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y}\rangle_{\mathfrak{h}} \\
&-i(1+\vartheta\overline{\omega_2(\{y+e_q,y\})})(1+\vartheta\overline{\omega_2(\{z,z-e_k\})})\langle \mathfrak{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_{z-e_k}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_x, \mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y}\rangle_{\mathfrak{h}}.
\end{aligned}$$

Proof. Fix in all the proof $k, q \in \{1, \ldots, d\}$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$, $\gamma \in \mathbb{R}$, $L \geq 2$, and $z \in \Lambda_{L/2}$. Since, by (33)–(34), for any $x, y \in \mathbb{Z}^d$, $2\Re\mathrm{e}\{S_{x,y}^{(\omega)}\} = \langle \mathfrak{e}_y, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}} P_{\{y\}} s_{y-x} P_{\{x\}} + \langle \mathfrak{e}_x, \Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}} P_{\{x\}} s_{x-y} P_{\{y\}}$, we deduce from (60) together with (28) and (33) that

$$\begin{aligned}
\boldsymbol{M}_k^{(L,\omega)}\mathfrak{e}_z &= \sum_{x,x+e_k\in\Lambda_L} (\delta_{z,x+e_k}\langle \mathfrak{e}_x, \Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}}\mathfrak{e}_x + \delta_{z,x}\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}}\mathfrak{e}_{x+e_k}) \\
&= \mathbf{1}[z\in\Lambda_L]\mathbf{1}[(z-e_k)\in\Lambda_L]\langle \mathfrak{e}_{z-e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_z\rangle_{\mathfrak{h}}\mathfrak{e}_{z-e_k} \\
&\qquad + \mathbf{1}[z\in\Lambda_L]\mathbf{1}[(z+e_k)\in\Lambda_L]\langle \mathfrak{e}_{z+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_z\rangle_{\mathfrak{h}}\mathfrak{e}_{z+e_k}.
\end{aligned}$$

If $z \in \Lambda_{L/2} \subseteq \Lambda_L$ and $L \geq 2$, then, obviously, $z, (z-e_k), (z+e_k) \in \Lambda_L$, and the last equality yields the first assertion.

By (33)–(34), for any $x, y \in \mathbb{Z}^d$, $2\Im\mathrm{m}\{S_{x,y}^{(\omega)}\} = i(\langle \mathfrak{e}_y, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}} P_{\{y\}} s_{y-x} P_{\{x\}} - \langle \mathfrak{e}_x, \Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}} P_{\{x\}} s_{x-y} P_{\{y\}})$, and we compute that, for any $x, y \in \mathbb{Z}^d$,

$$\begin{aligned}
&4i\big[\mathrm{e}^{-i\gamma h^{(\omega)}}\Im\mathrm{m}\{S_{y+e_q,y}^{(\omega)}\}\mathrm{e}^{i\gamma h^{(\omega)}}, \Im\mathrm{m}\{S_{x+e_k,x}^{(\omega)}\}\big] \\
&= i\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}}\langle \mathfrak{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}} s_{e_k} P_{\{x\}}\mathrm{e}^{-i\gamma h^{(\omega)}} s_{e_q} P_{\{y\}}\mathrm{e}^{i\gamma h^{(\omega)}} \\
&\quad - i\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}}\langle \mathfrak{e}_{y}, \Delta_{\omega,\vartheta}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}} s_{e_k} P_{\{x\}}\mathrm{e}^{-i\gamma h^{(\omega)}} s_{-e_q} P_{\{y+e_q\}}\mathrm{e}^{i\gamma h^{(\omega)}} \\
&\quad - i\langle \mathfrak{e}_{x}, \Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}} s_{-e_k} P_{\{x+e_k\}}\mathrm{e}^{-i\gamma h^{(\omega)}} s_{e_q} P_{\{y\}}\mathrm{e}^{i\gamma h^{(\omega)}} \\
&\quad + i\langle \mathfrak{e}_{x}, \Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_{y}, \Delta_{\omega,\vartheta}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}} s_{-e_k} P_{\{x+e_k\}}\mathrm{e}^{-i\gamma h^{(\omega)}} s_{-e_q} P_{\{y+e_q\}}\mathrm{e}^{i\gamma h^{(\omega)}} \\
&\quad - i\langle \mathfrak{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}}\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}}\mathrm{e}^{-i\gamma h^{(\omega)}} s_{e_q} P_{\{y\}}\mathrm{e}^{i\gamma h^{(\omega)}} s_{e_k} P_{\{x\}} \\
&\quad + i\langle \mathfrak{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}}\langle \mathfrak{e}_{x}, \Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}}\mathrm{e}^{-i\gamma h^{(\omega)}} s_{e_q} P_{\{y\}}\mathrm{e}^{i\gamma h^{(\omega)}} s_{-e_k} P_{\{x+e_k\}} \\
&\quad + i\langle \mathfrak{e}_{y}, \Delta_{\omega,\vartheta}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}}\mathrm{e}^{-i\gamma h^{(\omega)}} s_{-e_q} P_{\{y+e_q\}}\mathrm{e}^{i\gamma h^{(\omega)}} s_{e_k} P_{\{x\}} \\
&\quad - i\langle \mathfrak{e}_{y}, \Delta_{\omega,\vartheta}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle \mathfrak{e}_{x}, \Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}}\mathrm{e}^{-i\gamma h^{(\omega)}} s_{-e_q} P_{\{y+e_q\}}\mathrm{e}^{i\gamma h^{(\omega)}} s_{-e_k} P_{\{x+e_k\}}.
\end{aligned}$$

Using this last equality together with (33)–(34) and (61), we thus get that

$$\begin{aligned}
&\boldsymbol{N}_{\gamma,q,k}^{(L,\omega)}\mathfrak{e}_z \\
&= \sum_{\substack{x,y\in\Lambda_L\\ x+e_k,y+e_q\in\Lambda_L}} \Big\{ i\langle\mathfrak{e}_{x+e_k},\Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}}\langle\mathfrak{e}_{y+e_q},\Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}}\langle\mathfrak{e}_x,\mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle\mathfrak{e}_y,\mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_z\rangle_{\mathfrak{h}}\mathfrak{e}_{x+e_k} \\
&\qquad -i\langle\mathfrak{e}_{x+e_k},\Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}}\langle\mathfrak{e}_y,\Delta_{\omega,\vartheta}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle\mathfrak{e}_x,\mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_y\rangle_{\mathfrak{h}}\langle\mathfrak{e}_{y+e_q},\mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_z\rangle_{\mathfrak{h}}\mathfrak{e}_{x+e_k} \\
&\qquad -i\langle\mathfrak{e}_x,\Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle\mathfrak{e}_{y+e_q},\Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}}\langle\mathfrak{e}_{x+e_k},\mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle\mathfrak{e}_y,\mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_z\rangle_{\mathfrak{h}}\mathfrak{e}_x \\
&\qquad +i\langle\mathfrak{e}_x,\Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle\mathfrak{e}_y,\Delta_{\omega,\vartheta}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle\mathfrak{e}_{x+e_k},\mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_y\rangle_{\mathfrak{h}}\langle\mathfrak{e}_{y+e_q},\mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_z\rangle_{\mathfrak{h}}\mathfrak{e}_x \\
&\qquad -i\delta_{x,z}\langle\mathfrak{e}_{y+e_q},\Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}}\langle\mathfrak{e}_{x+e_k},\Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}}\langle\mathfrak{e}_y,\mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}}\,\mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y+e_q} \\
&\qquad +i\delta_{x+e_k,z}\langle\mathfrak{e}_{y+e_q},\Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}}\langle\mathfrak{e}_x,\Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle\mathfrak{e}_y,\mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_x\rangle_{\mathfrak{h}}\,\mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y+e_q} \\
&\qquad +i\delta_{x,z}\langle\mathfrak{e}_y,\Delta_{\omega,\vartheta}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle\mathfrak{e}_{x+e_k},\Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}}\langle\mathfrak{e}_{y+e_q},\mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}}\,\mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_y \\
&\qquad -i\delta_{x+e_k,z}\langle\mathfrak{e}_y,\Delta_{\omega,\vartheta}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle\mathfrak{e}_x,\Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}}\langle\mathfrak{e}_{y+e_q},\mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_x\rangle_{\mathfrak{h}}\,\mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_y\Big\}.
\end{aligned}$$

By using (2) and (42)–(43) together with

$$\sum_{z\in\mathbb{Z}^d}\mathrm{e}^{-2\mu_\eta(|x-z|+|y-z|)}\leq \mathrm{e}^{-\mu_\eta|x-y|}\sum_{z\in\mathbb{Z}^d}\mathrm{e}^{-\mu_\eta(|x-z|+|y-z|)}\leq \mathrm{e}^{-\mu_\eta|x-y|}\sum_{z\in\mathbb{Z}^d}\mathrm{e}^{-2\mu_\eta|z|},$$

which are simple consequences of the Cauchy–Schwarz and triangle inequalities, all the above summands are absolutely summable, uniformly with respect to $L\in\mathbb{R}^+$, $\omega\in\Omega$, $\lambda\in\mathbb{R}_0^+$, and ϑ, γ in compact subsets of $\mathbb{R}_0^+$ and $\mathbb{R}$, respectively. For instance, for any (characteristic) functions $f, g:\mathbb{Z}^d\to\{0,1\}$, one estimates

$$\begin{aligned}
&\sum_{x,y\in\mathbb{Z}^d} f(x)^2g(y)^2\left|\langle\mathfrak{e}_{x+e_k},\Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}}\langle\mathfrak{e}_{y+e_q},\Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}}\langle\mathfrak{e}_x,\mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}}\langle\mathfrak{e}_y,\mathrm{e}^{i\gamma h^{(\omega)}}\mathfrak{e}_z\rangle_{\mathfrak{h}}\right|\|\mathfrak{e}_{x+e_k}\|_{\mathfrak{h}} \\
&\quad\leq 36^2(1+\vartheta)^2\,\mathrm{e}^{2|\gamma\eta|}\sum_{x,y\in\mathbb{Z}^d} f(x)^2g(y)^2\,\mathrm{e}^{-2\mu_\eta(|x-e_q-y|+|z-y|)} \\
&\quad\leq 36^2(1+\vartheta)^2\,\mathrm{e}^{2|\gamma\eta|}\left(\sum_{u\in\mathbb{Z}^d} g(u+z)^2\,\mathrm{e}^{-2\mu_\eta|u|}\right)^{1/2} \\
&\qquad\qquad\times\sum_{x\in\mathbb{Z}^d} f(x)^2\,\mathrm{e}^{-\mu_\eta|x-e_q-z|}\left(\sum_{y\in\mathbb{Z}^d} g(y+x-e_q)^2\,\mathrm{e}^{-2\mu_\eta|y|}\right)^{1/2}<\infty.
\end{aligned}$$

(Recall that $\mu_\eta>0$, by (43).) In fact, by the same arguments combined with

$$\|C\|_{\mathcal{B}(\mathfrak{h})}\leq\sup_{x\in\mathbb{Z}^d}\sum_{z\in\mathbb{Z}^d}|\langle\mathfrak{e}_x,C\mathfrak{e}_z\rangle_{\mathfrak{h}}|,\qquad C\in\mathcal{B}(\mathfrak{h}),$$

(see [Aza et al. 2019, Lemma 4.1]), the absolutely summable sum

$$\mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_w=\sum_{u\in\mathbb{Z}^d}\mathfrak{e}_u\langle\mathfrak{e}_u,\mathrm{e}^{-i\gamma h^{(\omega)}}\mathfrak{e}_w\rangle_{\mathfrak{h}},\qquad w\in\mathbb{Z}^d, \tag{63}$$

(see (42)–(43)) and Lebesgue's dominated convergence theorem, in the limit $L\to\infty$ and for any $z\in\Lambda_{L/2}$, there is an operator $\boldsymbol{R}_{\gamma,q,k}^{(L,\omega)}\in\mathcal{B}(\mathfrak{h})$ with vanishing operator norm as $L\to\infty$, uniformly with respect to

$\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, and ϑ, γ in compact subsets of $\mathbb{R}_0^+$ and $\mathbb{R}$, respectively, such that

$$\boldsymbol{N}_{\gamma,q,k}^{(L,\omega)} \mathfrak{e}_z = \big(\boldsymbol{N}_{\gamma,q,k}^{(\infty,\omega)} + \boldsymbol{R}_{\gamma,q,k}^{(L,\omega)}\big)\mathfrak{e}_z,$$

where

$$\begin{aligned}
\boldsymbol{N}_{\gamma,q,k}^{(\infty,\omega)} \mathfrak{e}_z \doteq \sum_{x,y\in\mathbb{Z}^d} \Big\{ & i\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}} \langle \mathfrak{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}}, \langle \mathfrak{e}_x, \mathrm{e}^{-i\gamma h^{(\omega)}} \mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}} \langle \mathfrak{e}_y, \mathrm{e}^{i\gamma h^{(\omega)}} \mathfrak{e}_z\rangle_{\mathfrak{h}} \mathfrak{e}_{x+e_k} \\
& -i\langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}} \langle \mathfrak{e}_y, \Delta_{\omega,\vartheta}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}} \langle \mathfrak{e}_x, \mathrm{e}^{-i\gamma h^{(\omega)}} \mathfrak{e}_y\rangle_{\mathfrak{h}} \langle \mathfrak{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}} \mathfrak{e}_z\rangle_{\mathfrak{h}} \mathfrak{e}_{x+e_k} \\
& -i\langle \mathfrak{e}_x, \Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}} \langle \mathfrak{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}} \langle \mathfrak{e}_{x+e_k}, \mathrm{e}^{-i\gamma h^{(\omega)}} \mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}} \langle \mathfrak{e}_y, \mathrm{e}^{i\gamma h^{(\omega)}} \mathfrak{e}_z\rangle_{\mathfrak{h}} \mathfrak{e}_x \\
& +i\langle \mathfrak{e}_x, \Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}} \langle \mathfrak{e}_y, \Delta_{\omega,\vartheta}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}} \langle \mathfrak{e}_{x+e_k}, \mathrm{e}^{-i\gamma h^{(\omega)}} \mathfrak{e}_y\rangle_{\mathfrak{h}} \langle \mathfrak{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}} \mathfrak{e}_z\rangle_{\mathfrak{h}} \mathfrak{e}_x \\
& -i\delta_{x,z}\langle \mathfrak{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}} \langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}} \langle \mathfrak{e}_y, \mathrm{e}^{i\gamma h^{(\omega)}} \mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}} \,\mathrm{e}^{-i\gamma h^{(\omega)}} \mathfrak{e}_{y+e_q} \\
& +i\delta_{x+e_k,z}\langle \mathfrak{e}_{y+e_q}, \Delta_{\omega,\vartheta}\mathfrak{e}_y\rangle_{\mathfrak{h}} \langle \mathfrak{e}_x, \Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}} \langle \mathfrak{e}_y, \mathrm{e}^{i\gamma h^{(\omega)}} \mathfrak{e}_x\rangle_{\mathfrak{h}} \,\mathrm{e}^{-i\gamma h^{(\omega)}} \mathfrak{e}_{y+e_q} \\
& +i\delta_{x,z}\langle \mathfrak{e}_y, \Delta_{\omega,\vartheta}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}} \langle \mathfrak{e}_{x+e_k}, \Delta_{\omega,\vartheta}\mathfrak{e}_x\rangle_{\mathfrak{h}} \langle \mathfrak{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}} \mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}} \,\mathrm{e}^{-i\gamma h^{(\omega)}} \mathfrak{e}_y \\
& -i\delta_{x+e_k,z}\langle \mathfrak{e}_y, \Delta_{\omega,\vartheta}\mathfrak{e}_{y+e_q}\rangle_{\mathfrak{h}} \langle \mathfrak{e}_x, \Delta_{\omega,\vartheta}\mathfrak{e}_{x+e_k}\rangle_{\mathfrak{h}} \langle \mathfrak{e}_{y+e_q}, \mathrm{e}^{i\gamma h^{(\omega)}} \mathfrak{e}_x\rangle_{\mathfrak{h}} \,\mathrm{e}^{-i\gamma h^{(\omega)}} \mathfrak{e}_y \Big\}.
\end{aligned}$$

It suffices now to use again (2) and (63) together with elementary manipulations in each sum of $\boldsymbol{N}_{\gamma,q,k}^{(\infty,\omega)}$ in order to arrive at the second assertion. □

We are now in a position to show (57), at least for $|\gamma|, \vartheta \ll 1$, as a consequence of the next two lemmata:

Lemma 4.6 (Asymptotics for $\vartheta \ll 1$). *For all $k, q \in \{1, \ldots, d\}$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$, $\gamma \in \mathbb{R}$, and $z \in \mathbb{Z}^d$,*

$$\sum_{y\in\mathbb{Z}^d} \zeta_{z,y,z} = 2\Im\mathrm{m}\langle (s_{e_k} - s_{-e_k})\mathfrak{e}_z, \mathrm{e}^{-i\gamma h^{(\omega)}} (s_{e_q} - s_{-e_q})\, \mathrm{e}^{i\gamma h^{(\omega)}} \mathfrak{e}_z\rangle_{\mathfrak{h}} + \mathcal{O}(\vartheta), \quad \text{as } \vartheta \to 0,$$

uniformly with respect to $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and γ in compact subsets of $\mathbb{R}$. Note that ϑ is not necessarily 0 in the definition of $h^{(\omega)}$.

Proof. By Lemma 4.5 at $\vartheta = 0$, one directly computes that, for any $k, q \in \{1, \ldots, d\}$, $\lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$, $\gamma \in \mathbb{R}$, $z \in \mathbb{Z}^d$, and $\vartheta = 0$,

$$\sum_{y\in\mathbb{Z}^d} \zeta_{z,y,z} = \sum_{y\in\mathbb{Z}^d} 2\Im\mathrm{m}\langle \mathfrak{e}_{z+e_k} - \mathfrak{e}_{z-e_k}, \mathrm{e}^{-i\gamma h^{(\omega)}} (\mathfrak{e}_{y+e_q} - \mathfrak{e}_{y-e_q})\rangle_{\mathfrak{h}} \langle \mathfrak{e}_y, \mathrm{e}^{i\gamma h^{(\omega)}} \mathfrak{e}_z\rangle_{\mathfrak{h}}\,.$$

If $\vartheta \neq 0$, then one performs the same kind of computation in order to (trivially) deduce the assertion, by (33), Lemma 4.5, and (42)–(43). □

Lemma 4.7 (Asymptotics for $|\gamma| \ll 1$). *For all $k, q \in \{1, \ldots, d\}$, $\vartheta, \lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$, $\gamma \in \mathbb{R}$, and $z \in \mathbb{Z}^d$,*

$$\begin{aligned}
&2\Im\mathrm{m}\langle (s_{e_k} - s_{-e_k})\mathfrak{e}_z, \mathrm{e}^{-i\gamma h^{(\omega)}} (s_{e_q} - s_{-e_q})\, \mathrm{e}^{i\gamma h^{(\omega)}} \mathfrak{e}_z\rangle_{\mathfrak{h}} \\
&\qquad = 2\gamma\lambda\delta_{k,q}\{2\omega_1(z) - \omega_1(z+e_k) - \omega_1(z-e_k)\} + \mathcal{O}(\gamma^2),
\end{aligned}$$

as $|\gamma| \to 0$, uniformly with respect to $\omega \in \Omega$ and ϑ, λ in compact subsets of $\mathbb{R}_0^+$.

Proof. By (58), for any $\gamma \in \mathbb{R}$,

$$\mathrm{e}^{i\gamma h^{(\omega)}} = \mathbf{1}_{\mathfrak{h}} + \sum_{n\in\mathbb{N}} \frac{(i\gamma h^{(\omega)})^n}{n!} = \mathbf{1}_{\mathfrak{h}} + i\gamma h^{(\omega)} + \mathcal{O}(\gamma^2), \quad \text{as } |\gamma| \to 0,$$

in the Banach space $\mathcal{B}(\mathfrak{h})$, uniformly with respect to $\omega \in \Omega$ and ϑ, λ in compact subsets of $\mathbb{R}_0^+$. The assertion then follows by direct computations using (2)–(3), (33), and the last equality. □

Lemma 4.8 (Lower bounds on the Hilbert–Schmidt norm of $K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}$). *Take $\vartheta, \lambda, T \in \mathbb{R}_0^+$, $T \in \mathbb{R}^+$, $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$ with support in $[-T, 0]$, and $\vec{w} \doteq (w_1, \ldots, w_d) \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$. If T, ϑ are sufficiently small, then*

$$\lim_{L\to\infty} \frac{1}{|\Lambda_L|} \mathbb{E}\big[\mathrm{Tr}_{\mathfrak{h}}\big(\big(K^{(\cdot,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\big)^* K^{(\cdot,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\big)\big] \geq \frac{\lambda^2}{2} \mathrm{Var}\bigg[\int_{-\infty}^0 \langle w^{(\cdot)}, \mathcal{E}(\alpha)\rangle_{\mathbb{R}^d} \alpha^2\, d\alpha\bigg] + \mathcal{O}(\vartheta^2) + \mathcal{O}(T^4),$$

uniformly with respect to λ in compact subsets of $\mathbb{R}_0^+$, where $w^{(\cdot)} \doteq (w_1^{(\cdot)}, \ldots, w_d^{(\cdot)}) \in \mathbb{R}^d$ is the random vector defined by

$$w_k^{(\omega)} \doteq (2\omega_1(0) - \omega_1(e_k) - \omega_1(-e_k))w_k, \quad k \in \{1, \ldots, d\}, \omega \in \Omega. \tag{64}$$

Proof. Fix all parameters of the lemma. Take any $L \geq 2$. Note that

$$\mathrm{Tr}_{\mathfrak{h}}\big(\big(K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\big)^* K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\big) \geq \sum_{z\in\Lambda_{L/2}} \big\| K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \mathfrak{e}_z \big\|_{\mathfrak{h}}^2 \geq \sum_{z\in\Lambda_{L/2}} \big|\langle \mathfrak{e}_z, K^{(\omega,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \mathfrak{e}_z\rangle_{\mathfrak{h}}\big|^2. \tag{65}$$

By using (59)–(61) and Lemma 4.5, for any $z \in \Lambda_{L/2}$, we have that

$$\langle \mathfrak{e}_z, K^{(\cdot,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \mathfrak{e}_z\rangle_{\mathfrak{h}} = \sum_{k,q=1}^d w_k \int_{-\infty}^0 \{\mathcal{E}(\alpha)\}_q \int_0^{-\alpha} \sum_{y\in\mathbb{Z}^d} \zeta_{z,y,z}\, d\gamma\, d\alpha + \sum_{k,q=1}^d w_k \int_{-\infty}^0 \{\mathcal{E}(\alpha)\}_q \int_0^{-\alpha} \langle \mathfrak{e}_z, \boldsymbol{R}^{(L,\omega)}_{\gamma,q,k} \mathfrak{e}_z\rangle_{\mathfrak{h}}\, d\gamma\, d\alpha,$$

with $\boldsymbol{R}^{(L,\omega)}_{\gamma,q,k} \in \mathcal{B}(\mathfrak{h})$ satisfying (62). Note that $\zeta_{z,y,z}$ is γ-dependent, and its explicit expression is found in Lemma 4.5. If T, ϑ are sufficiently small then, by Lemmata 4.6–4.7, we deduce that, for any $z \in \Lambda_{L/2}$,

$$\langle \mathfrak{e}_z, K^{(\cdot,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}} \mathfrak{e}_z\rangle_{\mathfrak{h}} = \lambda \sum_{k=1}^d w_k \int_{-\infty}^0 \{2\omega_1(z) - \omega_1(z+e_k) - \omega_1(z-e_k)\}\{\mathcal{E}(\alpha)\}_k \alpha^2\, d\alpha + \mathcal{O}(\vartheta) + \mathcal{O}(T^2) + \sum_{k,q=1}^d w_k \int_{-\infty}^0 \{\mathcal{E}(\alpha)\}_q \int_0^{-\alpha} \langle \mathfrak{e}_z, \boldsymbol{R}^{(L,\omega)}_{\gamma,q,k} \mathfrak{e}_z\rangle_{\mathfrak{h}}\, d\gamma\, d\alpha,$$

uniformly with respect to $\omega \in \Omega$ and λ in compact subsets of $\mathbb{R}_0^+$. By the translation invariance of the distribution $\mathfrak{a}_\Omega$ (see [Aza et al. 2019, Equations (1)–(2)]) and (62), it follows that

$$\lim_{L\to\infty} \mathbb{E}\Big[\big|\langle \mathfrak{e}_z, K^{(\,\cdot\,,\mathcal{E})}_{\{\Lambda_L\},\{\mathbb{Z}^d\}}\mathfrak{e}_z\rangle_{\mathfrak{h}}\big|^2\Big] = \lambda^2 \mathbb{E}\left[\left|\int_{-\infty}^0 \langle w^{(\,\cdot\,)}, \mathcal{E}(\alpha)\rangle_{\mathbb{R}^d}\alpha^2\,d\alpha\right|^2\right] + \mathcal{O}(\vartheta^2) + \mathcal{O}(T^4)$$
$$= \lambda^2 \operatorname{Var}\Big[\int_{-\infty}^0 \langle w^{(\,\cdot\,)}, \mathcal{E}(\alpha)\rangle_{\mathbb{R}^d}\alpha^2\,d\alpha\Big] + \mathcal{O}(\vartheta^2) + \mathcal{O}(T^4),$$

uniformly with respect to λ in compact subsets of $\mathbb{R}_0^+$. Thanks to (65), the assertion then follows. Note that

$$\mathbb{E}\left[\int_{-\infty}^0 \langle w^{(\,\cdot\,)}, \mathcal{E}(\alpha)\rangle_{\mathbb{R}^d}\alpha^2\,d\alpha^2\right] = 0. \qquad \square$$

By combining Lemmata 4.4, 4.8, and 4.3, we directly obtain that, for any $\vartheta, \lambda, T \in \mathbb{R}_0^+$, $T, \beta \in \mathbb{R}^+$, $\mathcal{E} \in C_0^0(\mathbb{R}; \mathbb{R}^d)$ with support in $[-T, 0]$, and $\vec{w} \in \mathbb{R}^d$ with $\|\vec{w}\|_{\mathbb{R}^d} = 1$,

$$\partial_s^2\, \mathrm{J}^{(s\mathcal{E})}\,|_{s=0} \geq \frac{1}{2\big(1+\mathrm{e}^{\beta(2d(2+\vartheta)+\lambda)}\big)^2}\left(\lambda^2 \operatorname{Var}\left[\int_{-\infty}^0 \langle w^{(\,\cdot\,)}, \mathcal{E}(\alpha)\rangle_{\mathbb{R}^d}\alpha^2\,d\alpha\right] + \mathcal{O}(\vartheta^2) + \mathcal{O}(T^4)\right), \tag{66}$$

provided that T, ϑ are sufficiently small. In particular, if

$$\operatorname{Var}\left[\int_{-\infty}^0 \langle w^{(\,\cdot\,)}, \mathcal{E}(\alpha)\rangle_{\mathbb{R}^d}\alpha^2\,d\alpha\right] > 0, \tag{67}$$

then $\partial_s^2\, \mathrm{J}^{(s\mathcal{E})}\,|_{s=0} > 0$. This last condition is easily satisfied: Because the variance of the sum (or the difference) of uncorrelated random variables is the sum of their variances, if the random variables $\omega_1(0), \omega_1(e_1), \omega_1(-e_1), \ldots, \omega_1(e_d), \omega_1(-e_d)$ are independently and identically distributed (i.i.d.), then

$$\mathbb{E}\left[\left|\int_{-\infty}^0 \langle w^{(\omega)}, \mathcal{E}(\alpha)\rangle_{\mathbb{R}^d}\alpha^2\,d\alpha\right|^2\right] = 2\operatorname{Var}[(\,\cdot\,)_1(0)] \times \left(2\left(\int_{-\infty}^0 \langle w, \mathcal{E}(\alpha)\rangle_{\mathbb{R}^d}\alpha^2\,d\alpha\right)^2 + \sum_{k=1}^d \left(w_k \int_{-\infty}^0 (\mathcal{E}(\alpha))_k \alpha^2\,d\alpha\right)^2\right), \tag{68}$$

which is strictly positive as soon as $\mathcal{E} \neq 0$ and $\omega_1(0)$ is not almost surely constant, by Chebyshev's inequality.

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References

[Araki 1970/71] H. Araki, "On quasifree states of CAR and Bogoliubov automorphisms", *Publ. Res. Inst. Math. Sci.* **6** (1970/71), 385–442. MR Zbl

[Aza et al. 2017] N. J. B. Aza, J.-B. Bru, W. de Siqueira Pedra, and L. C. P. A. M. Müssnich, "Large deviations in weakly interacting fermions I - generating functions as Gaussian Berezin integrals and bounds on large pfaffians", preprint, 2017, available at https://web.ma.utexas.edu/mp_arc/c/17/17-70.pdf.

[Aza et al. 2019] N. J. B. Aza, J.-B. Bru, W. de Siqueira Pedra, and A. Ratsimanetrimanana, "Accuracy of classical conductivity theory at atomic scales for free fermions in disordered media", *J. Math. Pures Appl.* (9) **125** (2019), 209–246. MR Zbl

[Bellissard et al. 1994] J. Bellissard, A. van Elst, and H. Schulz-Baldes, "The noncommutative geometry of the quantum Hall effect", *J. Math. Phys.* **35**:10 (1994), 5373–5451. MR Zbl

[Bouclet et al. 2005] J.-M. Bouclet, F. Germinet, A. Klein, and J. H. Schenker, "Linear response theory for magnetic Schrödinger operators in disordered media", *J. Funct. Anal.* **226**:2 (2005), 301–372. MR Zbl

[Bratteli and Robinson 1997] O. Bratteli and D. W. Robinson, *Operator algebras and quantum statistical mechanics. 2*, 2nd ed., Texts and Monographs in Physics, Springer, Berlin, 1997. MR Zbl

[Bru and de Siqueira Pedra 2015a] J.-B. Bru and W. de Siqueira Pedra, "From the second law of thermodynamics to AC-conductivity measures of interacting fermions in disordered media", *Math. Models Methods Appl. Sci.* **25**:14 (2015), 2587–2632. MR Zbl

[Bru and de Siqueira Pedra 2015b] J.-B. Bru and W. de Siqueira Pedra, "Microscopic foundations of Ohm and Joule's laws—the relevance of thermodynamics", pp. 151–163 in *Mathematical results in quantum mechanics* (Berlin, 2013), edited by P. Exner et al., World Sci. Publ., Hackensack, NJ, 2015. MR Zbl

[Bru and de Siqueira Pedra 2016] J.-B. Bru and W. de Siqueira Pedra, "Microscopic conductivity of lattice fermions at equilibrium. Part II: Interacting particles", *Lett. Math. Phys.* **106**:1 (2016), 81–107. MR Zbl

[Bru and de Siqueira Pedra 2017a] J.-B. Bru and W. de Siqueira Pedra, *Lieb–Robinson bounds for multi-commutators and applications to response theory*, SpringerBriefs in Mathematical Physics **13**, Springer, Cham, 2017. MR Zbl

[Bru and de Siqueira Pedra 2017b] J.-B. Bru and W. de Siqueira Pedra, "Universal bounds for large determinants from non-commutative Hölder inequalities in fermionic constructive quantum field theory", *Math. Models Methods Appl. Sci.* **27**:10 (2017), 1963–1992. MR Zbl

[Bru et al. 2014] J.-B. Bru, W. de Siqueira Pedra, and C. Hertling, "Macroscopic conductivity of free fermions in disordered media", *Rev. Math. Phys.* **26**:5 (2014), 1450008, 25. MR Zbl

[Bru et al. 2015a] J.-B. Bru, W. de Siqueira Pedra, and C. Hertling, "Heat production of noninteracting fermions subjected to electric fields", *Comm. Pure Appl. Math.* **68**:6 (2015), 964–1013. MR Zbl

[Bru et al. 2015b] J.-B. Bru, W. de Siqueira Pedra, and C. Hertling, "Microscopic conductivity of lattice fermions at equilibrium. I. Non-interacting particles", *J. Math. Phys.* **56**:5 (2015), 051901, 51. MR Zbl

[Bru et al. 2016] J.-B. Bru, W. de Siqueira Pedra, and C. Hertling, "AC-conductivity measure from heat production of free fermions in disordered media", *Arch. Ration. Mech. Anal.* **220**:2 (2016), 445–504. MR Zbl

[Brynildsen and Cornean 2013] M. H. Brynildsen and H. D. Cornean, "On the Verdet constant and Faraday rotation for graphene-like materials", *Rev. Math. Phys.* **25**:4 (2013), 1350007, 28. MR Zbl

[Dembo and Zeitouni 1998] A. Dembo and O. Zeitouni, *Large deviations techniques and applications*, 2nd ed., Applications of Mathematics (New York) **38**, Springer, New York, 1998. MR Zbl

[Deuschel and Stroock 1989] J.-D. Deuschel and D. W. Stroock, *Large deviations*, Pure and Applied Mathematics **137**, Academic Press, Boston, 1989. MR Zbl

[Dombrowski and Germinet 2008] N. Dombrowski and F. Germinet, "Linear response theory for random Schrödinger operators and noncommutative integration", *Markov Process. Related Fields* **14**:3 (2008), 403–426. MR Zbl

[Ferry 2012] D. K. Ferry, "Ohm's law in a quantum world", *Science* **335**:6064 (2012), 45–46.

[Goderis et al. 1989a] D. Goderis, A. Verbeure, and P. Vets, "About the mathematical theory of quantum fluctuations", pp. 31–47 in *Mathematical methods in statistical mechanics*, edited by M. Fannes and A. Verbeure, Leuven Notes Math. Theoret. Phys. Ser. A Math. Phys. **1**, Leuven Univ. Press, 1989. MR Zbl

[Goderis et al. 1989b] D. Goderis, A. Verbeure, and P. Vets, "Noncommutative central limits", *Probab. Theory Related Fields* **82**:4 (1989), 527–544. MR Zbl

[Goderis et al. 1989c] D. Goderis, A. Verbeure, and P. Vets, "Theory of quantum fluctuations and the Onsager relations", *J. Statist. Phys.* **56**:5–6 (1989), 721–746. MR

[Goderis et al. 1990a] D. Goderis, A. Verbeure, and P. Vets, "Dynamics of fluctuations for quantum lattice systems", *Comm. Math. Phys.* **128**:3 (1990), 533–549. MR Zbl

[Goderis et al. 1990b] D. Goderis, A. Verbeure, and P. Vets, "Quantum central limit and coarse graining", pp. 178–193 in *Quantum probability and applications, V*, edited by L. Accardi and W. von Waldenfels, Lecture Notes in Math. **1442**, Springer, Berlin, 1990. MR Zbl

[Goderis et al. 1991] D. Goderis, A. Verbeure, and P. Vets, "About the exactness of the linear response theory", *Comm. Math. Phys.* **136**:2 (1991), 265–283. MR Zbl

[Klein and Müller 2008] A. Klein and P. Müller, "The conductivity measure for the Anderson model", *Zh. Mat. Fiz. Anal. Geom.* **4**:1 (2008), 128–150. MR Zbl

[Klein and Müller 2015] A. Klein and P. Müller, "AC-conductivity and electromagnetic energy absorption for the Anderson model in linear response theory", *Markov Process. Related Fields* **21**:3, part 1 (2015), 575–590. MR

[Klein et al. 2007] A. Klein, O. Lenoble, and P. Müller, "On Mott's formula for the ac-conductivity in the Anderson model", *Ann. of Math.* (2) **166**:2 (2007), 549–577. MR Zbl

[Pillet 2006] C.-A. Pillet, "Quantum dynamical systems", pp. 107–182 in *Open quantum systems. I*, edited by S. Attal et al., Lecture Notes in Math. **1880**, Springer, Berlin, 2006. MR Zbl

[Prodan 2013] E. Prodan, "Quantum transport in disordered systems under magnetic fields: a study based on operator algebras", *Appl. Math. Res. Express. AMRX* **2013**:2 (2013), 176–265. MR Zbl

[Ratsimanetrimanana 2019] A. Ratsimanetrimanana, *Equilibrium and transport properties of quantum many-body systems*, Ph.D. thesis, Universidad del País Vasco, 2019, available at http://hdl.handle.net/20.500.11824/1037.

[Rudin 1991] W. Rudin, *Functional analysis*, Second ed., International Series in Pure and Applied Mathematics, McGraw-Hill, New York, 1991. MR Zbl

[Schulz-Baldes and Bellissard 1998] H. Schulz-Baldes and J. Bellissard, "A kinetic theory for quantum transport in aperiodic media", *J. Statist. Phys.* **91**:5-6 (1998), 991–1026. MR Zbl

[Verbeure 2011] A. F. Verbeure, *Many-body boson systems*, Theoretical and Mathematical Physics, Springer, London, 2011. MR Zbl

[Weber et al. 2012] B. Weber, S. Mahapatra, H. Ryu, S. Lee, A. Fuhrer, T. C. G. Reusch, D. L. Thompson, W. C. T. Lee, G. Klimeck, L. C. L. Hollenberg, and M. Y. Simmons, "Ohm's law survives to the atomic scale", *Science* **335**:6064 (2012), 64–67.

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Guidelines for Authors

Authors may submit manuscripts in PDF format on-line at the submission page.

Originality. Submission of a manuscript acknowledges that the manuscript is original and and is not, in whole or in part, published or under consideration for publication elsewhere. It is understood also that the manuscript will not be submitted elsewhere while under consideration for publication in this journal.

Language. Articles are usually in English or French, but articles written in other languages are welcome.

Required items. A brief abstract of about 150 words or less must be included. It should be self-contained and not refer to bibliography keys. If the article is not in English, two versions of the abstract must be included, one in the language of the article and one in English. Also required are keywords and a Mathematics Subject Classification for the article, and, for each author, affiliation (if appropriate) and email address.

Format. Authors are encouraged to use LaTeX and the standard amsart class, but submissions in other varieties of TeX, and exceptionally in other formats, are acceptable. Initial uploads should normally be in PDF format; after the refereeing process we will ask you to submit all source material.

References. Bibliographical references should be complete, including article titles and page ranges. All references in the bibliography should be cited in the text. The use of BibTeX is preferred but not required. Tags will be converted to the house format, however, for submission you may use the format of your choice. Links will be provided to all literature with known web locations and authors are encouraged to provide their own links in addition to those supplied in the editorial process.

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Most drawing and graphing packages — Mathematica, Adobe Illustrator, Corel Draw, MATLAB, etc. — allow the user to save files in one of these formats. Make sure that what you are saving is vector graphics and not a bitmap. If you need help, please write to graphics@msp.org with as many details as you can about how your graphics were generated.

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