PURE and APPLIED ANALYSIS

PAA

msp

vol. 1 no. 2 2019

PURE and APPLIED ANALYSIS

msp.org/paa

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.

See inside back cover or msp.org/paa for submission instructions.

The subscription price for 2019 is US $495/year for the electronic version, and $555/year (+$25, if shipping outside the US) for print and electronic. Subscriptions, requests for back issues and changes of subscriber address should be sent to MSP.

Pure and Applied Analysis (ISSN 2578-5885 electronic, 2578-5893 printed) at Mathematical Sciences Publishers, 798 Evans Hall #3840, c/o University of California, Berkeley, CA 94720-3840 is published continuously online. Periodical rate postage paid at Berkeley, CA 94704, and additional mailing offices.

PAA peer review and production are managed by EditFlow® from MSP.

PUBLISHED BY

mathematical sciences publishers

nonprofit scientific publishing

http://msp.org/

PURE and APPLIED
ANALYSIS

Vol. 1, No. 2, 2019
dx.doi.org/10.2140/paa.2019.1.149

ABOUT SMALL EIGENVALUES OF THE WITTEN LAPLACIAN

LAURENT MICHEL

We study the low-lying eigenvalues of the semiclassical Witten Laplacian associated to a Morse function φ. Compared to previous works we allow general distributions of critical values of φ, for instance allowing all the local minima to be absolute. The motivation comes from metastable dynamics described by the Kramers–Smoluchowski equation.

1. Introduction

1A. ***Motivation.*** The Witten Laplacian, Δ_φ was introduced by Witten [1982] to give an analytic proof of Morse inequalities. Its study led to many mathematical developments, most notably the Helffer–Sjöstrand theory [1985] of potential wells in the semiclassical limit. It is defined by twisting the operator d (acting on forms) by a Morse function φ:

$$\Delta_\varphi := d_\varphi^* d_\varphi + d_\varphi d_\varphi^*, \quad d_\varphi := e^{-\varphi/h} h d e^{\varphi/h}. \tag{1-1}$$

It takes a simple form on functions and for the Euclidean metric on $\mathbb{R}^d$ we then have

$$\Delta_\varphi = -h^2\Delta + |\partial_x\varphi|^2 - h\Delta\varphi. \tag{1-2}$$

Even in that case using the action on 1-forms is highly beneficial — see [Michel and Zworski 2018] for an introduction in the simple one-dimensional setting.

MSC2010: 35P20.
Keywords: metastability, semiclassical analysis.

More recently the Witten Laplacian appeared in quantitative studies of metastability for kinetic equations — see for instance [Hérau and Nier 2004; Helffer, Klein and Nier 2004; Hérau, Hitrik and Sjöstrand 2011; Di Gesù, Lelièvre, Le Peutrec and Nectoux 2017].

Other interesting developments also include connecting the "Arrhenius rates" (exponential widths S of small eigenvalues λ_h in (1-8)) with barcodes of the Morse–Barannikov complex in [Le Peutrec, Nier and Viterbo 2013] and showing that (in the case of compact manifolds) the eigenvalues of the Witten Laplacian converge, as $h \to 0$, to the Ruelle resonances of the gradient flow of φ in [Dang and Rivière 2017].

This paper continues the study of the Witten Laplacian by considering functions φ with *general* distributions on critical values, in particular functions with several equal minima and equal values at saddle points. (In works related to Morse theory it is natural to assume that all critical values are distinct.) As emphasized in [Michel and Zworski 2018] such functions lead to interesting effective dynamics for the Kramers–Smoluchowski equation (1-6) — see Figure 2 and Section 1B. This, and more general situations in which equal critical values are allowed (see Figure 4 for a schematic illustration of an allowed landscape), leads to new subtle difficulties.

To explain metastable dynamics consider a particle evolving in an energy landscape φ and submitted to random forces. The position X_t of such a particle at time t satisfies the over-damped Langevin equation

$$\dot{X}_t = -2\nabla\varphi(X_t) + \sqrt{2h}\,\dot{B}_t, \tag{1-3}$$

where h is the temperature of the system and B_t is a Brownian force. This equation appears for instance in physics to describe the microscopic evolution of a charged gas assuming the mass of the particles is negligible.

Assuming that the potential φ has several wells, a particle starting at a local minimum of the function φ can, due to the presence of the random force, move over a saddle point and reach another energy well — see Figure 1 for a schematic illustration.

The celebrated Eyring–Kramers law describes the average time it takes to escape from a well, in the regime of low temperature, $h \to 0$. In his pioneering work, Kramers [1940] considered a one-dimensional model, see Figure 1, and predicted that the average transition time, τ_φ, from a local minimum A to the

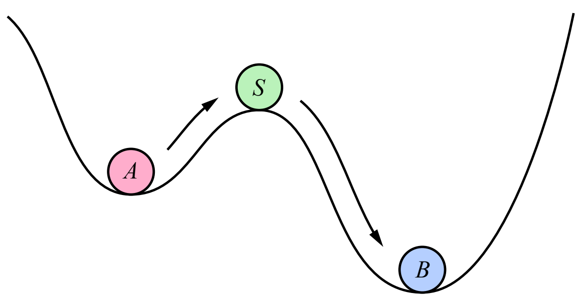

Figure 1. Metastable dynamics: random force allows a state localized near one minimum A to reach another minimum B passing a saddle point (a local maximum in dimension 1).

nearest saddle point S is exponentially large with respect to h^{-1}:

$$\tau_\varphi \simeq a_\varphi e^{\kappa_\varphi/h}, \quad \kappa_\varphi = \varphi(S) - \varphi(A), \quad a_\varphi = 2\pi|\varphi''(A)\varphi''(B)|^{-1/2}. \tag{1-4}$$

Hence, for h small this average transition time is large and this explains the terminology of A being a *metastable state*. (Once we get past S, the transition time to B is bounded and hence τ_φ is effectively the transition time from the state A to the state B.)

The Eyring–Kramers law has important applications in which the trajectory (1-3) is used to implement computational algorithms. Roughly speaking it proceeds as follows: in order to compute some thermodynamical quantities

$$\mathbb{E}_\mu(f) = \int_{\mathbb{R}^d} f(x)\, d\mu(x) \tag{1-5}$$

associated with a measure μ and an observable f, we introduce a random dynamics X_t which is ergodic with respect to μ. We then use the Monte Carlo method to approximate $\mathbb{E}_\mu(f)$ by the long-time average of f along any trajectory — see [Lelièvre, Rousset and Stoltz 2010] for an introduction. In many situations $d\mu(x) = Z_h e^{-\varphi(x)/h}$ for some potential φ and the over-damped Langevin dynamics (1-3) can be used as X_t. The time needed for the process X_t to explore the whole space $\mathbb{R}^d$ (which ensures the validity of the Monte Carlo approximation method) is directly linked to the metastable properties discussed previously. Understanding this metastable behavior is then of interest if, for instance, we need to evaluate the stopping time or to accelerate the convergence.

The mathematical proof of Eyring–Kramers law in a generic setting was first obtained by a potential-theory approach in [Bovier, Gayrard and Klein 2005] and then by semiclassical methods in [Helffer, Klein and Nier 2004]. The semiclassical point of view and connection to the Witten Laplacian can be seen by considering the Langevin equation (1-3) at the macroscopic level. In that case statistical distributions $\rho(t,x)$ of particles are governed by the Kramers–Smoluchowski equation

$$\partial_t \rho - h\Delta\rho - 2\,\mathrm{div}(\rho\nabla\varphi) = 0. \tag{1-6}$$

This is equivalent to

$$h\partial_t\tilde\rho + \Delta_\varphi\tilde\rho = 0, \quad \tilde\rho := e^{\varphi/h}\rho,$$

where Δ_φ is the Witten Laplacian (1-2) associated to φ. In view of (1-1), Δ_φ is nonnegative and under a confining assumption on the function φ, it has a nontrivial kernel corresponding to the global equilibrium of (1-6). (Confining assumption means that φ grows fast enough so that $e^{-\varphi/h} \in L^2$.) As a consequence, the behavior of $\tilde\rho$ when $t \to \infty$ is determined by the small eigenvalues of Δ_φ. In particular, any state associated to a small eigenvalue is stable for exponentially long times. These are the metastable states, and the inverses of the corresponding eigenvalues yield their lifetimes. Helffer, Klein and Nier [2004] obtained a full description of the small eigenvalues of the Witten Laplacian in a general setting. For the Kramers–Smoluchowski equation, their result implies that if the initial probability distribution ρ_0 belongs to $L^2(e^{2\varphi/h}\,dx)$, then the solution ρ of (1-6) converges exponentially fast to the equilibrium probability distribution $c_h^{-2}e^{-2\varphi/h}$ (where c_h is a normalizing factor)

$$\|\rho(t)-c_h^{-2}e^{-2\varphi/h}\|_{L^2(e^{2\varphi/h}\,dx)} \le e^{-\lambda_h t/h}\|\rho_0\|_{L^2(e^{2\varphi/h}\,dx)}. \tag{1-7}$$

Moreover, the rate of convergence

$$\lambda_h/h = b(h)e^{-2S/h}, \quad \lambda_h := \min\sigma(\Delta_\varphi)\setminus\{0\}, \tag{1-8}$$

is described by the Eyring–Kramers law, that is:

- S is the biggest height a particle has to pass in order to reach the unique global minimum.
- The prefactor $b(h)$ has an asymptotic expansion with respect to the parameter h, $b(h)\sim\sum_k b_k h^k$ and its leading term is given by an explicit formula in terms of the Hessian of φ.

More precisely, the assumptions made in [Helffer, Klein and Nier 2004] imply that there exist a unique minimum m and a unique saddle point s of φ such that $S=\varphi(s)-\varphi(m)$. Then, the leading term of $b(h)$ is

$$b_0 = \frac{|\mu_1(s)|}{\pi}\sqrt{\frac{\det \mathrm{Hess}(\varphi)(m)}{|\det \mathrm{Hess}(\varphi)(s)|}}, \tag{1-9}$$

where $\mu_1(s)$ denotes the negative eigenvalue of $\mathrm{Hess}(\varphi)(s)$. In the case of a double well, this formula is exactly the one predicted by Kramers [1940]. In view of (1-7) the transmission time is approximately the inverse of λ_h of (1-8). Hence the result of [Helffer, Klein and Nier 2004] is in agreement with (1-4). (Note that in dimension 1, $\varphi''(s)=\mu_1(s)$.)

The method developed in [Helffer, Klein and Nier 2004] to compute the small eigenvalues of the Witten Laplacian was successfully used on bounded domains in [Helffer and Nier 2006; Le Peutrec 2010] and in the study of semiclassical random walks [Bony, Hérau and Michel 2015].

The range of potential φ covered by these papers does not include many cases which are important in practice. Roughly speaking, Helffer, Klein and Nier [2004] make an assumption on the relative position of minima and saddle points that ensures that the small eigenvalues are all of different size. Among the limitations of this assumption is the fact that the potential φ cannot have saddle points or minima with the same value. In many physical applications the energy landscape may not satisfy that assumption. Also, the energy potential may have symmetries which again are not allowed by the assumptions in [Helffer, Klein and Nier 2004]. For instance this is the case of some homogeneous systems such as Lennard-Jones clusters — see [Wales 2006] for an example and a discussion.

The aim of this paper is to study the spectral properties of Δ_φ in the case where φ is a general Morse function without restrictions on the relative positions of the critical values.

1B. ***An example.*** A motivating example is given by $\varphi:\mathbb{R}^d\to\mathbb{R}$ which has n_0 minima all at the same level and n_1 saddle points all at the same level — see Figure 2, where the x represent minima and the o local maxima. Denote by $S=\varphi(s)-\varphi(m)$ the difference of the value at the saddle points and at the minima. To simplify the setting further, we assume also that the function $\mathrm{Hess}(\varphi)(x)$ has eigenvalues ±1 when x belongs to the set of minima and saddle points.

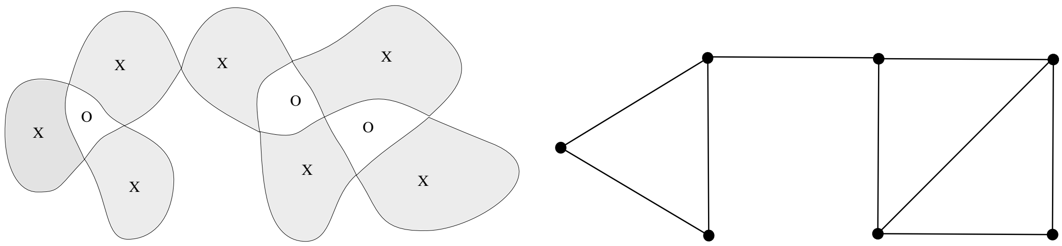

Figure 2. Left: the sublevel set $\{\varphi < \sigma\}$ (shaded region) associated to a potential φ having a unique saddle value σ. The x's represent local minima, the o's, local maxima. Right: the graph associated to the potential on the left.

This case is not allowed under the assumptions of [Helffer, Klein and Nier 2004] yet it displays some interesting phenomena. More precisely, in the very simplified case discussed in this section, a consequence of Theorem 7.1 below is the following:

Theorem 1.1. *Under the assumptions of this subsection, there exist $\epsilon_0 > 0$ and $h_0 > 0$ such that for all $h \in]0, h_0]$, Δ_φ has exactly n_0 eigenvalues $\lambda_k,\ k = 1, \dots, n_0$, in the interval $[0, \epsilon_0 h]$. The lowest eigenvalue is $\lambda_1 = 0$ and*

$$\lambda_k = h b_k(h) e^{-2S/h}, \quad k = 2, \dots, n_0.$$

The prefactors $b_k(h)$ satisfy $b_k(h) \sim \sum_{j=0}^{\infty} h^j b_{k,j}$ and the terms $b_{k,0}$ are given by the nonzero eigenvalues of the graph Laplacian for the graph $\mathcal{G}$ whose vertices are the minima of φ and whose edges are the saddle points joining two minima (*see Figure 2*).

In terms of the Kramers–Smoluchowski equation (1-6), Theorem 1.1 exhibits metastable states whose lifetimes (given by the inverse of the above eigenvalues) are described by the graph $\mathcal{G}$. At the level of particles, these new rules of computation can be understood as follows. Since all the minima are at the same level, the equilibrium state is equidistributed among all the minima. Moreover, since all the saddle points are at the same level, an ergodic trajectory of (1-3) will visit all the minima in the same time scale, by traveling along the edges of the graph $\mathcal{G}$. Hence, the effective long-time dynamics of the Kramers–Smoluchowski equation is given by the heat equation for the graph Laplacian of $\mathcal{G}$ — see [Michel and Zworski 2018, Theorem 3].

Earlier results, in dimension 1 and for finite times, on effective dynamics were obtained in [Peletier, Savaré and Veneroni 2012] using Γ-convergence, in [Herrmann and Niethammer 2011] using Wasserstein gradient flows and in [Evans and Tabrizian 2016]. We also remark that the same graph Laplacian was constructed in [Landim, Misturini and Tsunoda 2015] in a discrete setting.

Under our special assumptions the coefficients b_k do not depend on the second derivative of φ as in the usual case. In the more general case of arbitrary Hessians, $\mathcal{G}$ has to be replaced by a weighted graph with weights depending on the Hessians in an explicit way — see Theorem 7.1.

To motivate objects introduced in the next section, we now discuss what happens if we modify the potential φ in the following way: suppose that φ has the structure shown in Figure 2 but one of the minimal

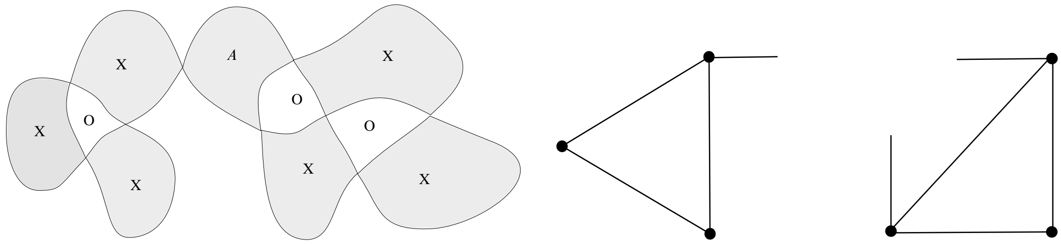

Figure 3. Left: the sublevel set $\{\varphi < \sigma\}$ (shaded region) associated to a potential φ having a unique saddle value σ. The x's represent local minima, the o's, local maxima. Right: the two hypergraphs associated to the potential on the left (the missing vertex corresponds to the minimum A).

values is made higher or lower. In Figure 3, the modified minimum is denoted by A. Then, we can associate to this potential the two hypergraphs corresponding to minima at the same level and linked by a saddle value (see Figure 3). If A is an absolute minimum, then equilibrium distribution is concentrated in A and the prefactor $b_k(h)$ will be given by the smallest nonzero eigenvalue of the two hypergraphs introduced above (roughly speaking this represents the maximum time needed to reach A). In the opposite case, A is no longer a global minimum and the equilibrium state is uniformly distributed among all the absolute minima. In order to visit each site of the equilibrium state, a particle will necessarily pass through the point A. This heuristic explains why the computation of the prefactor $b_k(h)$ will involve a more complicated procedure describing the interaction between the two hypergraphs via the well A.

The main contribution of this paper is to describe these phenomena in a quantitative way.

2. Framework and results

Let X be either $\mathbb{R}^d$ or a compact manifold of dimension d without boundary and let $\varphi : X \to \mathbb{R}$ be a smooth Morse function. Consider the semiclassical Witten Laplacian associated to φ:

$$\Delta_\varphi = -h^2\Delta + |\nabla\varphi|^2 - h\Delta\varphi, \tag{2-1}$$

where $h \in]0, 1]$ denotes the semiclassical parameter.

If X is a compact manifold, the operator Δ_φ is selfadjoint with domain $H^2(X)$ and its resolvent is compact. In the case $X = \mathbb{R}^d$ we make the additional assumption that there exist $C > 0$ and a compact $K \subset \mathbb{R}^d$ such that for all $x \in \mathbb{R}^d \setminus K$, we have

$$|\nabla\varphi(x)| \geq \frac{1}{C}, \quad |\operatorname{Hess}(\varphi(x))| \leq C|\nabla\varphi|^2 \quad \text{and} \quad \varphi(x) \geq C|x|. \tag{2-2}$$

Then, Δ_φ is essentially selfadjoint on $\mathcal{C}_c^\infty(\mathbb{R}^d)$ and thanks to (2-2), there exist $h_0 > 0$ and $c_0 > 0$ such that for all $h \in]0, h_0]$, we have

$$\sigma_{\text{ess}}(\Delta_\varphi) \subset [c_0, \infty[.$$

In both situations X compact or $X = \mathbb{R}^d$, it is well known that Δ_φ is nonnegative. Hence $\sigma(\Delta_\varphi) \subset [0, \infty[$ and it follows from the above remarks that $\sigma(\Delta_\varphi) \cap [0, c_0[$ is made of eigenvalues with no accumulation point except maybe c_0. Moreover $e^{-\varphi/h}$ is clearly in the kernel of Δ_φ and belongs to $L^2(\mathbb{R}^d)$ thanks to (2-2), so that the lowest eigenvalue of Δ_φ is clearly 0.

Since φ is a Morse function (and thanks to assumption (2-2) in the case $X = \mathbb{R}^d$), the set $\mathcal{U}$ of critical points is finite. In the following, for $p = 0, \dots, d$, we will denote by $\mathcal{U}^{(p)}$ the set of critical points of φ of index p. Hence, $\mathcal{U}^{(0)}$ is the set of minima and $\mathcal{U}^{(1)}$ the set of saddle points of φ. Throughout the paper, we will write $n_j = \#\mathcal{U}^{(j)}$.

From the pioneering work [Witten 1982], it is well known that for small h, there is a correspondence between the small eigenvalues of Δ_φ and the critical points of φ. More precisely, by standard localization arguments one can show that there exists $\epsilon_0 > 0$ such that for $h > 0$ small enough, Δ_φ has exactly n_0 eigenvalues in the interval $[0, \epsilon_0 h]$, which we denote by $0 = \lambda_1 \le \lambda_2 \le \cdots \le \lambda_{n_0}$. This result is easily proved in [Cycon, Froese, Kirsch and Simon 1987] with $\epsilon_0 h$ replaced by $h^{3/2}$. The proof with $\epsilon_0 h$ can be found in [Helffer and Sjöstrand 1985, Proposition 1.7] (see also [Michel and Zworski 2018, Proposition 1] for a self-contained proof). Moreover, these eigenvalues are actually exponentially small; that is, they live in an interval $[0, e^{-C/h}]$ for some $C > 0$ (see [Helffer 1988] for a proof). From a topological point of view, this information (together with the equivalent estimates for the Witten Laplacian $\Delta_\varphi^{(p)}$ acting on p-forms) is sufficient to establish a correspondence between the small eigenvalues of $\Delta_\varphi^{(p)}$ and the critical points of φ of index p (this was the key point in the Witten's proof of Morse inequalities). However, for applications to the description of metastable dynamics, it is important to get some accurate description of the λ_j. Our main theorem will give some asymptotic of these eigenvalues for any Morse function φ, without any assumption on the relative position of minimal and saddle values of φ.

Before going further, we introduce notation used in this paper. For $x_0 \in X$ and $r > 0$, introduce the geodesic ball $B(x_0, r) = \{x \in X : d(x, x_0) < r\}$.

Throughout, we will say that $\boldsymbol{s}$ is a saddle point if it is a critical point of index 1.

Given $a(h), b(h) > 0$, two functions of the semiclassical parameter, we say that $a(h) \asymp b(h)$ if there exists some constant $c_1, c_2 > 0$ such that for all $h > 0$ small we have $c_1 b(h) \le a(h) \le c_2 b(h)$. We say that a family of vectors $(a(h))_{h\in]0,1]}$ in a normed vector space V admits a classical expansion if there exists a sequence of vectors $(a_n)_{n\in\mathbb{N}}$ independent of h and such that for all $N \in \mathbb{N}$, there exists some constant $C_N > 0$ such that

$$\Big\| a(h) - \sum_{n=0}^{N} h^n a_n \Big\|_V \le C_N h^{N+1} \quad \text{for all } h \in]0, 1].$$

We set $a(h) \sim \sum_{n=0}^{\infty} h^n a_n$.

As we shall see later, we will have to analyze carefully some finite-dimensional matrices which are strongly related to the critical points of φ. Given any subsets $\mathcal{B}_1, \mathcal{B}_2$ of $\mathcal{U}$, it will be convenient to introduce the finite-dimensional vector space $\mathscr{F}(\mathcal{B}_j)$ of real-valued functions on $\mathcal{B}_j$. We shall then denote by $\mathscr{M}(\mathcal{B}_1, \mathcal{B}_2)$ the vector space of linear operators from $\mathscr{F}(\mathcal{B}_1)$ into $\mathscr{F}(\mathcal{B}_2)$.

2A. ***Labeling of minima.*** Let us now recall the general labeling of minima introduced in [Helffer, Klein and Nier 2004] and generalized in [Hérau, Hitrik and Sjöstrand 2011]. The main ingredient is the notion of separating saddle point, which is defined as follows. Given a saddle point $\boldsymbol{s}$ of φ, and $r > 0$ small

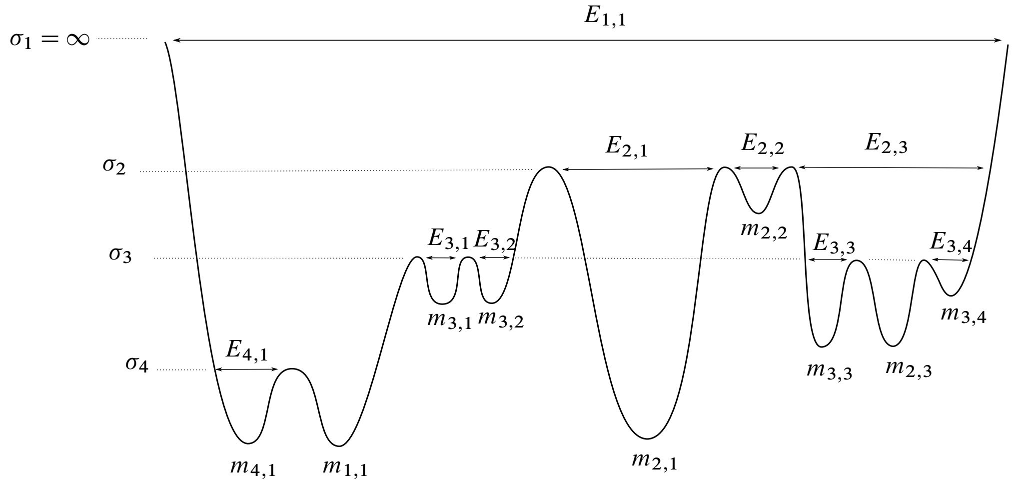

Figure 4. Labeling procedure.

enough, the set

$$\{x \in B(\boldsymbol{s}, r) : \varphi(x) < \varphi(\boldsymbol{s})\}$$

has exactly two connected components $C_j(\boldsymbol{s}, r)$, $j = 1, 2$. The following definition is taken from [Hérau, Hitrik and Sjöstrand 2011, Definition 4.1].

Definition 2.1. We say that $\boldsymbol{s} \in X$ is a separating saddle point (ssp) if it is a saddle point and if $C_1(\boldsymbol{s}, r)$ and $C_2(\boldsymbol{s}, r)$ are contained in two different connected components of $\{x \in X : \varphi(x) < \varphi(\boldsymbol{s})\}$. We will denote by $\mathcal{V}^{(1)}$ the set of separating saddle points.

We say that $\sigma \in \mathbb{R}$ is a separating saddle value (ssv) if it is of the form $\sigma = \varphi(\boldsymbol{s})$ with $\boldsymbol{s} \in \mathcal{V}^{(1)}$. We denote by $\underline{\Sigma} = \varphi(\mathcal{V}^{(1)})$ the set of separating saddle values.

We say that $E \subset X$ is a critical component if there exists $\sigma \in \underline{\Sigma}$ such that E is a connected component of $\{\varphi < \sigma\}$ and if $\partial E \cap \mathcal{V}^{(1)} \neq \varnothing$. We denote by $\mathscr{C}$ the set of critical components.

Let us now describe the labeling procedure of [Hérau, Hitrik and Sjöstrand 2011]. Since φ is a Morse function, it has finitely many critical points and so $\underline{\Sigma}$ is finite. We denote by $\sigma_2 > \sigma_3 > \cdots > \sigma_N$ its elements and for convenience we also introduce a fictive infinite saddle value $\sigma_1 = +\infty$ and write $\Sigma = \underline{\Sigma} \cup \{\sigma_1\}$. Starting from σ_1, we will recursively associate to each σ_i a finite family of local minima $(\boldsymbol{m}_{i,j})_j$ and a finite family of critical components $(E_{i,j})_j$ (see Figure 4):

- Let $X_{\sigma_1} = \{x \in X : \varphi(x) < \sigma_1 = \infty\} = X$. We let $\boldsymbol{m}_{1,1}$ be any global minimum of φ (not necessarily unique) and $E_{1,1} = X$.

- Next we consider $X_{\sigma_2} = \{x \in X : \varphi(x) < \sigma_2\}$. This is the union of its finitely many connected components. Exactly one of these components contains $\boldsymbol{m}_{1,1}$ and the other components are denoted by $E_{2,1}, \ldots, E_{2,N_2}$. In each component $E_{2,j}$, we pick up a point $\boldsymbol{m}_{2,j}$ which is a global minimum of $\varphi_{|E_{2,j}}$.

- Suppose now that the families $(\boldsymbol{m}_{k,j})_j$ and $(E_{k,j})_j$ have been constructed until rank $k = i - 1$. The set $X_{\sigma_i} = \{x \in X : \varphi(x) < \sigma_i\}$ has again finitely many connected components and we label by $E_{i,j}$,

$j = 1, \dots, N_i$, those that do not contain any $\boldsymbol{m}_{k,l}$ with $k < i$. In each $E_{i,j}$ we pick a point $\boldsymbol{m}_{i,j}$ which is a global minimum of $\varphi_{|E_{i,j}}$. Observe that for all $i \geq 2$, the components $E_{i,j}$ are all critical.

We run the procedure until all the minima have been labeled.

Remark 2.2. The above labeling satisfies the following property. For any $\sigma_i \in \Sigma$ and any connected component A_i of $\{\varphi < \sigma_i\}$, there exists a unique (k, l) such that $k \leq i$ and $\boldsymbol{m}_{k,l} \in A_i$.

Proof. Let us start with the existence part of the result. If A_i is one of the $E_{i,j}$ for some j, then take $k = i$ and $l = j$. Otherwise, this means that in the labeling procedure, A_i already contained a minimum $\boldsymbol{m}_{k,l}$ with $k < i$.

Let us prove the uniqueness part. Assume that $\boldsymbol{m}_{k,l}, \boldsymbol{m}_{k',l'} \in A_i$ with $k \leq k' \leq i$. Then $A_i \cap E_{k',l'} \neq \varnothing$ and since A_i is a connected component of $\{\varphi < \sigma_i\}$ with $\sigma_i \leq \sigma_{k'}$ it follows that $A_i \subset E_{k',l'}$. Since $\boldsymbol{m}_{k,l} \in A_i$, it follows that $\boldsymbol{m}_{k,l} \in E_{k',l'}$ which is impossible unless $(k, l) = (k', l')$. □

Using the above labeling, Hérau, Hitrik and Sjöstrand [2011] made some significant progress (in the more general situation of Kramers–Fokker–Planck operators, but this applies to Witten Laplacian). First, they showed in Theorem 7.1 of that paper that the exponentially small eigenvalues $(\lambda_{\boldsymbol{m}}(h))_{\boldsymbol{m}\in\mathcal{U}^{(0)}}$ of Δ_φ (indexed by the sequence of local minima) satisfy $\lambda_{\boldsymbol{m}}(h) \asymp he^{-2S(\boldsymbol{m})/h}$ for the sequence of Arrhenius numbers $(S(\boldsymbol{m}))_{\boldsymbol{m}\in\mathcal{U}^{(0)}}$ defined by $S(\boldsymbol{m}_{i,j}) = \sigma_i - f(\boldsymbol{m}_{i,j})$ with the above notation. However, their method does not work to prove that $h^{-1}\lambda_{\boldsymbol{m}}(h)e^{2S(\boldsymbol{m})/h}$ admits a limit when $h \to 0$. In order to compute the asymptotic expansion of the eigenvalues $\lambda_{\boldsymbol{m}}(h)$, they need to make some additional assumption on the interaction between minima and saddle points (see Assumption 5.1 in [Hérau, Hitrik and Sjöstrand 2011]). This hypothesis, which is a generalization of the one made in [Helffer, Klein and Nier 2004], can be formulated as follows with the notation of the preceding section:

Generic Assumption. For all $i = 1, \dots, N$, $j = 1, \dots, N_i$, the following hold true:

(i) $\boldsymbol{m}_{i,j}$ is the unique global minimum of the application $\varphi_{|E_{i,j}}$.

(ii) If E is a connected component of $\{\varphi < \sigma_i\}$ such that $E \cap \mathcal{V}^{(1)} \neq \varnothing$, there exists a unique $\boldsymbol{s} \in \mathcal{V}^{(1)}$ such that $\varphi(\boldsymbol{s}) = \sup \varphi(E \cap \mathcal{V}^{(1)})$. In particular, $\varphi^{-1}(]-\infty, \varphi(\boldsymbol{s})[) \cap E$ is the union of exactly two different connected components.

Throughout the paper, we denote this assumption by (GA).

Under this assumption, there exists a bijection between $\mathcal{U}^{(0)}$ and $\mathcal{V}^{(1)} \cup \{\boldsymbol{s}_1\}$, where $\boldsymbol{s}_1$ is a fictive saddle point associated to $\sigma_1 = \infty$ and for which by convention $\varphi(\boldsymbol{s}_1) = \infty$. Using this one-to-one correspondence, the authors exhibit some labeling $\mathcal{U}^{(0)} = \{\boldsymbol{m}_1, \dots, \boldsymbol{m}_{n_0}\}$ and $\mathcal{V}^{(1)} \cup \{\boldsymbol{s}_1\} = \{\boldsymbol{s}_1, \dots, \boldsymbol{s}_{n_0}\}$ such that the small eigenvalues $\lambda_i(h)$ are of the form $hb_i(h)e^{-2S_i/h}$ with $S_i = \varphi(\boldsymbol{s}_i) - \varphi(\boldsymbol{m}_i)$. Moreover, they prove that the $b_i(h)$ have a classical expansion and compute the leading term of this expansion; see [Hérau, Hitrik and Sjöstrand 2011, Theorem 5.10].

As it is stated above, (GA) is not exactly Assumption 5.1 stated in [Hérau, Hitrik and Sjöstrand 2011]. Indeed, it is supposed in that paper that (ii) holds true only for E being a critical component. However, as indicated by the anonymous referee, we can easily construct some function φ satisfying this assumption for which there is no bijection between $\mathcal{U}^{(0)}$ and $\mathcal{V}^{(1)}$. To see this, first consider in dimension 1 a potential φ with four minima m_j, $j=1,\dots,4$, and three saddle points s_j, $j=1,\dots,3$, such that $m_1 < s_1 < m_2 < s_2 < m_3 < s_3 < m_4$ and such that $\varphi(m_1) < \varphi(m_4) < \varphi(m_2) = \varphi(m_3)$ and $\varphi(s_1) = \varphi(s_2) < \varphi(s_3)$. Since the component of $\{\varphi < \varphi(s_3)\}$ containing m_1 is not critical, this function satisfies Assumption 5.1 in [Hérau, Hitrik and Sjöstrand 2011]. It doesn't satisfy (GA) as stated above. In higher dimensions, one can easily generalize this construction to obtain potentials satisfying Assumption 5.1 in [Hérau, Hitrik and Sjöstrand 2011], with a fixed number of minima and an arbitrarily large number of separating saddle points (think for instance of many saddle points between the well containing m_1 and the well containing m_2). This shows that Assumption 5.1 is not sufficient to ensure a bijection between minima and separating saddle points.

Let us emphasize that the above remark doesn't affect the rest of the work done in [Hérau, Hitrik and Sjöstrand 2011], where we can easily use the above corrected version of Assumption 5.1.

Let us observe that the Generic Assumption allows some degeneracy in the sequence (S_j); that is, there may exist j such that $S_j = S_{j+1}$. However, (GA) remains restrictive for the following reasons:

- It permits only potentials φ for which $\mathcal{U}^{(0)}$ and $\mathcal{V}^{(1)} \cup \{\boldsymbol{s}_1\}$ have the same cardinality.
- The eventual degenerate heights are associated to weakly interacting eigenstates in the following sense. Assume for instance that $S_j = S_{j+1}$ for some $j = 1,\dots,n_0-1$ and modify slightly the function φ near the minimum $\boldsymbol{m}_j$. Then the coefficient b_j is modified, whereas the classical expansion of b_{j+1} remains unchanged.

Figures 6 and 7 below present some examples of potentials where (GA) is not satisfied. These examples, as well as an example in higher dimensions, are discussed in detail in Section 7C.

In the present paper, we obtain an asymptotic expansion for the $\lambda_i(h)$ for general Morse functions φ without any additional assumptions on the relative position of minima and ssp's.

2B. *Main result.* In order to state our main result, we introduce some notation that will be used throughout the paper. First, using the above labeling, we define $\boldsymbol{\sigma} : \mathcal{U}^{(0)} \to \Sigma$ by $\boldsymbol{\sigma}(\boldsymbol{m}_{i,j}) = \sigma_i$ and $S : \mathcal{U}^{(0)} \to]0,+\infty]$ by $S(\boldsymbol{m}) = \boldsymbol{\sigma}(\boldsymbol{m}) - \varphi(\boldsymbol{m})$. We let $\mathcal{S} = S(\mathcal{U}^{(0)})$; then with the notation of the preceding section, we have

$$\mathcal{S} = \{\sigma_i - \varphi(\boldsymbol{m}_{i,j}) : i = 1,\dots,N,\ j = 1,\dots,N_i\}. \tag{2-3}$$

Throughout the paper, we denote by $\underline{\boldsymbol{m}} = \boldsymbol{m}_{1,1}$ the (not necessarily unique) absolute minimum of φ that was chosen at the first step of the labeling procedure, and we let

$$\underline{\mathcal{U}}^{(0)} = \mathcal{U}^{(0)} \setminus \{\underline{\boldsymbol{m}}\}. \tag{2-4}$$

Using again the above labeling, we can associate a critical component to any local minimum. More precisely, we define

$$E : \mathcal{U}^{(0)} \to \mathscr{C} \cup \{X\} \tag{2-5}$$

by $E(\boldsymbol{m}_{i,j}) = E_{i,j}$. Observe that by definition, this application is injective. Using this map, we can associate to each minimum $\boldsymbol{m} \in \mathcal{U}^{(0)}$ a boundary set given by $\Gamma(\boldsymbol{m}) = \partial E(\boldsymbol{m})$. Thanks to the fact that φ is a smooth Morse function, for any $\boldsymbol{m} \in \underline{\mathcal{U}}^{(0)}$, the set $\Gamma(\boldsymbol{m})$ is a finite union of compact submanifolds of X of dimension $d-1$ with conic singularities at the saddle points. For our construction of quasimodes, we also need to introduce the set

$$H(\boldsymbol{m}) := \{\boldsymbol{m}' \in E(\boldsymbol{m}) \cap \mathcal{U}^{(0)} : \varphi(\boldsymbol{m}') = \varphi(\boldsymbol{m})\}. \tag{2-6}$$

Given $\boldsymbol{m} \in \underline{\mathcal{U}}^{(0)}$, we have $\boldsymbol{\sigma}(\boldsymbol{m}) = \sigma_i$ for some $i \geq 2$. Moreover, since $\sigma_{i-1} > \sigma_i$, there exists a unique connected component of $\{\varphi < \sigma_{i-1}\}$ that contains $\boldsymbol{m}$ (observe that this component is not necessarily critical). We denote that component by $E_-(\boldsymbol{m})$, and by

$$E_- : \underline{\mathcal{U}}^{(0)} \to \Omega(X) \tag{2-7}$$

the corresponding application, where $\Omega(X)$ is the collection of connected open subsets of X. Thanks to Remark 2.2, we know that for any $\boldsymbol{m} \in \underline{\mathcal{U}}^{(0)}$, there exists a unique $\boldsymbol{m}' \in E_-(\boldsymbol{m}) \cap \mathcal{U}^{(0)}$, denoted by $\hat{\boldsymbol{m}}(\boldsymbol{m})$, such that $\boldsymbol{\sigma}(\boldsymbol{m}') > \boldsymbol{\sigma}(\boldsymbol{m})$. In particular,

$$\text{for all } \boldsymbol{m} \in \underline{\mathcal{U}}^{(0)}, \quad \varphi(\hat{\boldsymbol{m}}(\boldsymbol{m})) \leq \varphi(\boldsymbol{m}), \tag{2-8}$$

and we denote by $\widehat{E}(\boldsymbol{m})$ the connected component of $\{\varphi < \sigma(\boldsymbol{m})\}$ containing $\hat{\boldsymbol{m}}(\boldsymbol{m})$. It holds additionally $\widehat{E}(\boldsymbol{m}) \subset E_-(\boldsymbol{m})$ and we can easily see that $\widehat{E}(\boldsymbol{m})$ is always a critical component. Throughout, we denote by

$$\widehat{E} : \underline{\mathcal{U}}^{(0)} \to \mathscr{C}, \tag{2-9}$$

$$\hat{\boldsymbol{m}} : \underline{\mathcal{U}}^{(0)} \to \mathcal{U}^{(0)} \tag{2-10}$$

the corresponding applications. The fact that the inequality in (2-8) is large or strict plays an important role in our analysis.

Definition 2.3. Let $\boldsymbol{m} \in \underline{\mathcal{U}}^{(0)}$. We say that $\boldsymbol{m}$ is of type I if $\varphi(\hat{\boldsymbol{m}}(\boldsymbol{m})) < \varphi(\boldsymbol{m})$. If $\varphi(\hat{\boldsymbol{m}}(\boldsymbol{m})) = \varphi(\boldsymbol{m})$, we say that $\boldsymbol{m}$ is of type II. We define

$$\mathcal{U}^{(0),\mathrm{I}} = \{\boldsymbol{m} \in \underline{\mathcal{U}}^{(0)} : \boldsymbol{m} \text{ is of type I}\},$$
$$\mathcal{U}^{(0),\mathrm{II}} = \{\boldsymbol{m} \in \underline{\mathcal{U}}^{(0)} : \boldsymbol{m} \text{ is of type II}\}.$$

We have clearly the disjoint union $\underline{\mathcal{U}}^{(0)} = \mathcal{U}^{(0),\mathrm{I}} \cup \mathcal{U}^{(0),\mathrm{II}}$.

Example 2.4. Let us compute the preceding object in the case of the potential φ represented in Figure 4. The results are presented in Figure 5.

- Let us start with the object associated to σ_2. By definition, $\widehat{E}(\boldsymbol{m}_{2,1}) = \widehat{E}(\boldsymbol{m}_{2,2}) = \widehat{E}(\boldsymbol{m}_{2,3}) = \widetilde{E}_2$, where $\widetilde{E}_2$ is the connected component of $\{\varphi < \sigma_2\}$ that contains $\boldsymbol{m}_{1,1}$. Then we have $\hat{\boldsymbol{m}}(\boldsymbol{m}_{2,1}) = \hat{\boldsymbol{m}}(\boldsymbol{m}_{2,2}) = \hat{\boldsymbol{m}}(\boldsymbol{m}_{2,3}) = \boldsymbol{m}_{1,1}$.

  Since $\varphi(\boldsymbol{m}_{1,1}) = \varphi(\boldsymbol{m}_{2,1}) < \varphi(\boldsymbol{m}_{2,3}) < \varphi(\boldsymbol{m}_{2,2})$, we know $\boldsymbol{m}_{2,1}$ is of type II, whereas $\boldsymbol{m}_{2,2}$ and $\boldsymbol{m}_{2,3}$ are of type I.

- Consider now the level σ_3. We have $E_-(\boldsymbol{m}_{3,1}) = E_-(\boldsymbol{m}_{3,2}) = \widetilde{E}_2$ and $E_-(\boldsymbol{m}_{3,3}) = E_-(\boldsymbol{m}_{3,4}) = E_{2,3}$. Therefore, $\widehat{E}(\boldsymbol{m}_{3,1}) = \widehat{E}(\boldsymbol{m}_{3,2}) = \widetilde{E}_3$, where $\widetilde{E}_3$ is the connected component of $\{\varphi < \sigma_3\}$ that contains $m_{1,1}$. Similarly, we have $\widehat{E}(\boldsymbol{m}_{3,3}) = \widehat{E}(\boldsymbol{m}_{3,4}) = \widetilde{E}'_3$, where $\widetilde{E}'_3$ is the connected component of $\{\varphi < \sigma_3\}$ that contains $m_{2,3}$. From these computations, it follows that $\hat{\boldsymbol{m}}(\boldsymbol{m}_{3,1}) = \hat{\boldsymbol{m}}(\boldsymbol{m}_{3,2}) = \boldsymbol{m}_{1,1}$ and

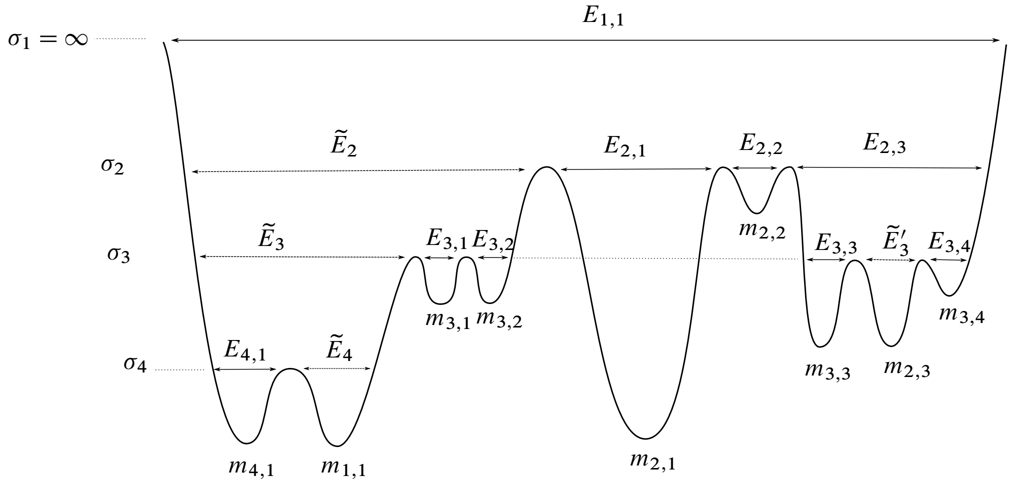

Figure 5. Computations of Example 2.4.

since $\varphi(\boldsymbol{m}_{1,1}) < \varphi(\boldsymbol{m}_{3,1}) = \varphi(\boldsymbol{m}_{3,2})$ it follows that $\boldsymbol{m}_{3,1}$ and $\boldsymbol{m}_{3,2}$ are both of type I. On the other hand, $\hat{\boldsymbol{m}}(\boldsymbol{m}_{3,3}) = \hat{\boldsymbol{m}}(\boldsymbol{m}_{3,4}) = \boldsymbol{m}_{2,3}$ and since $\varphi(\boldsymbol{m}_{2,3}) = \varphi(\boldsymbol{m}_{3,3}) < \varphi(\boldsymbol{m}_{3,4})$ it follows that $\boldsymbol{m}_{3,3}$ is of type II and $\boldsymbol{m}_{3,4}$ is of type I.

- Finally, $E_-(\boldsymbol{m}_{4,1}) = \widetilde{E}_3$, $\widehat{E}(\boldsymbol{m}_{4,1}) = \widetilde{E}_4$ as represented on Figure 5 and $\hat{\boldsymbol{m}}(\boldsymbol{m}_{4,1}) = \boldsymbol{m}_{1,1}$. Since $\varphi(\boldsymbol{m}_{1,1}) = \varphi(\boldsymbol{m}_{4,1})$, it follows that $\boldsymbol{m}_{4,1}$ is of type II.

The points of type II play an important role in our analysis. Given $\sigma \in \Sigma$, let $\Omega_\sigma = \Omega_\sigma^0 \cup \widehat{\Omega}_\sigma$, with

$$\Omega_\sigma^0 = \{E(\boldsymbol{m}) : \boldsymbol{m} \in \boldsymbol{\sigma}^{-1}(\sigma)\} \tag{2-11}$$

and $\widehat{\Omega}_\sigma$ be defined by $\widehat{\Omega}_\sigma = \varnothing$ if $\sigma = \sigma_1$ and

$$\widehat{\Omega}_\sigma = \{\widehat{E}(\boldsymbol{m}) : \boldsymbol{m} \in \boldsymbol{\sigma}^{-1}(\sigma) \cap \mathcal{U}^{(0),\mathrm{II}}\} \tag{2-12}$$

if $\sigma \in \underline{\Sigma}$.

Definition 2.5. We define an equivalence relation $\mathcal{R}$ on $\mathcal{U}^{(0)}$ by $\boldsymbol{m}\mathcal{R}\boldsymbol{m}'$ if and only if

$$\begin{cases} \boldsymbol{\sigma}(\boldsymbol{m}) = \boldsymbol{\sigma}(\boldsymbol{m}') = \sigma, \\ \exists \omega_1, \dots, \omega_K \in \Omega_\sigma \text{ such that } \boldsymbol{m} \in \omega_1, \boldsymbol{m}' \in \omega_K \text{ and } \forall k = 1, \dots, K-1,\ \bar{\omega}_k \cap \bar{\omega}_{k+1} \neq \varnothing. \end{cases} \tag{2-13}$$

Throughout the paper, we denote by $\mathrm{Cl}(\boldsymbol{m})$ the equivalence class of $\boldsymbol{m}$ for the relation $\mathcal{R}$. Observe that since $\underline{\boldsymbol{m}}$ is the only minimum such that $\boldsymbol{\sigma}(\boldsymbol{m}) = \infty$, we have $\mathrm{Cl}(\underline{\boldsymbol{m}}) = \{\underline{\boldsymbol{m}}\}$.

Let us denote by $(\mathcal{U}_\alpha^{(0)})_{\alpha \in \mathcal{A}}$ the equivalence classes of $\mathcal{R}$ with $\mathcal{A}$ a finite set. We have evidently

$$\mathcal{U}^{(0)} = \bigsqcup_{\alpha \in \mathcal{A}} \mathcal{U}_\alpha^{(0)}. \tag{2-14}$$

We need also to consider the set $\underline{\mathcal{A}}$ defined by $\underline{\mathcal{A}} = \mathcal{A} \setminus \{\underline{\alpha}\}$, where $\mathcal{U}_{\underline{\alpha}}^{(0)} = \{\underline{\boldsymbol{m}}\}$ is the equivalence class of the absolute minimum chosen for φ. Throughout, we will write $q_\alpha = \#\mathcal{U}_\alpha^{(0)}$. We will also use the following partition of $\mathcal{U}_\alpha^{(0)}$ for any $\alpha \in \underline{\mathcal{A}}$:

$$\mathcal{U}_\alpha^{(0),\mathrm{I}} := \mathcal{U}_\alpha^{(0)} \cap \mathcal{U}^{(0),\mathrm{I}}, \quad \mathcal{U}_\alpha^{(0),\mathrm{II}} := \mathcal{U}_\alpha^{(0)} \cap \mathcal{U}^{(0),\mathrm{II}}. \tag{2-15}$$

Proposition 2.6. *Let $\alpha \in \underline{\mathcal{A}}$. The applications $\boldsymbol{\sigma}$, E_-, $\widehat{E}$ and $\hat{\boldsymbol{m}}$ are constant on $\mathcal{U}_\alpha^{(0)}$.*

Proof. For $\boldsymbol{\sigma}$, it is a direct consequence of the definition. Suppose now that $\boldsymbol{m}, \boldsymbol{m}' \in \underline{\mathcal{U}}^{(0)}$ satisfy $\boldsymbol{m}\mathcal{R}\boldsymbol{m}'$ and $\boldsymbol{m} \neq \boldsymbol{m}'$. Then, $\boldsymbol{m}$ and $\boldsymbol{m}'$ belong to the same connected component of $\{\varphi \leq \sigma(\boldsymbol{m})\}$. Hence, the uniqueness part in the definition of E_- shows that $E_-(\boldsymbol{m}) = E_-(\boldsymbol{m}')$. Since $E_-(\boldsymbol{m}) = E_-(\boldsymbol{m}')$, the identity $\hat{\boldsymbol{m}}(\boldsymbol{m}) = \hat{\boldsymbol{m}}(\boldsymbol{m}')$ follows directly from the definition of $\hat{\boldsymbol{m}}$. This implies automatically $\widehat{E}(\boldsymbol{m}) = \widehat{E}(\boldsymbol{m}')$. ☐

Thanks to the above proposition, given $\alpha \in \underline{\mathcal{A}}$, we will write respectively $\boldsymbol{\sigma}(\alpha)$, $E_-(\alpha)$, $\widehat{E}(\alpha)$ and $\hat{\boldsymbol{m}}(\alpha)$ instead of $\boldsymbol{\sigma}(\boldsymbol{m})$, $E_-(\boldsymbol{m})$, $\widehat{E}(\boldsymbol{m})$, $\hat{\boldsymbol{m}}(\boldsymbol{m})$ for some $\boldsymbol{m} \in \mathcal{U}_\alpha^{(0)}$.

Definition 2.7. We say that

- α is of type I if $\varphi(\hat{\boldsymbol{m}}(\alpha)) < \varphi(\boldsymbol{m})$ for all $\boldsymbol{m} \in \mathcal{U}_\alpha^{(0)}$,
- α is of type II if there exists $\boldsymbol{m} \in \mathcal{U}_\alpha^{(0)}$ such that $\varphi(\hat{\boldsymbol{m}}(\alpha)) = \varphi(\boldsymbol{m})$.

Recall that the height function $S : \mathcal{U}^{(0)} \to \mathbb{R}$ and the set of heights $\mathcal{S} = S(\mathcal{U}^{(0)})$ were defined by (2-3) and above. For any $\alpha \in \mathcal{A}$, we let

$$\mathcal{S}_\alpha = S(\mathcal{U}_\alpha^{(0)}) \quad \text{and} \quad p(\alpha) = \#\mathcal{S}_\alpha. \tag{2-16}$$

There exist some integers $\nu_1^\alpha < \nu_2^\alpha < \cdots < \nu_{p(\alpha)}^\alpha$ such that

$$\mathcal{S}_\alpha = \{S_{\nu_1^\alpha}, \ldots, S_{\nu_{p(\alpha)}^\alpha}\}.$$

In the theorem below, proved in Sections 5 and 6, we sum up in a rather vague way the description of the small eigenvalues that we obtained.

Theorem 2.8. *There exist $c > 0$ and some symmetric positive definite matrices $\mathcal{M}^\alpha$, $\alpha \in \mathcal{A}$, such that counted with multiplicity, we have $\sigma(\Delta_\varphi) \setminus \{0\} = \bigcup_{\alpha\in\mathcal{A}} \sigma(\mathcal{M}^\alpha)(1 + \mathcal{O}(e^{-c/h}))$, with*

$$\sigma(\mathcal{M}^\alpha) = \bigcup_{j=1}^{p(\alpha)} he^{-2h^{-1}S_{\nu_j^\alpha}} \sigma(M^{\alpha,j})$$

for some symmetric positive definite matrices $M^{\alpha,j}$ having a classical expansion with invertible leading term given in Theorem 5.8. Moreover 0 *is a multiplicity*-1 *eigenvalue.*

Let us make a few comments on this theorem.

First, observe that since $M^{\alpha,j}$ has a classical expansion with invertible leading term $M_0^{\alpha,j}$, its eigenvalues $\zeta_r^{\alpha,j}$, $r = 1, \ldots, r^{\alpha,j}$, have a classical expansion

$$\zeta_r^{\alpha,j}(h) \sim \sum_k h^k \zeta_{r,k}^{\alpha,j},$$

with $\zeta_{r,0}^{\alpha,j}$ eigenvalue of the matrix $M_0^{\alpha,j}$.

Compared to previous results obtained under the Generic Assumption, the main difference is that the prefactors $\zeta_{r,k}^{\alpha,j}$ are more difficult to compute since they are obtained as the eigenvalues of the matrices $M^{\alpha,j}$. When (GA) is satisfied, the $M^{\alpha,j}$ are 1×1 matrices whose spectrum is direct to obtain. In the general case, this is not true anymore and the construction of the matrices $M^{\alpha,j}$ is more involved. In particular, it depends dramatically on the number $p(\alpha)=\#S(\mathcal{U}_\alpha^{(0)})$. Observe that this number is also equal to the number of different values taken by φ on the equivalence class $\mathcal{U}_\alpha^{(0)}$.

If $p(\alpha)=1$, the coefficients of $M^{\alpha,j}$ depend only on the pairs $(\boldsymbol{m},\boldsymbol{s})$ for which $\varphi(\boldsymbol{s})-\varphi(\boldsymbol{m})=S_{\nu_j^\alpha}$. Except for the fact that the different eigenvalues $\zeta_r^{\alpha,j}$, $r=1,\dots,r^{\alpha,j}$, are linked together, the situation is similar to that encountered in the generic case. Actually, we prove in Appendix B that if (GA) is satisfied then $\mathrm{Cl}(\boldsymbol{m})$ is reduced to one point for any $\boldsymbol{m}$, and in particular $p(\alpha)=1$ for all α.

In the case where $p(\alpha)\geq 2$, the matrix is more difficult to compute. It comes from an application of the Schur complement method and it depends on some pairs $(\boldsymbol{m},\boldsymbol{s})$ for which the height $\varphi(\boldsymbol{s})-\varphi(\boldsymbol{m})$ is smaller than $S_{\nu_j^\alpha}$. In other words, the lifetime of the metastable state $\boldsymbol{m}$ is not entirely described by the height that is needed to jump over in order to reach the nearest lower-energy position. It depends also on some interactions with some higher-energy states that are not present in the classical Eyring–Kramers formula. To our knowledge, this is the first time that such a phenomena is exhibited.

Let us now compute $p(\alpha)$ on explicit examples. Let us fix $n=2$ and consider the potentials φ given respectively by Figures 6 and 7. In both cases, $\hat{\boldsymbol{m}}(\boldsymbol{m}_{2,1})=\hat{\boldsymbol{m}}(\boldsymbol{m}_{2,2})=\hat{\boldsymbol{m}}(\boldsymbol{m}_{2,3})=\boldsymbol{m}_{1,1}$, which we denote by $\hat{\boldsymbol{m}}$ for short. Since $\varphi(\hat{\boldsymbol{m}})<\varphi(\boldsymbol{m}_{2,j})$ for all j, there is no point of type II, $\mathcal{U}^{(0),\mathrm{II}}=\varnothing$ and hence $\Omega_{\sigma_2}=\{E_{2,1},E_{2,2},E_{2,3}\}$. Therefore, we can compute easily the equivalence classes of $\mathcal{R}$ in both cases:

- In the case of Figure 6, we have three equivalence classes: $c_1=\{\boldsymbol{m}_{1,1}\}$, $c_2=\{\boldsymbol{m}_{2,1},\boldsymbol{m}_{2,2}\}$ and $c_3=\{\boldsymbol{m}_{2,3}\}$. The potential φ is constant on each equivalence class, and hence $p(c_1)=p(c_2)=p(c_3)=1$.

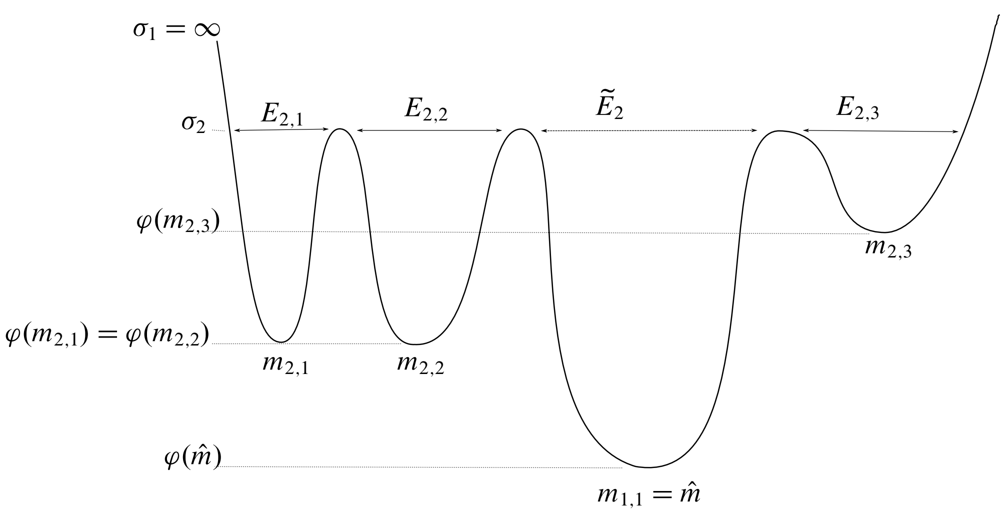

Figure 6. A potential with $p(\alpha)=1$.

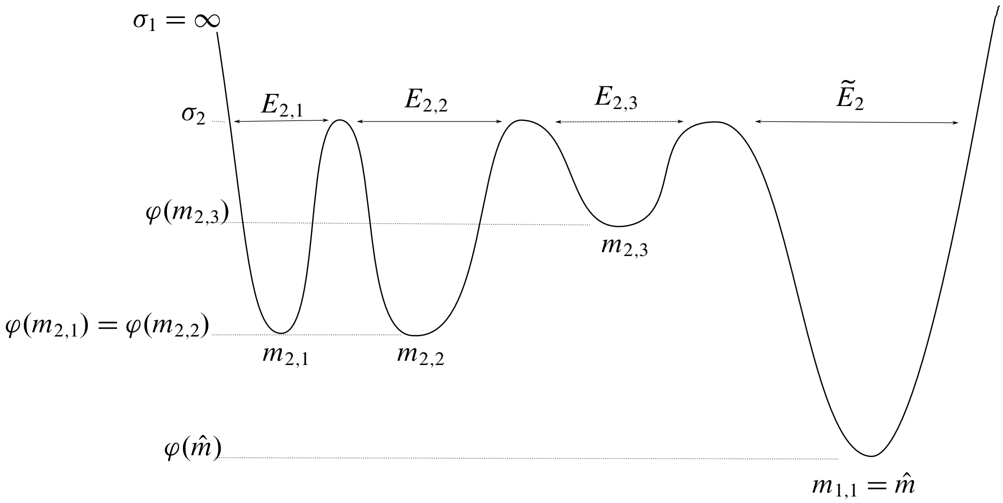

Figure 7. A potential with $p(\alpha) = 2$.

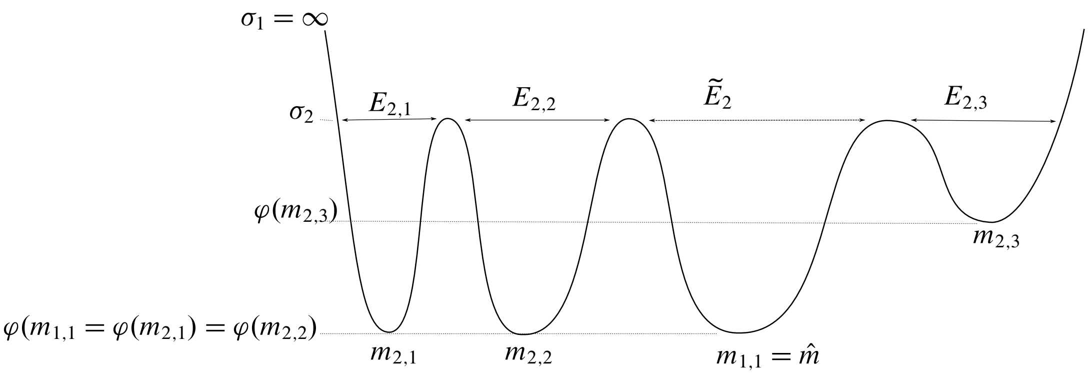

Figure 8. An example with points of type II.

- In the case of Figure 7, we have two equivalence classes: $c_1 = \{\boldsymbol{m}_{1,1}\}$ and $c_2 = \{\boldsymbol{m}_{2,1}, \boldsymbol{m}_{2,2}, \boldsymbol{m}_{2,3}\}$. The potential φ takes two different values on c_2: $p(c_2) = 2$.

We will come back to these examples at the end of the paper and compute explicitly the spectrum of Δ_φ in both cases.

Let us finish this discussion with an example where $\mathcal{U}^{(0),\mathrm{II}} \neq \varnothing$. Consider the potential given by Figure 8. In that case $\hat{\boldsymbol{m}}(\boldsymbol{m}_{2,1}) = \hat{\boldsymbol{m}}(\boldsymbol{m}_{2,2}) = \hat{\boldsymbol{m}}(\boldsymbol{m}_{2,2}) = \boldsymbol{m}_{1,1}$, which we denote by $\hat{\boldsymbol{m}}$ for short. Since $\varphi(\hat{\boldsymbol{m}}) = \varphi(\boldsymbol{m}_{2,1}) = \varphi(\boldsymbol{m}_{2,2}) < \varphi(\boldsymbol{m}_{2,3})$, we know $\boldsymbol{m}_{2,1}$ and $\boldsymbol{m}_{2,2}$ are of type II and $\boldsymbol{m}_{2,3}$ is of type I. We still have $\Omega^0_{\sigma_2} = \{E_{2,1}, E_{2,2}, E_{2,3}\}$ but contrary to the previous case $\widehat{\Omega}_{\sigma_2} = \{\widetilde{E}_2\}$ is nonempty. It follows that $\Omega_{\sigma_2} = \{E_{2,1}, E_{2,2}, E_{2,3}, \widetilde{E}_2\}$ and $\mathcal{R}$ admits two equivalence classes: $c_1 = \{\boldsymbol{m}_{1,1}\}$ and $c_2 = \{\boldsymbol{m}_{2,1}, \boldsymbol{m}_{2,2}, \boldsymbol{m}_{2,3}\}$. The potential φ takes two different values on c_2 and hence $p(c_2) = 2$.

2C. ***General strategy of the proof.*** Let us recall the general strategy followed in [Helffer, Klein and Nier 2004]. The starting point is to use the supersymmetric structure of the Witten Laplacian. For $0 \le k \le n$, let $\Omega^k(X) = \mathcal{C}^\infty(X, \Lambda^k T^* X)$ be the space of k-differential forms and denote by $d : \Omega^k(X) \to \Omega^{k+1}(X)$ the exterior derivative and by $d^* : \Omega^k(X) \to \Omega^{k-1}(X)$ its adjoint for the natural pairing. The Witten complex associated to the function φ is defined by the semiclassical weighted de Rham differentiation

$$d_{\varphi,h} = e^{-\varphi/h} \circ hd \circ e^{\varphi/h} = hd + d\varphi^\wedge$$

and its adjoint

$$d^*_{\varphi,h} = e^{\varphi/h} \circ hd^* \circ e^{-\varphi/h} = hd^* + d\varphi^\lrcorner.$$

Then the semiclassical Witten Laplacian is defined on the forms of any degree by

$$\Delta_\varphi = d^*_{\varphi,h} \circ d_{\varphi,h} + d_{\varphi,h} \circ d^*_{\varphi,h}. \tag{2-17}$$

When restricted to the space of p-forms we denote this operator by $\Delta_\varphi^{(p)}$ (observe that in the case $p = 0$, the above formula yields easily (2-1)). Then, we have the intertwining relation

$$d_{\varphi,h} \Delta_\varphi^{(p)} = \Delta_\varphi^{(p+1)} d_{\varphi,h} \tag{2-18}$$

and its analogue for the coderivative

$$d^*_{\varphi,h} \Delta_\varphi^{(p+1)} = \Delta_\varphi^{(p)} d^*_{\varphi,h}. \tag{2-19}$$

For any $p = 0, \dots, d$, it follows from (2-2) that $\Delta_\varphi^{(p)}$ (as an unbounded operator on L^2) is essentially self-adjoint on the space of compactly supported smooth forms. We still denote by $\Delta_\varphi^{(p)}$ its unique self-adjoint extension. Then $\Delta_\varphi^{(p)}$ is nonnegative and thanks to (2-2), there exists $c_0 > 0$ such that $\sigma_{\text{ess}}(\Delta_\varphi^{(p)}) \subset [c_0, +\infty[$ for any $h > 0$ small enough (in the case where X is a compact manifold, $\Delta_\varphi^{(p)}$ has actually compact resolvent). Moreover, there exists $\epsilon_p > 0$ such that for $h > 0$ small enough, it has exactly n_p eigenvalues in the interval $[0, \epsilon_p h]$, where n_p denotes the number of critical points of index p of φ. We shall denote by $E^{(p)}$ the spectral subspace associated to these small eigenvalues of $\Delta_\varphi^{(p)}$. Then $\dim E^{(p)} = n_p$ and relations (2-18), (2-19) show that

$$d_{\varphi,h}(E^{(p)}) \subset E^{(p+1)} \quad \text{and} \quad d^*_{\varphi,h}(E^{(p+1)}) \subset E^{(p)}. \tag{2-20}$$

This shows in particular that $d_{\varphi,h}$ acts from $E^{(0)}$ into $E^{(1)}$ and we shall denote by $\mathcal{L}$ this operator. Similarly $\Delta_\varphi^{(0)}$ acts on $E^{(0)}$ and we denote by $\mathcal{M}$ this operator. By (2-17), we get

$$\mathcal{M} = \mathcal{L}^* \mathcal{L}.$$

The general strategy used in [Helffer, Klein and Nier 2004] (that we will follow in the present work), is to construct appropriate bases of $E^{(0)}$ and $E^{(1)}$ in which one can compute handily the singular values of $\mathcal{L}$. The main idea to construct such bases is to build accurate quasimodes for Δ_φ and to project them on the spaces $E^{(j)}$. The construction of the quasimodes is performed in Section 3. The quasimodes for 1-forms are the ones constructed in [Helffer and Sjöstrand 1985]. The main properties of these quasimodes will be recalled in Section 3C. Concerning the quasimodes on 0-forms, we cannot use the ones constructed in

[Helffer, Klein and Nier 2004] since many important properties that are required for our analysis fail to be true in the present situation (for instance, the quasiorthogonality). In Section 3B, we use the partition of $\mathcal{U}^{(0)}$ into equivalence classes of $\mathcal{R}$ to construct a family of quasimodes on 0-forms adapted to our setting. Each quasimode will be associated to a minimum $\boldsymbol{m} \in \mathcal{U}^{(0)}$.

In Section 4, we compute the matrix $\mathcal{L}$ in the above basis. One arrives at a block diagonal matrix $\operatorname{diag}(\mathcal{L}^{\alpha}, \alpha \in \mathcal{A})$ whose singular values are the singular values of each block.

Section 5 is devoted to the computation of singular values of the above blocks. The main difficulty is that given two minima $\boldsymbol{m}, \boldsymbol{m}'$ in the same equivalence class, we do not necessarily have $S(\boldsymbol{m}) = S(\boldsymbol{m}')$. For equivalence classes satisfying this property (that is, $p(\alpha) = 1$), each block $\mathcal{L}^{\alpha}$ of the matrix $\mathcal{L}$ has a typical size $e^{-S(\alpha)/h}$ and the situation could be handled quite easily. But more complicated cases may arise where quasimodes yielding different heights $S(\boldsymbol{m})$ are interacting. In order to treat the full general case, we use the Schur complement method combined with an induction on $p(\alpha)$. Running the induction step requires exhibiting a specific structure of the matrices under consideration (see Sections 5A and 5B). In Section 5C, we prove a general result for such matrices, which we use to conclude in Section 5D.

In Section 6, we prove Theorem 2.8.

In the Appendices, we collect several results linear algebra. We also provide a list of notation used in the paper.

3. Construction of adapted quasimodes

3A. ***Gathering minima by equivalence class.*** Let us start this section with a proposition collecting some elementary facts about E, E_- and $\widehat{E}$.

Proposition 3.1. *Let $\boldsymbol{m}, \boldsymbol{m}' \in \mathcal{U}^{(0)}$ such that $\boldsymbol{m} \neq \boldsymbol{m}'$. Then, we have the following*:

- (i) *If $\sigma(\boldsymbol{m}) = \sigma(\boldsymbol{m}')$, then*
  - (i.a) $E(\boldsymbol{m}) \cap E(\boldsymbol{m}') = \varnothing$,
  - (i.b) *either $E_-(\boldsymbol{m}) = E_-(\boldsymbol{m}')$ or $E_-(\boldsymbol{m}) \cap E_-(\boldsymbol{m}') = \varnothing$,*
  - (i.c) *if $E_-(\boldsymbol{m}) = E_-(\boldsymbol{m}')$ then $\widehat{E}(\boldsymbol{m}) = \widehat{E}(\boldsymbol{m}')$; otherwise $\widehat{E}(\boldsymbol{m}) \cap \widehat{E}(\boldsymbol{m}') = \varnothing$.*
- (ii) *If $\sigma(\boldsymbol{m}) > \sigma(\boldsymbol{m}')$, then*
  - (ii.a) *either $E(\boldsymbol{m}) \cap E(\boldsymbol{m}') = \varnothing$ or $E_-(\boldsymbol{m}') \subset E(\boldsymbol{m})$,*
  - (ii.b) *either $E_-(\boldsymbol{m}) \cap E_-(\boldsymbol{m}') = \varnothing$ or $E_-(\boldsymbol{m}') \subset E_-(\boldsymbol{m})$.*

Proof. Let $\boldsymbol{m} \neq \boldsymbol{m}'$ be two minima. Assume first that $\sigma(\boldsymbol{m}) = \sigma(\boldsymbol{m}') = \sigma$. Since $\boldsymbol{m} \neq \boldsymbol{m}'$ and $\boldsymbol{\sigma}^{-1}(\infty) = \{\underline{\boldsymbol{m}}\}$, we have necessarily $\boldsymbol{m}, \boldsymbol{m}' \in \underline{\mathcal{U}}^{(0)}$. In particular, $E_-(\nu), \widehat{E}(\nu)$, $\nu = \boldsymbol{m}, \boldsymbol{m}'$, are well-defined. Moreover, since $E(\boldsymbol{m})$ and $E(\boldsymbol{m}')$ are two connected components of $\{\varphi < \sigma\}$, we have either $E(\boldsymbol{m}) = E(\boldsymbol{m}')$ or $E(\boldsymbol{m}) \cap E(\boldsymbol{m}') = \varnothing$. Since $\boldsymbol{m} \neq \boldsymbol{m}'$ and E is injective, $E(\boldsymbol{m}) \cap E(\boldsymbol{m}') = \varnothing$, which proves (i.a).

Since $E_-(\boldsymbol{m})$ and $E_-(\boldsymbol{m}')$ are two connected component of the same set $\{\varphi < \tau\}$ for some $\tau > \sigma(\boldsymbol{m})$, (i.b) is obvious.

Suppose now that $E_-(\boldsymbol{m}) = E_-(\boldsymbol{m}')$. Since $\sigma(\boldsymbol{m}) = \sigma(\boldsymbol{m}')$, we have $\hat{\boldsymbol{m}}(\boldsymbol{m}) = \hat{\boldsymbol{m}}(\boldsymbol{m}')$. Moreover, since $\widehat{E}(\boldsymbol{m})$ is the unique connected component of $\{\varphi < \sigma(\boldsymbol{m})\}$ containing $\hat{\boldsymbol{m}}(\boldsymbol{m})$, we get $\widehat{E}(\boldsymbol{m}) = \widehat{E}(\boldsymbol{m}')$.

If $E_-(\boldsymbol{m})$ and $E_-(\boldsymbol{m}')$ are disjoint, then $\widehat{E}(\boldsymbol{m})$ and $\widehat{E}(\boldsymbol{m}')$ are also disjoint since $\widehat{E}(\boldsymbol{m}) \subset E_-(\boldsymbol{m})$ and $\widehat{E}(\boldsymbol{m}') \subset E_-(\boldsymbol{m}')$. This completes the proof of (i.c).

Let us now prove (ii) and assume that $\sigma(\boldsymbol{m}) > \sigma(\boldsymbol{m}')$. Once again, since $\boldsymbol{\sigma}^{-1}(\infty) = \{\underline{\boldsymbol{m}}\}$, we have $\boldsymbol{m}' \in \underline{\mathcal{U}}^{(0)}$. If $E(\boldsymbol{m}') \cap E(\boldsymbol{m}) \neq \varnothing$, then $E_-(\boldsymbol{m}') \cap E(\boldsymbol{m}) \neq \varnothing$. Moreover, $E_-(\boldsymbol{m}')$ is a connected component of $\{\varphi < \tau\}$ for some $\tau \leq \sigma(\boldsymbol{m})$. Since $E(\boldsymbol{m})$ is a connected component of $\{\varphi < \sigma(\boldsymbol{m})\} \supset \{\varphi < \tau\}$, we have $E_-(\boldsymbol{m}') \subset E(\boldsymbol{m})$ which proves (ii.a).

The point (ii.b) is proved by similar arguments. □

Let us now decompose the set of separating saddle points according to the equivalence classes. Given $\alpha \in \underline{\mathcal{A}}$, introduce the closed set

$$G(\alpha) = \bigcup_{\boldsymbol{m} \in \mathcal{U}_\alpha^{(0)}} \overline{E(\boldsymbol{m})} \tag{3-1}$$

and for any $\alpha \in \underline{\mathcal{A}}$ let

$$\mathcal{V}_\alpha^{(1)} = \{\boldsymbol{s} \in \mathcal{V}^{(1)} : \varphi(\boldsymbol{s}) = \boldsymbol{\sigma}(\alpha)\} \cap G(\alpha). \tag{3-2}$$

For any $\alpha \in \underline{\mathcal{A}}$, let

$$\widehat{\mathcal{U}}_\alpha^{(0)} = \mathcal{U}_\alpha^{(0)} \cup \{\hat{\boldsymbol{m}}(\alpha)\} \tag{3-3}$$

and define an application Γ_α from $\widehat{\mathcal{U}}_\alpha^{(0)}$ into the closed subsets of X by

$$\begin{cases} \Gamma_\alpha(\boldsymbol{m}) = \Gamma(\boldsymbol{m}) & \text{if } \boldsymbol{m} \in \mathcal{U}_\alpha^{(0)}, \\ \Gamma_\alpha(\hat{\boldsymbol{m}}(\alpha)) = \partial \widehat{E}(\alpha), \end{cases} \tag{3-4}$$

where Γ is defined below (2-5).

Remark 3.2. Since $\widehat{E}(\boldsymbol{m}) \subsetneq E(\hat{\boldsymbol{m}})$, the application Γ_α is slightly different from the application Γ defined in below (2-5). Observe also that for all $\boldsymbol{m} \in \widehat{\mathcal{U}}_\alpha^{(0)}$, $\Gamma_\alpha(\boldsymbol{m})$ is the boundary of the connected component of $\{\varphi < \varphi(\boldsymbol{s})\}$ that contains $\boldsymbol{m}$.

Lemma 3.3. *The collection $(\mathcal{V}_\alpha^{(1)})_{\alpha \in \underline{\mathcal{A}}}$ is a partition of $\mathcal{V}^{(1)}$. Moreover, for all $\alpha \in \underline{\mathcal{A}}$ and $\boldsymbol{s} \in \mathcal{V}_\alpha^{(1)}$, there exists $\boldsymbol{m}_1(\boldsymbol{s}) \in \mathcal{U}_\alpha^{(0)}$ and $\boldsymbol{m}_2(\boldsymbol{s}) \in \widehat{\mathcal{U}}_\alpha^{(0)}$ such that*

$$\boldsymbol{s} \in \Gamma_\alpha(\boldsymbol{m}_1) \cap \Gamma_\alpha(\boldsymbol{m}_2). \tag{3-5}$$

One can chose $\boldsymbol{m}_1, \boldsymbol{m}_2$ in order that $S(\boldsymbol{m}_1) \leq S(\boldsymbol{m}_2)$ (that is, $\varphi(\boldsymbol{m}_1) \geq \varphi(\boldsymbol{m}_2)$). Up to permutation, the pair $(\boldsymbol{m}_1(\boldsymbol{s}), \boldsymbol{m}_2(\boldsymbol{s}))$ is unique.

Proof. Let $\boldsymbol{s} \in \mathcal{V}^{(1)}$; then $\varphi(\boldsymbol{s}) \in \underline{\Sigma}$ and there exists $k \geq 2$ such that $\varphi(\boldsymbol{s}) = \sigma_k$. By definition, there exist two different connected components E_1, E_2 of $\{\varphi < \sigma_k\}$ such that $\boldsymbol{s} \in \overline{E}_1 \cap \overline{E}_2$. From the existence part of Remark 2.2 there exist $\boldsymbol{m}_{l,i} \in E_1$ and $\boldsymbol{m}_{l',i'} \in E_2$ with $l' \leq l \leq k$. Moreover, one has necessarily $l = k$. Otherwise $\boldsymbol{\sigma}(\boldsymbol{m}_{l,i}) > \sigma_k$ and since $\overline{E}_1 \cap \overline{E}_2 \neq \varnothing$, this would imply that $\boldsymbol{m}_{l',i'} \in E(\boldsymbol{m}_{l,i})$, which is impossible since $l' \leq l$. Hence we have $l = k$. Therefore E_1 is equal to $E(\boldsymbol{m}_{l,i})$ with $\boldsymbol{m}_{l,i} \in \mathcal{U}_\alpha^{(0)}$, which proves that $\boldsymbol{s} \in \mathcal{V}_\alpha^{(1)}$. Moreover, E_2 is either of the form $E_2 = E(\boldsymbol{m}_{l',i'})$ with $\boldsymbol{m}_{l',i'} \in \mathcal{U}_\alpha^{(0)}$ (if $l' = k$) or $E_2 = \widehat{E}(\boldsymbol{m}_{l,i})$ (if $l' < k$). Setting $\boldsymbol{m}_1(\boldsymbol{s}) = \boldsymbol{m}_{l,i} \in \mathcal{U}_\alpha^{(0)}$ and $\boldsymbol{m}_2(\boldsymbol{s}) = \boldsymbol{m}_{l',i'} \in \widehat{\mathcal{U}}_\alpha^{(0)}$, one has $\boldsymbol{s} \in \Gamma_\alpha(\boldsymbol{m}_1) \cap \Gamma_\alpha(\boldsymbol{m}_2)$ and since $l \geq l'$ one has also $\varphi(\boldsymbol{m}_1) \geq \varphi(\boldsymbol{m}_2)$.

Let us now prove that the union of the $\mathcal{V}_\alpha^{(1)}$ for $\alpha \in \underline{\mathcal{A}}$ is disjoint. Suppose that $\boldsymbol{s} \in \mathcal{V}_\alpha^{(1)} \cap \mathcal{V}_\beta^{(1)}$. Then $\sigma(\alpha) = \varphi(\boldsymbol{s}) = \sigma(\beta)$. Moreover, there exist $\boldsymbol{m} \in \mathcal{U}_\alpha^{(0)}$ and $\boldsymbol{m}' \in \mathcal{U}_\beta^{(0)}$ such that $\boldsymbol{s} \in \overline{E(\boldsymbol{m})} \cap \overline{E(\boldsymbol{m}')}$. This proves that $\boldsymbol{m}\mathcal{R}\boldsymbol{m}'$ and hence $\alpha = \beta$.

The uniqueness of $(\boldsymbol{m}_1, \boldsymbol{m}_2)$ up to permutation is obvious. □

Let us now introduce an extra partition that will be useful in the sequel.

Lemma 3.4. *For all $\alpha \in \mathcal{A}$ there exists a partition $\mathcal{V}_\alpha^{(1)} = \mathcal{V}_\alpha^{(1),\boldsymbol{b}} \sqcup \mathcal{V}_\alpha^{(1),\boldsymbol{i}}$ such that the following hold true*:

(i) *For any $\boldsymbol{s} \in \mathcal{V}_\alpha^{(1),\boldsymbol{i}}$, $\boldsymbol{m}_1(\boldsymbol{s})$ and $\boldsymbol{m}_2(\boldsymbol{s})$ belong to $\mathcal{U}_\alpha^{(0)}$.*

(ii) *The set $\mathcal{V}_\alpha^{(1),b}$ is nonempty and for all $\boldsymbol{s} \in \mathcal{V}_\alpha^{(1),b}$ one has $\boldsymbol{m}_1(\boldsymbol{s}) \in \mathcal{U}_\alpha^{(0)}$, $\boldsymbol{m}_2(\boldsymbol{s}) = \hat{\boldsymbol{m}}(\alpha)$ and*

$$\boldsymbol{s} \in \Gamma_\alpha(\boldsymbol{m}_1(\boldsymbol{s})) \cap \Gamma_\alpha(\hat{\boldsymbol{m}}(\alpha)).$$

Proof. Define $\mathcal{V}_\alpha^{(1),\boldsymbol{i}} = \{\boldsymbol{s} \in \mathcal{V}_\alpha^{(1)} : \boldsymbol{m}_1(\boldsymbol{s}), \boldsymbol{m}_2(\boldsymbol{s}) \in \mathcal{U}_\alpha^{(0)}\}$. Then (i) is true by definition. Moreover, defining $\mathcal{V}_\alpha^{(1),\boldsymbol{b}} = \mathcal{V}_\alpha^{(1)} \setminus \mathcal{V}_\alpha^{(1),\boldsymbol{i}}$, one has automatically the partition property and it remains to prove (ii).

Since $\alpha \in \underline{\mathcal{A}}$, the set $\overline{\widehat{E}(\alpha)} \cap \big(\bigcup_{\boldsymbol{m}\in\mathcal{U}_\alpha^{(0)}} \overline{E(\boldsymbol{m})}\big)$ is nonempty and contained in $\mathcal{V}_\alpha^{(1),\boldsymbol{b}}$. This proves that $\mathcal{V}_\alpha^{(1),\boldsymbol{b}}$ is not empty. Suppose now that $\boldsymbol{s} \in \mathcal{V}_\alpha^{(1),b}$. It follows from Lemma 3.3 that $\boldsymbol{m}_1(\boldsymbol{s}) \in \mathcal{U}_\alpha^{(0)}$ and $\boldsymbol{m}_2(\boldsymbol{s}) \in \widehat{\mathcal{U}}_\alpha^{(0)}$. But by the definition of $\mathcal{V}_\alpha^{(1),\boldsymbol{b}}$, $\boldsymbol{m}_2(\boldsymbol{s})$ cannot belong to $\mathcal{U}_\alpha^{(0)}$, which implies by definition that $\boldsymbol{m}_2(\boldsymbol{s}) = \hat{\boldsymbol{m}}(\alpha)$. This completes the proof of (ii). □

3B. *Quasimodes for* 0*-forms.* In this section we construct a family of quasimodes of $\Delta_\varphi^{(0)}$ associated to the minima of φ. Each of these quasimodes will be of the form $x \mapsto h^{-d/4}\chi_{\boldsymbol{m}}(x)e^{-(\varphi(x)-\varphi(\boldsymbol{m}))/h}$ with some suitable cut-off functions $\chi_{\boldsymbol{m}}$ associated to a minimum $\boldsymbol{m} \in \mathcal{U}^{(0)}$.

Following [Helffer, Klein and Nier 2004], we can associate to each minimum $\boldsymbol{m} \in \mathcal{U}^{(0)}$ a cut-off function $\chi_{\boldsymbol{m}}$ in the following way. For $\boldsymbol{m} = \underline{\boldsymbol{m}}$, we simply take $\chi_{\underline{\boldsymbol{m}}} = 1$. For $\boldsymbol{m} \in \underline{\mathcal{U}}^{(0)}$ we introduce some small parameters $\epsilon, \tilde{\epsilon}, \delta > 0$ with $\tilde{\epsilon} < \epsilon$ and we define

$$E_{\epsilon,\tilde{\epsilon},\delta}(\boldsymbol{m}) = \Bigg(\bigg(E(\boldsymbol{m}) \setminus \bigcup_{\boldsymbol{s}\in\mathcal{V}^{(1)}\cap\Gamma(\boldsymbol{m})} B(\boldsymbol{s},\epsilon)\bigg) + B(0,\tilde{\epsilon})\Bigg) \cup \Bigg(\bigcup_{\boldsymbol{s}\in(\mathcal{U}^{(1)}\setminus\mathcal{V}^{(1)})\cap\Gamma(\boldsymbol{m})} B(\boldsymbol{s},\delta)\Bigg). \tag{3-6}$$

Proposition 3.5. *Let $\chi_{\boldsymbol{m}}$ be any function in $\mathscr{C}_c^\infty(E_{\epsilon,2\tilde{\epsilon},2\delta}(\boldsymbol{m}))$ such that $\chi_{\boldsymbol{m}} = 1$ on $E_{\epsilon,\tilde{\epsilon},\delta}(\boldsymbol{m})$. There exist $\epsilon_0 > 0$, $\delta_0 > 0$ and $C > 0$ such that for all $0 < \delta < \delta_0$, all $0 < \epsilon < \epsilon_0$ and all $0 < \tilde{\epsilon} < \epsilon/4$, the following hold true*:

(a) *If $x \in \operatorname{supp}(\chi_{\boldsymbol{m}})$ and $\varphi(x) < \sigma(\boldsymbol{m})$, then $x \in E(\boldsymbol{m})$.*

(b) *There exists $c_\epsilon > 0$ such that for all $x \in \operatorname{supp}(\nabla\chi_{\boldsymbol{m}})$, we have*

- *either $x \notin \bigcup_{\boldsymbol{s}\in\mathcal{V}^{(1)}\cap\Gamma(\boldsymbol{m})} B(\boldsymbol{s},\epsilon)$ and*

$$\sigma(\boldsymbol{m}) + c_\epsilon^{-1} < \varphi(x) < \sigma(\boldsymbol{m}) + c_\epsilon,$$

- *or $x \in \bigcup_{\boldsymbol{s}\in\mathcal{V}^{(1)}\cap\Gamma(\boldsymbol{m})} B(\boldsymbol{s},\epsilon)$ and*

$$|\varphi(x) - \sigma(\boldsymbol{m})| \le C\epsilon.$$

(c) *For all* $s \in \mathcal{U}^{(1)} \setminus (\mathcal{V}^{(1)} \cap \Gamma(\boldsymbol{m}))$, *one has* $\operatorname{dist}(s, \operatorname{supp} \nabla \chi_{\boldsymbol{m}}) \geq \delta$. *If moreover* $s \in \operatorname{supp}(\chi_{\boldsymbol{m}})$ *then* $s \in \overline{E(\boldsymbol{m})}$ *and* $\chi_{\boldsymbol{m}} = 1$ *near* s.

(d) *Suppose that* $\boldsymbol{m} \in \mathcal{U}_\alpha^{(0)}$, $\alpha \in \mathcal{A}$, *and let* $s \in \mathcal{V}^{(1)} \cap \operatorname{supp}(\chi_{\boldsymbol{m}})$. *Then, there exists* $\beta \in \underline{\mathcal{A}}$ *such that* $\boldsymbol{\sigma}(\beta) < \boldsymbol{\sigma}(\alpha)$, $s \in \mathcal{V}_\beta^{(1)}$ *and* $\bigcup_{\boldsymbol{m}' \in \mathcal{U}_\beta^{(0)}} E(\boldsymbol{m}') \subset \{x \in X : \chi_{\boldsymbol{m}}(x) = 1\}$.

Proof. Observe that the construction of the cut-off functions $\chi_{\boldsymbol{m}}$ is slightly different to that of the $\chi_{k,\epsilon}$ in Proposition 4.2 in [Helffer, Klein and Nier 2004] (in particular because there can exist more than one separating saddle point on $\partial E(\boldsymbol{m})$).

Let $\delta_1 = \min\{|s - s'| : s, s' \in \mathcal{U}^{(1)},\ s \neq s'\}$ and $\delta_2 = \min\{\operatorname{dist}(s, \Gamma(\boldsymbol{m})) : s \in E(\boldsymbol{m}) \cap \mathcal{U}^{(1)}\}$. Let $0 < \delta < \frac{1}{4}\min(\delta_1, \delta_2)$ and $\epsilon_0 > 0$ such that there exists $C > 0$ such that for all $0 < \epsilon < \epsilon_0$ and all $s \in \mathcal{V}^{(1)}$, one has

$$|\varphi(x) - \varphi(s)| < C\epsilon \quad \text{for all } x \in B(s, \epsilon).$$

This is possible since φ is a smooth function. Then (a) and (b) above can be proved much as Proposition 4.2 in [Helffer, Klein and Nier 2004] and (c) is a direct consequence of our choice of δ.

Let us now prove (d). By definition, if $s \in \mathcal{V}^{(1)} \cap \operatorname{supp}(\chi_{\boldsymbol{m}})$, then $s \in E(\boldsymbol{m})$ (here we use the condition $0 < \tilde{\epsilon} < \epsilon/4$). Hence, there exists $\beta \neq \alpha$ such that $s \in \mathcal{V}_\beta^{(1)}$ and one has additionally $\boldsymbol{\sigma}(\beta) < \boldsymbol{\sigma}(\alpha)$. By definition of the sets $E(\boldsymbol{m})$, this implies that

$$\bigcup_{\boldsymbol{m}' \in \mathcal{U}_\beta^{(0)}} E(\boldsymbol{m}') \subset E(\boldsymbol{m}) \setminus \bigcup_{s' \in \mathcal{V}^{(1)} \cap \Gamma(\boldsymbol{m})} B(s', \epsilon)$$

for any $\epsilon \in]0, \epsilon_0[$ with $\epsilon_0 > 0$ small enough independent of δ. This implies the results. □

We are now in position to define the quasimodes in a recursive way on the values of $\boldsymbol{\sigma}(\alpha)$.

- We start with the quasimode associated to $\underline{\boldsymbol{m}}$. We set

$$f_{\underline{\boldsymbol{m}}}^{(0)}(x) = c(\underline{\boldsymbol{m}}, h) h^{-d/4} e^{(\varphi(\underline{\boldsymbol{m}}) - \varphi(x))/h}, \tag{3-7}$$

where $c(\underline{\boldsymbol{m}}, h)$ is a normalizing constant such that $\| f_{\underline{\boldsymbol{m}}} \|_{L^2} = 1$. Due to the fact that φ may have several global minima, the function $f_{\underline{\boldsymbol{m}}}^{(0)}$ does not concentrate only on $\underline{\boldsymbol{m}}$ but on the reunion of all global minima. Hence the normalizing factor $c(\underline{\boldsymbol{m}}, h)$ is computed by adding the contributions coming from each of these minima via quadratic approximation. More precisely, it follows from the Laplace method that $c(\underline{\boldsymbol{m}}, h) \sim \sum_{k=0}^{\infty} h^k \gamma_k(\underline{\boldsymbol{m}})$ with the function γ_0 given by

$$\gamma_0(\boldsymbol{m})^{-2} = \pi^{d/2} \sum_{\boldsymbol{m}' \in H(\boldsymbol{m})} |\det \operatorname{Hess} \varphi(\boldsymbol{m}')|^{-1/2}, \tag{3-8}$$

where by definition (2-6) one has

$$H(\boldsymbol{m}) := \{\boldsymbol{m}' \in E(\boldsymbol{m}) \cap \mathcal{U}^{(0)} : \varphi(\boldsymbol{m}') = \varphi(\boldsymbol{m})\}.$$

Finally, observe that $f_{\underline{\boldsymbol{m}}}^{(0)}$ is an exact quasimode: $\Delta_\varphi f_{\underline{\boldsymbol{m}}}^{(0)} = 0$.

• Suppose now that $k \in \{2, \dots, K\}$ and that the quasimodes $f_{\boldsymbol{m}}^{(0)}$ have been constructed for $\boldsymbol{m} \in \bigcup_{\alpha' \in \underline{\mathcal{A}}, \boldsymbol{\sigma}(\alpha') \leq \sigma_{k-1}} \mathcal{U}_{\alpha}^{(0)}$, and let us define $f_{\boldsymbol{m}}^{(0)}$ for $\boldsymbol{m} \in \mathcal{U}_{\alpha}^{(0)}$ with $\boldsymbol{\sigma}(\alpha) = \sigma_k$. The form of the quasimode associated to $\boldsymbol{m}$ depends on the type of $\boldsymbol{m}$ as introduced in Definition 2.3.

– If $\boldsymbol{m}$ is of type I, then we define $f_{\boldsymbol{m}}^{(0)}$ as in [Helffer, Klein and Nier 2004] by

$$f_{\boldsymbol{m}}^{(0)}(x) = c(\boldsymbol{m}, h) h^{-d/4} \chi_{\boldsymbol{m}}(x) e^{(\varphi(\boldsymbol{m}) - \varphi(x))/h}, \tag{3-9}$$

where $\chi_{\boldsymbol{m}}$ is the cut-off function associated to $\boldsymbol{m}$ defined in Proposition 3.5 and $c(\boldsymbol{m}, h)$ is again a normalizing constant such that $\| f_{\boldsymbol{m}}^{(0)} \|_{L^2} = 1$. As before, we have to add all the contributions of minima in $E(\boldsymbol{m})$ at the same height as $\boldsymbol{m}$. We get $c(\boldsymbol{m}, h) \sim \sum_{k=0}^{\infty} h^k \gamma_k(\boldsymbol{m})$ with $\gamma_0(\boldsymbol{m})$ given by (3-8).

– Let us now construct quasimodes associated to minima $\boldsymbol{m}$ of type II. We assume here that $\mathcal{U}^{(0),\mathrm{II}} \neq \varnothing$ and we define

$$\widehat{\mathcal{U}}_{\alpha}^{(0),\mathrm{II}} = \mathcal{U}_{\alpha}^{(0),\mathrm{II}} \cup \{\hat{\boldsymbol{m}}\}, \tag{3-10}$$

where for short, we write $\hat{\boldsymbol{m}} = \hat{\boldsymbol{m}}(\alpha)$ and $q_{\alpha}^{\mathrm{II}} = \# \mathcal{U}_{\alpha}^{(0),\mathrm{II}}$.

Let us introduce an additional cut-off function around $\hat{\boldsymbol{m}}$ that we define as follows. Recall that $\widehat{E}(\alpha)$ denotes the connected component of $\{x \in E_-(\boldsymbol{m}) : \varphi(x) < \sigma(\boldsymbol{m})\}$ that contains $\hat{\boldsymbol{m}}$. As before, we introduce some parameters $\epsilon, \tilde{\epsilon}, \delta > 0$ with $\tilde{\epsilon} < \epsilon$ and we define

$$\widehat{E}_{\epsilon,\tilde{\epsilon},\delta}(\alpha) = \left(\left(\widehat{E}(\alpha) \setminus \bigcup_{\boldsymbol{s} \in \mathcal{V}^{(1)} \cap \partial \widehat{E}(\alpha)} B(\boldsymbol{s}, \epsilon) \right) + B(0, \tilde{\epsilon}) \right) \cup \left(\bigcup_{\boldsymbol{s} \in (\mathcal{U}^{(1)} \setminus \mathcal{V}^{(1)}) \cap \partial \widehat{E}(\alpha)} B(\boldsymbol{s}, \delta) \right).$$

Then, we let $\hat{\chi}_{\hat{\boldsymbol{m}}}$ be any function in $\mathscr{C}_c^{\infty}(\widehat{E}_{\epsilon,2\tilde{\epsilon},2\delta}(\alpha))$ such that $\hat{\chi}_{\hat{\boldsymbol{m}}} = 1$ on $\widehat{E}_{\epsilon,\tilde{\epsilon},\delta}(\alpha)$. For $\boldsymbol{m} \in \mathcal{U}_{\alpha}^{(0),\mathrm{II}}$, we let $\hat{\chi}_{\boldsymbol{m}} = \chi_{\boldsymbol{m}}$, with $\chi_{\boldsymbol{m}}$ defined in Proposition 3.5. We want to construct the quasimode as a linear combination of the $\hat{\chi}_{\boldsymbol{m}} e^{-\varphi/h}$, $\boldsymbol{m} \in \widehat{\mathcal{U}}_{\alpha}^{(0),\mathrm{II}}$. In order to chose the coefficients, let us introduce $\mathcal{F}_{\alpha} = \mathscr{F}(\widehat{\mathcal{U}}_{\alpha}^{(0),\mathrm{II}})$, the finite vector space of functions from $\widehat{\mathcal{U}}_{\alpha}^{(0),\mathrm{II}}$ into $\mathbb{R}$. This space has dimension $q_{\alpha}^{\mathrm{II}} + 1$ and is endowed with the usual Euclidean structure

$$\langle \theta, \theta' \rangle_{\mathcal{F}_{\alpha}} = \sum_{\boldsymbol{m} \in \widehat{\mathcal{U}}_{\alpha}^{(0),\mathrm{II}}} \theta(\boldsymbol{m}) \theta'(\boldsymbol{m}).$$

We denote by N the associated norm. Eventually, we define $\theta_0^{\alpha} \in \mathcal{F}_{\alpha}$ by

$$\theta_0^{\alpha}(\boldsymbol{m}) = \frac{c_0^{\alpha}(h)}{c(\boldsymbol{m}, h)}, \tag{3-11}$$

where $c(\boldsymbol{m}, h)$ is the unique positive constant such that the function

$$\tilde{f}_{\boldsymbol{m}} := c(\boldsymbol{m}, h) h^{-d/4} \hat{\chi}_{\boldsymbol{m}} e^{(\varphi(\boldsymbol{m}) - \varphi(x))/h}$$

satisfies $\| \tilde{f}_{\boldsymbol{m}} \|_{L^2} = 1$ and $c_0^{\alpha}(h)$ is defined by $N(\theta_0^{\alpha}) = 1$. Let us now extend the definition of the set $H(\boldsymbol{m})$ in the following way. Given $\alpha \in \mathcal{A}$ and $\boldsymbol{m} \in \widehat{\mathcal{U}}_{\alpha}^{(0),\mathrm{II}}$ we define

$$\widehat{H}_{\alpha}(\boldsymbol{m}) = \begin{cases} H(\boldsymbol{m}) & \text{if } \boldsymbol{m} \in \mathcal{U}_{\alpha}^{(0)}, \\ \{\boldsymbol{m}' \in \widehat{E}(\alpha) \cap \mathcal{U}^{(0)} : \varphi(\boldsymbol{m}') = \varphi(\hat{\boldsymbol{m}})\} & \text{if } \boldsymbol{m} \in \widehat{\mathcal{U}}_{\alpha}^{(0),\mathrm{II}} \setminus \mathcal{U}_{\alpha}^{(0)}. \end{cases} \tag{3-12}$$

Observe that if α is of type II, since $E(\hat{\boldsymbol{m}}(\alpha))$ is larger than $\widehat{E}(\alpha)$, the sets $H(\hat{\boldsymbol{m}}(\alpha))$ and $\widehat{H}_\alpha(\hat{\boldsymbol{m}}(\alpha))$ may be different. From the preceding definition, it follows that for all $\boldsymbol{m} \in \widehat{\mathcal{U}}_\alpha^{(0),\mathrm{II}}$, the normalizing factor $c(\boldsymbol{m},h)$ admits a classical expansion $c(\boldsymbol{m},h) = \sum_k h^k \gamma_k(\boldsymbol{m})$ with

$$\gamma_0(\boldsymbol{m})^{-2} = \pi^{d/2} \sum_{\boldsymbol{m}' \in \widehat{H}_\alpha(\boldsymbol{m})} |\det \operatorname{Hess} \varphi(\boldsymbol{m}')|^{-1/2}. \tag{3-13}$$

Therefore, we can compute the constant $c_0^\alpha(h)$, and we get

$$c_0^\alpha(h) = \pi^{-d/4} \Bigg(\sum_{\nu \in \widehat{\mathcal{U}}_\alpha^{(0),\mathrm{II}}} \sum_{\boldsymbol{m}' \in \widehat{H}_\alpha(\nu)} |\det \operatorname{Hess} \varphi(\boldsymbol{m}')|^{-1/2} \Bigg)^{-1/2} + \mathcal{O}(h).$$

Here the index α is used to indicate that the function is associated to $\mathcal{U}_\alpha^{(0),\mathrm{II}}$.

Lemma 3.6. *There exist some functions $\theta_1^\alpha, \dots, \theta_{q_\alpha^{\mathrm{II}}}^\alpha \in \mathcal{F}_\alpha$ such that the following hold true*:

(i) *$\{\theta_j^\alpha, j = 0, \dots, q_\alpha^{\mathrm{II}}\}$ is an orthonormal basis of $\mathcal{F}_\alpha$.*

(ii) *The functions θ_j^α admit a classical expansion*

$$\theta_j^\alpha = \sum_{k \ge 0} h^k \theta_j^{\alpha,k}$$

and for all $j \ge 1$, the leading terms $\theta_j^{\alpha,0}$ are orthogonal to the function $\theta_0^{\alpha,0}(\boldsymbol{m}) = c_0^\alpha(0)/\gamma_0(\boldsymbol{m})$.

Proof. First observe that θ_0^α admits a classical expansion $\theta_0^\alpha \sim \sum_{j \ge 0} h^j \theta_0^{\alpha,j}$ with $\theta_0^{\alpha,0}(\boldsymbol{m}) = c_0^\alpha(0)/\gamma_0(\boldsymbol{m})$. Since $(\theta_0^{\alpha,0})^\perp$ is a q_α^{II}-dimensional subspace of $\mathcal{F}_\alpha$, it admits an orthonormal basis $(\tilde{\theta}_j^{\alpha,0})$ independent of h. Then the functions $\tilde{\theta}_j^\alpha$ defined by

$$\tilde{\theta}_j^\alpha := \tilde{\theta}_j^{\alpha,0} - \langle \tilde{\theta}_j^{\alpha,0}, \theta_0^\alpha \rangle \theta_0^\alpha$$

form a basis of $(\theta_0^\alpha)^\perp$. Moreover, the $\tilde{\theta}_j^\alpha$ admit a classical expansion and since $\langle \tilde{\theta}_j^{\alpha,0}, \theta_0^\alpha \rangle = \mathcal{O}(h)$ for any j, they satisfy

$$\langle \tilde{\theta}_j^\alpha, \tilde{\theta}_k^\alpha \rangle = \delta_{jk} + \mathcal{O}(h^2).$$

Defining the (θ_j^α) as the Gram–Schmidt orthonormalization of the $(\tilde{\theta}_j^\alpha)$, we get the desired result. ☐

Observe that since $\mathcal{U}_\alpha^{(0),\mathrm{II}}$ has q_α^{II} elements, the functions $\theta_1^\alpha, \dots, \theta_{q_\alpha^{\mathrm{II}}}^\alpha$ can also be indexed by $\mathcal{U}_\alpha^{(0),\mathrm{II}}$ using any arbitrary bijection. We end up with a family of functions $(\theta_{\boldsymbol{m}}^\alpha)_{\boldsymbol{m} \in \mathcal{U}_\alpha^{(0),\mathrm{II}}}$ and for convenience we will also write $\theta_{\hat{\boldsymbol{m}}}^\alpha = \theta_0^\alpha$. Then, we define the q_α^{II} quasimodes associated to the $\boldsymbol{m} \in \mathcal{U}_\alpha^{(0),\mathrm{II}}$ by

$$f_{\boldsymbol{m}}^{(0)}(x) = h^{-d/4} \sum_{\boldsymbol{m}' \in \widehat{\mathcal{U}}_\alpha^{(0),\mathrm{II}}} \theta_{\boldsymbol{m}}^\alpha(\boldsymbol{m}') c(\boldsymbol{m}', h) \hat{\chi}_{\boldsymbol{m}'}(x) e^{(\varphi(\boldsymbol{m}) - \varphi(x))/h}, \tag{3-14}$$

where the normalization factor $c(\boldsymbol{m}', h)$ is defined above and ensures that

$$\| c(\boldsymbol{m}', h) h^{-d/4} \hat{\chi}_{\boldsymbol{m}'}(x) e^{(\varphi(\boldsymbol{m}) - \varphi(x))/h} \|_{L^2} = 1.$$

Before going further and as a preparation for the final analysis we would like to write the quasimode given by (3-9) and (3-14) in the same fashion. For this purpose, we define $\widehat{\mathcal{U}}_\alpha^{(0)}$ by

$$\widehat{\mathcal{U}}_\alpha^{(0)} = \mathcal{U}_\alpha^{(0),\mathrm{I}} \cup \widehat{\mathcal{U}}_\alpha^{(0),\mathrm{II}}, \tag{3-15}$$

with the convention that $\widehat{\mathcal{U}}_\alpha^{(0),\mathrm{II}} = \varnothing$ if $\mathcal{U}_\alpha^{(0),\mathrm{II}} = \varnothing$ (observe that $\widehat{\mathcal{U}}_\alpha^{(0)}$ is equal to the set $\widehat{\mathcal{U}}_\alpha^{(0)}$ defined in (3-3) if and only if $\mathcal{U}_\alpha^{(0),\mathrm{II}} \neq \varnothing$). Then, we define $\theta_{\boldsymbol{m}}^\alpha(\boldsymbol{m}')$ for any $\boldsymbol{m} \in \mathcal{U}_\alpha^{(0)}$, $\boldsymbol{m}' \in \widehat{\mathcal{U}}_\alpha^{(0})$ in the following way:

- If $\boldsymbol{m} \in \mathcal{U}_\alpha^{(0),\mathrm{II}}$ and $\boldsymbol{m}' \in \widehat{\mathcal{U}}_\alpha^{(0),\mathrm{II}}$, we keep the above definition.
- Otherwise, we set

$$\theta_{\boldsymbol{m}}^\alpha(\boldsymbol{m}') = \delta_{\boldsymbol{m},\boldsymbol{m}'}. \tag{3-16}$$

Then the formulas in (3-9) and (3-14) can be summarized in

$$f_{\boldsymbol{m}}^{(0)}(x) = h^{-d/4} \sum_{\boldsymbol{m}' \in \widehat{\mathcal{U}}_\alpha^{(0)}} \theta_{\boldsymbol{m}}^\alpha(\boldsymbol{m}') c(\boldsymbol{m}', h) \hat{\chi}_{\boldsymbol{m}'}(x) e^{(\varphi(\boldsymbol{m})-\varphi(x))/h}, \tag{3-17}$$

with $\widehat{\mathcal{U}}_\alpha^{(0)}$ and θ^α as above.

Definition 3.7. For any $\alpha \in \underline{\mathcal{A}}$, let us denote by $\mathscr{T}^\alpha \in \mathscr{M}(\mathcal{U}_\alpha^{(0)}, \widehat{\mathcal{U}}_\alpha^{(0)})$ the matrix given by

$$\mathscr{T}^\alpha = (\theta_{\boldsymbol{m}}^\alpha(\boldsymbol{m}'))_{\boldsymbol{m}' \in \widehat{\mathcal{U}}_\alpha^{(0)}, \boldsymbol{m} \in \mathcal{U}_\alpha^{(0)}}$$

Let us remark that if all points of $\mathcal{U}_\alpha^{(0)}$ are of type I, then $\mathscr{T}^\alpha$ is just the $q_\alpha \times q_\alpha$ identity matrix, whereas if $\mathcal{U}_\alpha^{(0),\mathrm{II}} \neq \varnothing$, it is a $(q_\alpha + 1) \times q_\alpha$ matrix. Observe also that the partitions $\mathcal{U}_\alpha^{(0)} = \mathcal{U}_\alpha^{(0),\mathrm{I}} \sqcup \mathcal{U}_\alpha^{(0),\mathrm{II}}$ and $\widehat{\mathcal{U}}_\alpha^{(0)} = \mathcal{U}_\alpha^{(0),\mathrm{I}} \sqcup \widehat{\mathcal{U}}_\alpha^{(0),\mathrm{II}}$ induce decompositions of the corresponding vector spaces:

$$\mathscr{F}(\mathcal{U}_\alpha^{(0)}) = \mathscr{F}(\mathcal{U}_\alpha^{(0),\mathrm{I}}) \oplus \mathscr{F}(\mathcal{U}_\alpha^{(0),\mathrm{II}}), \tag{3-18}$$

$$\mathscr{F}(\widehat{\mathcal{U}}_\alpha^{(0)}) = \mathscr{F}(\mathcal{U}_\alpha^{(0),\mathrm{I}}) \oplus \mathscr{F}(\widehat{\mathcal{U}}_\alpha^{(0),\mathrm{II}}). \tag{3-19}$$

From the above construction, one deduces that in a suitable basis the matrix $\mathscr{T}^\alpha$ is block diagonal with Id on the upper-left corner and a certain orthogonal matrix in the lower-right corner. More precisely, there exists an orthogonal matrix $\widehat{\mathscr{T}}^\alpha \in \mathscr{M}(\mathcal{U}_\alpha^{(0),\mathrm{II}}, \widehat{\mathcal{U}}_\alpha^{(0),\mathrm{II}})$ such that for any $f = f^{\mathrm{I}} + f^{\mathrm{II}}$ with $f^{\mathrm{I}} \in \mathscr{F}(\mathcal{U}_\alpha^{(0),\mathrm{I}})$ and $f^{\mathrm{II}} \in \mathscr{F}(\widehat{\mathcal{U}}_\alpha^{(0),\mathrm{II}})$, one has

$$\mathscr{T} f(\boldsymbol{m}) = f^{\mathrm{I}}(\boldsymbol{m}) + (\widehat{\mathscr{T}}^\alpha f^{\mathrm{II}})(\boldsymbol{m}). \tag{3-20}$$

Moreover, the matrix $\widehat{\mathscr{T}}^\alpha$ is just the matrix $(\theta_{\boldsymbol{m}}^\alpha(\boldsymbol{m}'))_{\boldsymbol{m} \in \mathcal{U}_\alpha^{(0),\mathrm{II}}, \boldsymbol{m}' \in \widehat{\mathcal{U}}_\alpha^{(0),\mathrm{II}}}$ whose coefficients are given by Lemma 3.6. In particular, Ran $\widehat{\mathscr{T}}^\alpha = (\mathbb{R}\theta_0^\alpha)^\perp$, where θ_0^α is defined by (3-11).

For any $\boldsymbol{m} \in \mathcal{U}^{(0)}$, let us introduce the set $F(\boldsymbol{m})$, defined as follows. If $\boldsymbol{m} = \underline{\boldsymbol{m}}$, let $F(\underline{\boldsymbol{m}}) = X$. If $\boldsymbol{m} \in \underline{\mathcal{U}}^{(0),\mathrm{I}} := \underline{\mathcal{U}}^{(0)} \cap \mathcal{U}^{(0),\mathrm{I}}$, let $F(\boldsymbol{m}) = \overline{E(\boldsymbol{m})}$ and if $\boldsymbol{m} \in \underline{\mathcal{U}}^{(0),\mathrm{II}} := \underline{\mathcal{U}}^{(0)} \cap \mathcal{U}^{(0),\mathrm{II}}$, let

$$F(\boldsymbol{m}) = \Bigg(\bigcup_{\boldsymbol{m}' \in \mathcal{U}_\alpha^{(0),\mathrm{II}}} \overline{E(\boldsymbol{m}')} \Bigg) \cup \overline{\widehat{E}(\boldsymbol{m})}, \tag{3-21}$$

where α is such that $\boldsymbol{m} \in \mathcal{U}_\alpha^{(0)}$. Observe that we always have $\overline{E(\boldsymbol{m})} \subset F(\boldsymbol{m})$.

Proposition 3.8. *Let $\boldsymbol{m},\boldsymbol{m}'\in\mathcal{U}^{(0)}$ be such that $\boldsymbol{m}\neq\boldsymbol{m}'$. The following hold true:*

(i) *If $\boldsymbol{m}\mathcal{R}\boldsymbol{m}'$ then*

(i.a) *if $\boldsymbol{m}$ or $\boldsymbol{m}'$ is of type I, then $F(\boldsymbol{m})\cap F(\boldsymbol{m}')\subset\mathcal{V}^{(1)}$,*

(i.b) *if $\boldsymbol{m}$ and $\boldsymbol{m}'$ are both of type II, then $F(\boldsymbol{m})=F(\boldsymbol{m}')$.*

(ii) *If $\boldsymbol{m}'\notin\mathrm{Cl}(\boldsymbol{m})$, then*

(ii.a) *if $\sigma(\boldsymbol{m})=\sigma(\boldsymbol{m}')$, then $F(\boldsymbol{m})\cap F(\boldsymbol{m}')=\varnothing$,*

(ii.b) *if $\sigma(\boldsymbol{m})>\sigma(\boldsymbol{m}')$, then either $F(\boldsymbol{m})\cap F(\boldsymbol{m}')=\varnothing$ or $F(\boldsymbol{m}')\subset\mathring{F}(\boldsymbol{m})$.*

Proof. Let $\boldsymbol{m}\mathcal{R}\boldsymbol{m}'$ with $\boldsymbol{m}\neq\boldsymbol{m}'$. As in the proof of Proposition 3.1, one has necessarily $\boldsymbol{m},\boldsymbol{m}'\neq\underline{\boldsymbol{m}}$. Assume first that $\boldsymbol{m}$ is of type I. Then $F(\boldsymbol{m})=\overline{E(\boldsymbol{m})}$. If $\boldsymbol{m}'$ is also of type I, then $F(\boldsymbol{m}')=\overline{E(\boldsymbol{m}')}$. Moreover since $\boldsymbol{m}\neq\boldsymbol{m}'$, it follows from (i.a) of Proposition 3.1 that $E(\boldsymbol{m})\cap E(\boldsymbol{m}')=\varnothing$. Therefore, $F(\boldsymbol{m})\cap F(\boldsymbol{m}')$ is either empty or is reduced to a union of saddle points which are separating by definition. If $\boldsymbol{m}'$ is of type II, the same proof works. This completes the proof of (i.a).

Suppose now that $\boldsymbol{m}$ and $\boldsymbol{m}'$ are both of type II. Since $\boldsymbol{m}\mathcal{R}\boldsymbol{m}'$, it follows that $\widehat{E}(\boldsymbol{m})=\widehat{E}(\boldsymbol{m}')$ and hence $F(\boldsymbol{m})=F(\boldsymbol{m}')$ which shows (i.b).

Suppose now that $\boldsymbol{m}'\notin\mathrm{Cl}(\boldsymbol{m})$. Consider first the case where $\sigma(\boldsymbol{m})=\sigma(\boldsymbol{m}')$. Then, one has necessarily $F(\boldsymbol{m})\cap F(\boldsymbol{m}')=\varnothing$; otherwise we would have $\boldsymbol{m}\mathcal{R}\boldsymbol{m}'$.

Suppose now that $\sigma(\boldsymbol{m})>\sigma(\boldsymbol{m}')$ and that $F(\boldsymbol{m})\cap F(\boldsymbol{m}')\neq\varnothing$. If $\boldsymbol{m}=\underline{\boldsymbol{m}}$, then $F(\boldsymbol{m})=X$ and the conclusion is obvious. Suppose now that $\boldsymbol{m}\in\underline{\mathcal{U}}^{(0)}$ and consider first the case where $\boldsymbol{m}$ and $\boldsymbol{m}'$ are of type I. Then $F(\boldsymbol{m})=\overline{E(\boldsymbol{m})}$ and $F(\boldsymbol{m}')=\overline{E(\boldsymbol{m}')}$ and since $\sigma(\boldsymbol{m})>\sigma(\boldsymbol{m}')$, it follows that $E(\boldsymbol{m})\cap E(\boldsymbol{m}')\neq\varnothing$. Hence (ii.a) of Proposition 3.1 shows that $E_-(\boldsymbol{m}')\subset E(\boldsymbol{m})$ which yields $F(\boldsymbol{m}')\subset E(\boldsymbol{m})=\mathring{F}(\boldsymbol{m})$. If $\boldsymbol{m}$ is of type I and $\boldsymbol{m}'$ is of type II, then one has $E(\boldsymbol{m})\cap\widetilde{E}\neq\varnothing$ with either $\widetilde{E}=E(\boldsymbol{m}'')$ for some $\boldsymbol{m}''\in\mathrm{Cl}(\boldsymbol{m}')$ or $\widetilde{E}=\widehat{E}(\boldsymbol{m}')$. As before, $E(\boldsymbol{m})$ contains the connected component of $\{\varphi<\boldsymbol{\sigma}(\boldsymbol{m})\}$ that contains $\widetilde{E}$ and the same proof works.

Let us now suppose that $\boldsymbol{m}$ is of type II and $\boldsymbol{m}'$ is of type I. Then $E(\boldsymbol{m}')\cap\widetilde{E}\neq\varnothing$ with either $\widetilde{E}=E(\boldsymbol{m}'')$ for some $\boldsymbol{m}''\in\mathrm{Cl}(\boldsymbol{m})$ or $\widetilde{E}=\widehat{E}(\boldsymbol{m})$. In both cases one sees easily that $E_-(\boldsymbol{m}')\subset\widetilde{E}$, which proves the result.

The case where both $\boldsymbol{m}$ and $\boldsymbol{m}'$ are of type II is left to the reader. ☐

Let us now give some information on the support of the quasimodes. For $\boldsymbol{m}\in\underline{\mathcal{U}}^{(0)}$, let us introduce the set

$$F_{\epsilon,\tilde{\epsilon},\delta}(\boldsymbol{m})=\Bigg(\Bigg(F(\boldsymbol{m})\setminus\bigcup_{\boldsymbol{s}\in\mathcal{V}^{(1)}\cap\partial F(\boldsymbol{m})}B(\boldsymbol{s},\epsilon)\Bigg)+\overline{B(0,\tilde{\epsilon})}\Bigg)\cup\Bigg(\bigcup_{\boldsymbol{s}\in(\mathcal{U}^{(1)}\setminus\mathcal{V}^{(1)})\cap\partial F(\boldsymbol{m})}\overline{B(\boldsymbol{s},\delta)}\Bigg).\tag{3-22}$$

If $\boldsymbol{m}$ is of type I, it is clear that $F_{\epsilon,\tilde{\epsilon},\delta}(\boldsymbol{m})=\overline{E_{\epsilon,\tilde{\epsilon},\delta}(\boldsymbol{m})}$ and if $\boldsymbol{m}$ is of type II, one has

$$F_{\epsilon,\tilde{\epsilon},\delta}(\boldsymbol{m})=\overline{\widehat{E}_{\epsilon,\tilde{\epsilon},\delta}(\alpha)}\cup\Bigg(\bigcup_{\boldsymbol{m}'\in\mathcal{U}_\alpha^{(0),\mathrm{II}}}\overline{E_{\epsilon,\tilde{\epsilon},\delta}(\boldsymbol{m})}\Bigg).$$

From the above construction one deduces the following proposition.

Proposition 3.9. *There exists* $\epsilon_0, \delta_0 > 0$ *such that for all* $0 < \delta < \delta_0$ *and all* $0 < \tilde{\epsilon} < \epsilon/4 < \epsilon_0/4$, *the following hold true*:

(i) *For any* $\boldsymbol{m}, \boldsymbol{m}' \in \mathcal{U}^{(0)}$

$$F(\boldsymbol{m}) \cap F(\boldsymbol{m}') = \varnothing \quad \Longrightarrow \quad F_{\epsilon,\tilde{\epsilon},\delta}(\boldsymbol{m}) \cap F_{\epsilon,\tilde{\epsilon},\delta}(\boldsymbol{m}') = \varnothing.$$

(ii) *For any* $\alpha \in \underline{A}$ *and* $\boldsymbol{m} \in \mathcal{U}_\alpha^{(0)}$, *one has* $\operatorname{supp}(f_{\boldsymbol{m}}^{(0)}) \subset F_{\epsilon,2\tilde{\epsilon},2\delta}(\boldsymbol{m})$ *and*

$$\text{for all } \boldsymbol{s} \in \mathcal{U}^{(1)} \setminus (\mathcal{V}^{(1)} \cap \partial F(\boldsymbol{m})), \quad d_\varphi f_{\boldsymbol{m}}^{(0)} = 0 \quad \text{in } B(\boldsymbol{s}, \delta).$$

Proof. Observe that

$$F_{\epsilon,2\tilde{\epsilon},2\delta}(\boldsymbol{m}) \subset F(\boldsymbol{m}) + \overline{B(0, 2\max(\delta, \tilde{\epsilon}))}.$$

Since $F(\boldsymbol{m})$ and $F(\boldsymbol{m}')$ are compact, the first point of the proposition immediately follows. The second point of the proposition is a direct consequence of (c) of Proposition 3.5. □

Recall that the functions $f_{\boldsymbol{m}}^{(0)}$, $\boldsymbol{m} \in \mathcal{U}^{(0)}$, depend on $\epsilon, \tilde{\epsilon}, \delta$ via the definition of the cut-off function $\chi_{\boldsymbol{m}}$. This family is quasiorthonormal in the following sense.

Proposition 3.10. *There exist* $\epsilon_0, \delta_0, \beta > 0$ *such that for all* $0 < \delta < \delta_0$, $0 < \tilde{\epsilon} < \epsilon/4 < \epsilon_0/4$ *and all* $\boldsymbol{m}, \boldsymbol{m}' \in \mathcal{U}^{(0)}$, *one has*

$$\langle f_{\boldsymbol{m}}^{(0)}, f_{\boldsymbol{m}'}^{(0)} \rangle = \delta_{\boldsymbol{m},\boldsymbol{m}'} + \mathcal{O}(e^{-\beta/h}).$$

Proof. Throughout the proof, we assume that $0 < \delta < \delta_0$ and $0 < \tilde{\epsilon} < \epsilon/4 < \epsilon_0/4$ as in Proposition 3.5 and we decrease ϵ_0, δ_0 if necessary.

Let $\boldsymbol{m}, \boldsymbol{m}'$ be two minima.

- Consider first the case where $\boldsymbol{m}\mathcal{R}\boldsymbol{m}'$. If $\boldsymbol{m} = \underline{\boldsymbol{m}}$, one has necessarily $\boldsymbol{m}' = \boldsymbol{m}$ and hence

$$\langle f_{\boldsymbol{m}}^{(0)}, f_{\boldsymbol{m}'}^{(0)} \rangle = \| f_{\boldsymbol{m}}^{(0)} \|^2 = 1$$

by construction. Consider now the case where $\boldsymbol{m}, \boldsymbol{m}' \neq \underline{\boldsymbol{m}}$ and suppose first that $\boldsymbol{m}$ or $\boldsymbol{m}'$ is of type I. If $\boldsymbol{m} = \boldsymbol{m}'$, the definition of $c(\boldsymbol{m}, h)$ shows that $\| f_{\boldsymbol{m}} \| = 1$. If $\boldsymbol{m} \neq \boldsymbol{m}'$, it follows from (ii) of Proposition 3.9 that $f_{\boldsymbol{m}}^{(0)}$ and $f_{\boldsymbol{m}'}^{(0)}$ are supported in $F_{\epsilon,2\tilde{\epsilon},2\delta}(\boldsymbol{m})$ and $F_{\epsilon,2\tilde{\epsilon},2\delta}(\boldsymbol{m}')$ respectively. Moreover, thanks to (i) of Proposition 3.8, one has $F(\boldsymbol{m}) \cap F(\boldsymbol{m}') \subset \mathcal{V}^{(1)} \cap \partial F(\boldsymbol{m})$. Hence, one can choose ϵ_0 sufficiently small, so that $F_{\epsilon,2\tilde{\epsilon},2\delta}(\boldsymbol{m}) \cap F_{\epsilon,2\tilde{\epsilon},2\delta}(\boldsymbol{m}') = \varnothing$. Therefore, $\operatorname{supp}(f_{\boldsymbol{m}}^{(0)}) \cap \operatorname{supp}(f_{\boldsymbol{m}'}^{(0)}) = \varnothing$ and hence $f_{\boldsymbol{m}}^{(0)}$ and $f_{\boldsymbol{m}'}^{(0)}$ are orthogonal.

Suppose now that $\boldsymbol{m}$ and $\boldsymbol{m}'$ are both of type II. Then, we can write

$$f_{\boldsymbol{m}}^{(0)}(x) = h^{-d/4} \sum_{\nu_1 \in \widehat{\mathcal{U}}_\alpha^{(0)}} \theta_{\boldsymbol{m}}(\nu_1) c(\nu_1, h) \hat{\chi}_{\nu_1}(x) e^{(\varphi(\hat{\boldsymbol{m}}(\boldsymbol{m})) - \varphi(x))/h},$$

$$f_{\boldsymbol{m}'}^{(0)}(x) = h^{-d/4} \sum_{\nu_2 \in \widehat{\mathcal{U}}_\alpha^{(0)}} \theta_{\boldsymbol{m}'}(\nu_2) c(\nu_2, h) \hat{\chi}_{\nu_2}(x) e^{(\varphi(\hat{\boldsymbol{m}}(\boldsymbol{m})) - \varphi(x))/h}.$$

Since, for $\nu_2 \neq \nu_1$, $\hat\chi_{\nu_1}$ and $\hat\chi_{\nu_2}$ have again disjoint support for $\epsilon_0, \delta_0 > 0$ small enough, we get

$$\begin{aligned}\langle f_{\boldsymbol m}^{(0)}, f_{\boldsymbol m'}^{(0)}\rangle &= h^{-d/2} \sum_{\nu \in \widehat{\mathcal U}_\alpha^{(0)}} \theta_{\boldsymbol m}(\nu)\theta_{\boldsymbol m'}(\nu)|c(\nu,h)|^2 \int_X |\hat\chi_\nu(x)|^2 e^{2(\varphi(\hat{\boldsymbol m}(\boldsymbol m))-\varphi(x))/h}\,dx \\ &= \langle \theta_{\boldsymbol m}, \theta_{\boldsymbol m'}\rangle_{\mathcal F_\alpha} = \delta_{\boldsymbol m,\boldsymbol m'}.\end{aligned}$$

This shows in particular that $\|f_{\boldsymbol m}^{(0)}\|_{L^2} = 1$ for all $\boldsymbol m \in \mathcal U^{(0)}$.

• Suppose now, that $\boldsymbol m' \notin \mathrm{Cl}(\boldsymbol m)$ (in particular $\boldsymbol m \neq \boldsymbol m'$). If $\sigma(\boldsymbol m') = \sigma(\boldsymbol m)$ then $F(\boldsymbol m) \cap F(\boldsymbol m') = \varnothing$ thanks to (ii.a) of Proposition 3.8, and (i) of Proposition 3.9 implies that $F_{\epsilon,2\tilde\epsilon,2\delta}(\boldsymbol m) \cap F_{\epsilon,2\tilde\epsilon,2\delta}(\boldsymbol m') = \varnothing$. Then, the first part of (ii) of Proposition 3.9 proves that $f_{\boldsymbol m}^{(0)}$ and $f_{\boldsymbol m'}^{(0)}$ are orthogonal.

Consider now the case where $\sigma(\boldsymbol m) \neq \sigma(\boldsymbol m')$; say, $\sigma(\boldsymbol m) > \sigma(\boldsymbol m')$. From (ii.b) of Proposition 3.8, we know that either $F(\boldsymbol m')$ is disjoint from $F(\boldsymbol m)$ or $F(\boldsymbol m') \subset \mathring F(\boldsymbol m)$. In the first case, we get immediately $\langle f_{\boldsymbol m}^{(0)}, f_{\boldsymbol m'}^{(0)}\rangle = 0$ by the same argument as before. Suppose we are in the second situation, that is $F(\boldsymbol m') \subset \mathring F(\boldsymbol m)$. By definition, we have $\varphi(\boldsymbol m) \le \varphi(\boldsymbol m')$, and by taking $\epsilon_0, \delta_0 > 0$ small enough we can ensure that $F_{\epsilon,2\tilde\epsilon,2\delta}(\boldsymbol m') \subset \mathring F_{\epsilon,2\tilde\epsilon,2\delta}(\boldsymbol m)$.

Suppose first that $\varphi(\boldsymbol m) < \varphi(\boldsymbol m')$. A priori we don't know if $\boldsymbol m, \boldsymbol m'$ are of type I or II. However, since $F_{\epsilon,2\tilde\epsilon,2\delta}(\boldsymbol m') \subset \mathring F_{\epsilon,2\tilde\epsilon,2\delta}(\boldsymbol m)$,

$$\langle f_{\boldsymbol m}^{(0)}, f_{\boldsymbol m'}^{(0)}\rangle = \int_{F_{\epsilon,2\tilde\epsilon,2\delta}(\boldsymbol m')} f_{\boldsymbol m}^{(0)}(x) f_{\boldsymbol m'}^{(0)}(x)\,dx$$

and

$$(f_{\boldsymbol m}^{(0)})_{|F_{\epsilon,2\tilde\epsilon,2\delta}(\boldsymbol m')} = \tilde c(\boldsymbol m,h) h^{-d/4} e^{(\varphi(\boldsymbol m)-\varphi(x))/h}, \tag{3-23}$$

where the constant $\tilde c(\boldsymbol m,h)$ is uniformly bounded with respect to h. This is clear if $\boldsymbol m$ is of type I. If $\boldsymbol m$ is of type II and, say, $\boldsymbol m \in \mathcal U_\alpha^{(0)}$, then $F(\boldsymbol m') \subset \mathring F(\boldsymbol m)$ implies that there exists $\nu \in \widehat{\mathcal U}_\alpha^{(0)}$ such that $F(\boldsymbol m') \subset E(\nu)$ (or $\widehat E(\nu)$). Then the general formula (3-14) shows (3-23). Moreover, by construction, there exists a cut-off function $\psi \in \mathscr C_c^\infty(\mathring F_{\epsilon,2\tilde\epsilon,2\delta}(\boldsymbol m))$ independent of h such that $\inf_{\mathrm{supp}\,\psi} \varphi = \varphi(\boldsymbol m')$ and

$$|f_{\boldsymbol m'}^{(0)}(x)| \le h^{-d/4} \psi(x) e^{(\varphi(\boldsymbol m')-\varphi(x))/h}$$

and it follows that

$$|\langle f_{\boldsymbol m}^{(0)}, f_{\boldsymbol m'}^{(0)}\rangle| \le C h^{-d/2} \int \psi(x) e^{(\varphi(\boldsymbol m')+\varphi(\boldsymbol m)-2\varphi(x))/h}\,dx \le C' h^{-d/2} e^{(\varphi(\boldsymbol m)-\varphi(\boldsymbol m'))/h}.$$

Since $\varphi(\boldsymbol m') > \varphi(\boldsymbol m)$, this proves the result.

It remains to study the case where $\varphi(\boldsymbol m) = \varphi(\boldsymbol m')$. Let $\alpha, \alpha' \in \mathcal A$ be such that $\boldsymbol m \in \mathcal U_\alpha^{(0)}$ and $\boldsymbol m' \in \mathcal U_{\alpha'}^{(0)}$. From the above assumption, we also have $\sigma(\boldsymbol m) > \sigma(\boldsymbol m')$ and $F(\boldsymbol m') \subset \mathring F(\boldsymbol m)$. Since $\sigma(\boldsymbol m) > \sigma(\boldsymbol m')$ and $\varphi(\boldsymbol m) = \varphi(\boldsymbol m')$, we know $f_{\boldsymbol m'}^{(0)}$ is necessarily of type II. It has the form (3-14) and since $F_{\epsilon,2\tilde\epsilon,2\delta}(\boldsymbol m') \subset \mathring F_{\epsilon,2\tilde\epsilon,2\delta}(\boldsymbol m)$, (3-23) still holds true. Hence, we get

$$\langle f_{\boldsymbol m}^{(0)}, f_{\boldsymbol m'}^{(0)}\rangle = \tilde c(\boldsymbol m,h) h^{-d/2} \sum_{\nu \in \widehat{\mathcal U}_{\alpha'}^{(0),\mathrm{II}}} \theta_{\boldsymbol m'}(\nu) c(\nu,h) \int \hat\chi_\nu(x) e^{2(\varphi(x)-\varphi(\boldsymbol m))/h}\,dx. \tag{3-24}$$

On the other hand, by a standard argument based on the Laplace method, we know that there exist $r>0$ and $\beta>0$ such that for all $\nu\in\widehat{\mathcal{U}}_{\alpha'}^{(0),\mathrm{II}}$, we have

$$\begin{aligned}h^{-d/2}c(\nu,h)\int\hat{\chi}_\nu(x)e^{2(\varphi(x)-\varphi(\boldsymbol{m}))/h}\,dx&=h^{-d/2}c(\nu,h)\sum_{\nu'\in H(\nu)}\int_{B(\nu',r)}e^{2(\varphi(x)-\varphi(\boldsymbol{m}))/h}\,dx+\mathcal{O}(e^{-\beta/h})\\&=h^{-d/2}c(\nu,h)\int|\hat{\chi}_\nu(x)|^2e^{2(\varphi(x)-\varphi(\boldsymbol{m}))/h}\,dx+\mathcal{O}(e^{-\beta/h})\\&=\frac{1}{c(\nu,h)}+\mathcal{O}(e^{-\beta/h}).\end{aligned}$$

Plugging this in (3-24), we get

$$\langle f_{\boldsymbol{m}}^{(0)},f_{\boldsymbol{m}'}^{(0)}\rangle=\tilde{c}(\boldsymbol{m},h)\sum_{\nu\in\widehat{\mathcal{U}}_{\alpha'}^{(0),\mathrm{II}}}\theta_{\boldsymbol{m}'}(\nu)\frac{1}{c(\nu,h)}+\mathcal{O}(e^{-\beta/h})=\frac{\tilde{c}(\boldsymbol{m},h)}{c_0^{\alpha'}(h)}\langle\theta_{\boldsymbol{m}'},\theta_0^{\alpha'}\rangle_{\mathcal{F}_{\alpha'}}+\mathcal{O}(e^{-\beta/h}).\quad(3\text{-}25)$$

Since $\theta_{\boldsymbol{m}'}$ is orthogonal to $\theta_0^{\alpha'}$ by construction, the first term of the right-hand side above vanishes and we get $\langle f_{\boldsymbol{m}}^{(0)},f_{\boldsymbol{m}'}^{(0)}\rangle=\mathcal{O}(e^{-\beta/h})$. □

We end this section by giving an exponential estimate of the action of $d_{\varphi,h}$ on the quasimodes.

Lemma 3.11. *There exists $C>0$ such that for all $\epsilon>0$ small enough, we have*

$$d_{\varphi,h}f_{\boldsymbol{m}}^{(0)}=\mathcal{O}(e^{-(S(\boldsymbol{m})-C\epsilon)/h})$$

for all $\boldsymbol{m}\in\mathcal{U}^{(0)}$.

Proof. The result is classical, but since the quasimodes $f_{\boldsymbol{m}}^{(0)}$ are slightly different from the usual ones, we have to check the estimates. Let $\boldsymbol{m}\in\mathcal{U}^{(0)}$ and let us compute $d_{\varphi,h}f_{\boldsymbol{m}}^{(0)}$.

If $\boldsymbol{m}=\underline{\boldsymbol{m}}$, then $d_{\varphi,h}f_{\boldsymbol{m}}^{(0)}=0$ and there is nothing to do.

Suppose now that $\boldsymbol{m}\neq\underline{\boldsymbol{m}}$. From (3-17), one has

$$d_{\varphi,h}f_{\boldsymbol{m}}^{(0)}(x)=h^{1-d/4}\sum_{\boldsymbol{m}'\in\widehat{\mathcal{U}}_\alpha^{(0)}}\theta_{\boldsymbol{m}}(\boldsymbol{m}')c(\boldsymbol{m}',h)\nabla\hat{\chi}_{\boldsymbol{m}'}(x)e^{(\varphi(\boldsymbol{m})-\varphi(x))/h}.$$

All terms of the above sum corresponding to $\boldsymbol{m}\in\mathcal{U}_\alpha^{(0)}$ are $\mathcal{O}(e^{-(S(\boldsymbol{m})-C\epsilon)/h})$ by (b) of Proposition 3.5. The only new term is the one corresponding to $\hat{\boldsymbol{m}}(\boldsymbol{m})$. Since $\hat{\chi}_{\hat{\boldsymbol{m}}}\in\mathcal{C}_c^\infty(\widehat{E}_{\epsilon,2\tilde{\epsilon},2\delta})$ and is equal to 1 on $\widehat{E}_{\epsilon,\tilde{\epsilon},\delta}$, we have again

$$\varphi(x)-\varphi(\hat{\boldsymbol{m}})=\varphi(x)-\varphi(\boldsymbol{m})\geq S(\boldsymbol{m})-C\epsilon$$

on $\operatorname{supp}(\nabla\hat{\chi}_{\hat{\boldsymbol{m}}})$ and the proof is complete. □

3C. ***Quasimodes for* 1*-forms.*** This section is devoted to the quasimodes associated to low-lying eigenvalues of $\Delta_\varphi^{(1)}$. The construction of these quasimodes was done in [Helffer and Sjöstrand 1985] and we refer to that paper for all the proofs. Here, we just describe the main properties of these functions. In this section $\omega_{\boldsymbol{s}}$ denotes a small neighborhood of $\boldsymbol{s}\in\mathcal{U}^{(1)}$ that may be chosen as small as needed independently of ϵ_0 fixed in previous sections.

Given any saddle point $s \in \mathcal{U}^{(1)}$, and any appropriate open neighborhood ω_s of s, let $P_{\varphi,s}$ denote the operator $\Delta_\varphi^{(1)}$ restricted to ω_s with Dirichlet boundary conditions. Let u_s denote a normalized fundamental state of $P_{\varphi,s}$. The quasimodes $f_s^{(1)}$ are then defined by

$$f_s^{(1)}(x) := \epsilon_0 \|\psi_s u_s\|^{-1} \psi_s(x) u_s(x), \tag{3-26}$$

where ψ_s is a well-chosen C_0^∞ localization function supported in ω_s and equal to 1 near s and $\epsilon_0 = \pm 1$ will be fixed later. By taking ω_s sufficiently small, we can ensure that the $f_s^{(1)}$ have disjoint supports, and thanks to (c) of Proposition 3.5, we can also shrink ω_s so that

$$\text{for all } s \in \mathcal{U}^{(1)} \setminus \mathcal{V}^{(1)}, \ \text{ for all } m \in \mathcal{U}^{(0)}, \quad (s \in \operatorname{supp}(\chi_m) \implies \chi_m = 1 \text{ on } \omega_s). \tag{3-27}$$

Observe that this choice of ω_s depends on δ_0 but not on ϵ_0. From this construction, we immediately deduce that

$$\langle f_s^{(1)}, f_{s'}^{(1)} \rangle = \delta_{s,s'}, \tag{3-28}$$

and hence the family $\{f_s^{(1)} : s \in \mathcal{U}^{(1)}\}$ is a free family of 1-forms. From [Helffer 1988, Proposition 5.2.6], one knows that the eigenvalues of $P_{\varphi,s}$ are exponentially small. Using Agmon estimates, it follows that there exists $\beta > 0$ independent of ϵ such that

$$\Delta_\varphi^{(1)} f_s^{(1)} = \mathcal{O}(e^{-\beta/h}). \tag{3-29}$$

Combined with the spectral theorem, this proves that the n_1 eigenvalues of $\Delta_\varphi^{(1)}$ in $[0, \epsilon_1 h]$ are actually $\mathcal{O}(e^{-\beta/h})$ (see [Helffer 1988, Proposition 5.2.5] for details).

Furthermore, Theorem 2.5 of [Helffer and Sjöstrand 1985] implies that these quasimodes have a WKB expansion given by

$$f_s^{(1)}(x) = \epsilon_0 h^{-d/4} \psi_s(x) b_s^{(1)}(x,h) e^{-\varphi_{+,s}(x)/h}, \tag{3-30}$$

where $b_s^{(1)}(x,h)$ is a 1-form having a semiclassical asymptotic, and $\varphi_{+,s}$ is the phase generating the outgoing manifold of $|\xi|^2 - |\nabla_x \varphi(x)|^2$ at $(s, 0)$ (see [Dimassi and Sjöstrand 1999, Chapter 3] for details on such constructions). In particular, the phase function $\varphi_{+,s}$ satisfies the eikonal equation $|\nabla_x \varphi_{+,s}|^2 = |\nabla_x \varphi|^2$ and $\varphi_{+,s}(x) \asymp |x - s|^2$ near s (the notation $\asymp$ was defined in the paragraph before Section 2A). For other properties of $\varphi_{+,s}$ we refer to [Helffer and Sjöstrand 1985].

3D. ***Projection onto the eigenspaces.*** The next step in our analysis is to project the preceding quasimodes onto the generalized eigenspaces associated to exponentially small eigenvalues. Recall that we have built in the preceding section quasimodes $f_m^{(0)}$, $m \in \mathcal{U}^{(0)}$, with good orthogonality properties. To each of these quasimodes we will associate a function in $E^{(0)}$, the eigenspace associated to $o(h)$ eigenvalues. For this, we first define the spectral projector

$$\Pi^{(0)} = \frac{1}{2\pi i} \int_\gamma (z - \Delta_\varphi^{(0)})^{-1} \, dz, \tag{3-31}$$

where $\gamma = \partial B(0, \epsilon_0 h)$ and $\epsilon_0 > 0$ is such that $\sigma(\Delta_\varphi) \cap [0, 2\epsilon_0 h] \subset [0, e^{-C/h}]$. From the fact that $\Delta_\varphi^{(0)}$ is selfadjoint, we get that

$$\|\Pi^{(0)}\| = 1.$$

We now introduce the projection of the quasimodes constructed above, $e_{\boldsymbol{m}}^{(0)} = \Pi^{(0)}(f_{\boldsymbol{m}}^{(0)})$. We have the following:

Lemma 3.12. *The system $(e_{\boldsymbol{m}}^{(0)})_{\boldsymbol{m}\in\mathcal{U}^{(0)}}$ is free and spans $E^{(0)}$. Additionally, there exists $\beta > 0$ independent of ϵ_0 such that for all $0 < \tilde{\epsilon} < \epsilon/4 < \epsilon_0/4$, one has*

$$e_{\boldsymbol{m}}^{(0)} = f_{\boldsymbol{m}}^{(0)} + \mathcal{O}(e^{-\beta/h}) \quad \text{and} \quad \langle e_{\boldsymbol{m}}^{(0)}, e_{\boldsymbol{m}'}^{(0)} \rangle = \delta_{\boldsymbol{m},\boldsymbol{m}'} + \mathcal{O}(e^{-\beta/h})$$

for all $\boldsymbol{m}, \boldsymbol{m}' \in \mathcal{U}^{(0)}$.

Proof. The argument is very classical. We recall it for reader's convenience. One has

$$\begin{aligned} e_{\boldsymbol{m}}^{(0)} - f_{\boldsymbol{m}}^{(0)} = (\Pi^{(0)} - \mathrm{Id}) f_{\boldsymbol{m}}^{(0)} &= \frac{1}{2\pi i} \int_\gamma ((z - \Delta_\varphi^{(0)})^{-1} - z^{-1}) f_{\boldsymbol{m}}^{(0)} \, dz \\ &= \frac{1}{2\pi i} \int_\gamma (z - \Delta_\varphi^{(0)})^{-1} z^{-1} \Delta_\varphi^{(0)} f_{\boldsymbol{m}}^{(0)} \, dz. \end{aligned} \tag{3-32}$$

Since $(z - \Delta_\varphi^{(0)})^{-1} = \mathcal{O}(h^{-1})$ on γ, it follows from Lemma 3.11 that $e_{\boldsymbol{m}}^{(0)} - f_{\boldsymbol{m}}^{(0)} = \mathcal{O}(e^{-\beta/h})$ for some $\beta > 0$. This proves the first point. Combining this information with Proposition 3.10 we get immediately the second point. ☐

We can do a similar study for $\Delta_\varphi^{(1)}$, for which we know that the n_1 eigenvalues lying in $[0, \epsilon_1 h]$ are actually $\mathcal{O}(e^{-\alpha'/h})$. To the family of quasimodes $(f_{\boldsymbol{s}}^{(1)})_{\boldsymbol{s}\in\mathcal{U}^{(1)}}$, we now associate a family of functions in $E^{(1)}$, the eigenspace associated to eigenvalues of $\Delta_\varphi^{(1)}$ in $[0, \epsilon_1 h]$. Thanks to the spectral properties of the selfadjoint operator $\Delta_\varphi^{(1)}$, its spectral projector onto $E^{(1)}$ is given by

$$\Pi^{(1)} = \frac{1}{2\pi i} \int_\gamma (z - \Delta_\varphi^{(1)})^{-1} \, dz, \tag{3-33}$$

where $\gamma = \partial B(0, \epsilon_1 h)$ with ϵ_1 defined above. In the sequel, we write $e_{\boldsymbol{s}}^{(1)} = \Pi^{(1)}(f_{\boldsymbol{s}}^{(1)})$. The family $(e_{\boldsymbol{s}}^{(1)})_{\boldsymbol{s}}$ satisfies the following estimates.

Lemma 3.13. *The system $(e_{\boldsymbol{s}}^{(1)})_{\boldsymbol{s}\in\mathcal{U}^{(1)}}$ is free and spans $E^{(1)}$. Additionally, we have*

$$e_{\boldsymbol{s}}^{(1)} = f_{\boldsymbol{s}}^{(1)} + \mathcal{O}(e^{-\beta'/h}) \quad \text{and} \quad \langle e_{\boldsymbol{s}}^{(1)}, e_{\boldsymbol{s}'}^{(1)} \rangle = \delta_{\boldsymbol{s},\boldsymbol{s}'} + \mathcal{O}(e^{-\beta'/h}),$$

with $\beta' > 0$ independent of ϵ.

Proof. Using the orthonormality of the $f_j^{(1)}$ and (3-29), the proof is the same as that of Lemma 3.12. ☐

4. Preliminaries for singular values analysis

This section is a preparation for the study of the singular values of the operator $\mathcal{L} : E^{(0)} \to E^{(1)}$ defined below (2-20). We simplify the forthcoming study by several reductions and changes of basis. Let us denote by $\mathcal{L}^{\pi}$ the $n_1 \times n_0$ matrix given by

$$\mathcal{L}^{\pi}_{\boldsymbol{s},\boldsymbol{m}} = \langle e^{(1)}_{\boldsymbol{s}}, d_{\varphi,h} e^{(0)}_{\boldsymbol{m}} \rangle \quad \text{for all } \boldsymbol{s} \in \mathcal{U}^{(1)},\ \boldsymbol{m} \in \mathcal{U}^{(0)}, \tag{4-1}$$

with $e^{(1)}_{\boldsymbol{s}}$, $e^{(0)}_{\boldsymbol{m}}$ defined in the preceding section. Since $(e^{(0)}_{\boldsymbol{m}})$ and $(e^{(1)}_{\boldsymbol{s}})$ are almost orthonormal bases (thanks to Lemmas 3.12 and 3.13), this matrix is close to the matrix of the operator $\mathcal{L}$ in these bases. We first work on the matrix $\mathcal{L}^{\pi}$.

Recall that $\underline{\boldsymbol{m}}$ denotes the absolute minimum of φ associated to the connected component $E(\underline{\boldsymbol{m}}) = X$. Since $\Delta^{(0)}_{\varphi} e_{\underline{\boldsymbol{m}}} = 0$, the nonzero singular values of $\mathcal{L}^{\pi}$ are exactly the singular values of the reduced matrix $\mathcal{L}^{\pi,\prime}$ defined by $\mathcal{L}^{\pi,\prime}_{\boldsymbol{s},\boldsymbol{m}} = \mathcal{L}^{\pi}_{\boldsymbol{s},\boldsymbol{m}}$ for all $\boldsymbol{s} \in \mathcal{U}^{(1)}$, $\boldsymbol{m} \in \underline{\mathcal{U}}^{(0)}$ with $\underline{\mathcal{U}}^{(0)} = \mathcal{U}^{(0)} \setminus \{\underline{\boldsymbol{m}}\}$.

Lemma 4.1. *There exists $\beta'' > 0$ such that for $\epsilon > 0$ sufficiently small, one has*

$$\mathcal{L}^{\pi,\prime}_{\boldsymbol{s},\boldsymbol{m}} = \langle f^{(1)}_{\boldsymbol{s}}, d_{\varphi,h} f^{(0)}_{\boldsymbol{m}} \rangle + \mathcal{O}(e^{-(S(\boldsymbol{m})+\beta'')/h})$$

for all $\boldsymbol{s} \in \mathcal{U}^{(1)}$, $\boldsymbol{m} \in \underline{\mathcal{U}}^{(0)}$.

Proof. The trick to get the good error estimate above is now well-known (see for instance the proof of Proposition 5.8 in [Hérau, Hitrik and Sjöstrand 2011]) but we recall the proof for reader's convenience. Let $\boldsymbol{s} \in \mathcal{U}^{(1)}$, $\boldsymbol{m} \in \underline{\mathcal{U}}^{(0)}$; then thanks to (2-18) we have

$$\begin{aligned}\langle e^{(1)}_{\boldsymbol{s}}, d_{\varphi,h} e^{(0)}_{\boldsymbol{m}} \rangle &= \langle e^{(1)}_{\boldsymbol{s}}, d_{\varphi,h} \Pi^{(0)} f^{(0)}_{\boldsymbol{m}} \rangle = \langle e^{(1)}_{\boldsymbol{s}}, \Pi^{(1)} d_{\varphi,h} f^{(0)}_{\boldsymbol{m}} \rangle = \langle e^{(1)}_{\boldsymbol{s}}, d_{\varphi,h} f^{(0)}_{\boldsymbol{m}} \rangle \\ &= \langle f^{(1)}_{\boldsymbol{s}}, d_{\varphi,h} f^{(0)}_{\boldsymbol{m}} \rangle + \langle e^{(1)}_{\boldsymbol{s}} - f^{(1)}_{\boldsymbol{s}}, d_{\varphi,h} f^{(0)}_{\boldsymbol{m}} \rangle.\end{aligned}$$

But from Lemmas 3.11 and 3.13 and the Cauchy–Schwarz inequality one gets

$$|\langle e^{(1)}_{\boldsymbol{s}} - f^{(1)}_{\boldsymbol{s}}, d_{\varphi,h} f^{(0)}_{\boldsymbol{m}} \rangle| \le C e^{-(\beta' + S(\boldsymbol{m}) - C\epsilon)/h}.$$

Since β' is independent of ϵ, one can conclude by taking ϵ small enough and $\beta'' = \beta'/2$. ☐

Let us denote by $\mathcal{L}^{\text{bkw}} \in \mathscr{M}(\mathcal{U}^{(0)}, \mathcal{U}^{(1)})$ the matrix defined by

$$\mathcal{L}^{\text{bkw}}_{\boldsymbol{s},\boldsymbol{m}} = \langle f^{(1)}_{\boldsymbol{s}}, d_{\varphi,h} f^{(0)}_{\boldsymbol{m}} \rangle \quad \text{for all } \boldsymbol{s} \in \mathcal{U}^{(1)},\ \boldsymbol{m} \in \mathcal{U}^{(0)}. \tag{4-2}$$

Of course, the first column of this matrix is identically zero and it is more interesting to consider the matrix $\mathcal{L}^{\text{bkw},\prime} \in \mathscr{M}(\underline{\mathcal{U}}^{(0)}, \mathcal{U}^{(1)})$ defined by

$$\mathcal{L}^{\text{bkw},\prime}_{\boldsymbol{s},\boldsymbol{m}} = \langle f^{(1)}_{\boldsymbol{s}}, d_{\varphi,h} f^{(0)}_{\boldsymbol{m}} \rangle \quad \text{for all } \boldsymbol{s} \in \mathcal{U}^{(1)},\ \boldsymbol{m} \in \underline{\mathcal{U}}^{(0)}. \tag{4-3}$$

As we shall see later, the singular values of $\mathcal{L}^{\pi,\prime}$ and $\mathcal{L}^{\text{bkw},\prime}$ are exponentially close and it is natural to study the matrix $\mathcal{L}^{\text{bkw},\prime}$. For $\boldsymbol{s} \in \mathcal{U}^{(1)} \setminus \mathcal{V}^{(1)}$ and $\boldsymbol{m} \in \underline{\mathcal{U}}^{(0)}$, thanks to (ii) of Proposition 3.9 one has $d_{\varphi,h} f^{(0)}_{\boldsymbol{m}} = 0$ near $\boldsymbol{s}$, and hence

$$\langle f^{(1)}_{\boldsymbol{s}}, d_{\varphi,h} f^{(0)}_{\boldsymbol{m}} \rangle = 0. \tag{4-4}$$

Therefore, the singular values of $\mathcal{L}^{\text{bkw},\prime}$ are equal to the singular values of the reduced matrix $\mathcal{L}^{\text{bkw},\prime\prime} \in \mathscr{M}(\underline{\mathcal{U}}^{(0)}, \mathcal{V}^{(1)})$ defined by

$$\mathcal{L}^{\text{bkw},\prime\prime}_{\boldsymbol{s},\boldsymbol{m}} = \langle f^{(1)}_{\boldsymbol{s}}, d_{\varphi,h} f^{(0)}_{\boldsymbol{m}} \rangle \quad \text{for all } \boldsymbol{s} \in \mathcal{V}^{(1)},\ \boldsymbol{m} \in \underline{\mathcal{U}}^{(0)}. \tag{4-5}$$

In order to study this matrix, we need to introduce a new enumeration of critical points. Let us start with some abstract notation. Assume that $(\mathcal{I}, \leq)$ and $(\mathcal{J}, \leq)$ are two totally ordered sets and let $A = (a_{ij})_{i\in\mathcal{I}, j\in\mathcal{J}}$ be the associated matrix (with i, j enumerated in increasing order). Assume that we have partitions $\mathcal{P}_\mathcal{I}$ and $\mathcal{P}_\mathcal{J}$ of $\mathcal{I}$ and $\mathcal{J}$ respectively

$$\mathcal{P}_\mathcal{I} = (\mathcal{I}_1, \dots, \mathcal{I}_{N_\mathcal{I}}) \quad \text{and} \quad \mathcal{P}_\mathcal{J} = (\mathcal{J}_1, \dots, \mathcal{J}_{N_\mathcal{J}}).$$

Assume that each partition admits a total order $\preceq$ (that is, we can compare the subsets $\mathcal{I}_i$). Then we get a total order $\preceq$ on $\mathcal{I}$ (resp. $\mathcal{J}$) by using the associated lexicographical order:

$$i \preceq j \quad \Longleftrightarrow \quad (\exists \mathcal{I}_\alpha \preceq \mathcal{I}_\beta,\ i \in \mathcal{I}_\alpha \text{ and } j \in \mathcal{I}_\beta) \text{ or } (\exists \mathcal{I}_\alpha,\ i, j \in \mathcal{I}_\alpha \text{ and } i \leq j).$$

Hence, there exists a unique $\alpha : (\mathcal{I}, \leq) \to (\mathcal{I}, \preceq)$ which is strictly increasing (and hence bijective). Similarly, there is a unique $\beta : (\mathcal{J}, \leq) \to (\mathcal{J}, \preceq)$ which is strictly increasing. We denote by $A_{\mathcal{P}_\mathcal{I}, \mathcal{P}_\mathcal{J}}$ the matrix $(a_{\alpha(i),\beta(j)})_{i\in\mathcal{I}, j\in\mathcal{J}}$. This matrix is obtained from A by intertwining the basis vector; hence it has exactly the same singular values.

Let us go back to the matrix $\mathcal{L}^{\mathrm{bkw},\prime\prime}$. Consider the partitions of $\underline{\mathcal{U}}^{(0)}$ and $\mathcal{V}^{(1)}$ given by

$$\mathcal{P}^{(0)} = \{\mathcal{U}_\alpha^{(0)},\ \alpha \in \underline{\mathcal{A}}\} \quad \text{and} \quad \mathcal{P}^{(1)} = \{\mathcal{V}_\beta^{(1)},\ \beta \in \underline{\mathcal{A}}\}.$$

At this stage of our analysis, we do not need any specific choice of order on these partitions. We just endow $\underline{\mathcal{A}}$ with any total order and for all $\alpha, \beta \in \underline{\mathcal{A}}$ we choose any arbitrary total order on $\mathcal{U}_\alpha^{(0)}$ and $\mathcal{V}_\beta^{(1)}$. This gives an order on the above partitions and we denote by $\mathscr{L} = (\mathscr{L}^{\alpha,\beta})_{\alpha,\beta\in\underline{\mathcal{A}}}$ the matrix $\mathcal{L}^{\mathrm{bkw},\prime\prime}$ associated to these partitions. Observe here that each $\mathscr{L}^{\alpha,\beta}$ is itself a matrix $\mathscr{L}^{\alpha,\beta} = (\mathscr{L}^{\alpha,\beta}_{\boldsymbol{s},\boldsymbol{m}})_{\boldsymbol{s}\in\mathcal{V}_\beta^{(1)}, \boldsymbol{m}\in\mathcal{U}_\alpha^{(0)}}$.

Lemma 4.2. *For all $\alpha \neq \beta$, we have $\mathscr{L}^{\alpha,\beta} = 0$.*

Proof. Let $\alpha, \beta \in \underline{\mathcal{A}}$ such that $\alpha \neq \beta$ and let $\boldsymbol{m} \in \mathcal{U}_\alpha^{(0)}$ and $\boldsymbol{s} \in \mathcal{V}_\beta^{(1)}$. If $\boldsymbol{\sigma}(\alpha) = \boldsymbol{\sigma}(\beta)$ then $\alpha \neq \beta$ implies that $\boldsymbol{s} \notin F(\boldsymbol{m})$. Shrinking if necessary (by taking $\epsilon_0, \delta_0 > 0$ small enough) the support of $f_{\boldsymbol{m}}^{(0)}$ and $f_{\boldsymbol{s}}^{(1)}$, it follows that these functions have disjoint supports so that their scalar product vanishes.

If $\boldsymbol{\sigma}(\alpha) \neq \boldsymbol{\sigma}(\beta)$, then by construction $d_{\varphi,h} f_{\boldsymbol{m}}^{(0)}$ is supported near $\{\varphi = \boldsymbol{\sigma}(\alpha)\}$ whereas $e_{\boldsymbol{s}}^{(1)}$ is supported near $\{\varphi = \boldsymbol{\sigma}(\beta)\}$. Since this two sets are disjoint we get $\langle f_{\boldsymbol{s}}^{(1)}, d_{\varphi,h} e_{\boldsymbol{m}}^{(0)}\rangle = 0$ and the proof is complete. □

From this lemma we deduce that the matrix $\mathscr{L}$ admits a block-diagonal structure

$$\mathscr{L} = \mathrm{diag}(\mathscr{L}^\alpha, \alpha \in \underline{\mathcal{A}}), \tag{4-6}$$

with $\mathscr{L}^\alpha := \mathscr{L}^{\alpha,\alpha}$. Recall from Definition 3.7 that for any $\alpha \in \underline{\mathcal{A}}$, the matrix $\mathscr{T}^\alpha \in \mathscr{M}(\mathcal{U}_\alpha^{(0)}, \widehat{\mathcal{U}}_\alpha^{(0)})$ is given by $\mathscr{T}^\alpha = (\theta_{\boldsymbol{m}}^\alpha(\boldsymbol{m}'))_{\boldsymbol{m}'\in\widehat{\mathcal{U}}_\alpha^{(0)}, \boldsymbol{m}\in\mathcal{U}_\alpha^{(0)}}$. We have the following factorization result on $\mathscr{L}^\alpha$.

Lemma 4.3. *We have $\mathscr{L}^\alpha = \widehat{\mathscr{L}}^\alpha \mathscr{T}^\alpha$, where the matrix $\widehat{\mathscr{L}}^\alpha = (\hat{\ell}^\alpha_{\boldsymbol{s},\boldsymbol{m}'})_{\boldsymbol{s},\boldsymbol{m}'} \in \mathscr{M}(\widehat{\mathcal{U}}_\alpha^{(0)}, \mathcal{V}_\alpha^{(1)})$ is given by*

$$\hat{\ell}^\alpha_{\boldsymbol{s},\boldsymbol{m}'} = \langle f_{\boldsymbol{s}}^{(1)}, d_{\varphi,h} g_{\boldsymbol{m}'}^{(0)}\rangle \quad \text{for all } \boldsymbol{s} \in \mathcal{V}_\alpha^{(1)},\ \boldsymbol{m}' \in \widehat{\mathcal{U}}_\alpha^{(0)},$$

with $g_{\boldsymbol{m}'}^{(0)}(x) = h^{-d/4} c(\boldsymbol{m}', h) \hat{\chi}_{\boldsymbol{m}'}(x) e^{\varphi(\boldsymbol{m}')-\varphi(x)/h}$.

Proof. Let $s \in \mathcal{V}_\alpha^{(1)}$, $m \in \mathcal{U}_\alpha^{(0)}$. From (3-17), one has

$$\langle f_s^{(1)}, d_{\varphi,h} f_m^{(0)}\rangle = h^{-d/4} \sum_{m' \in \widehat{\mathcal{U}}_\alpha^{(0)}} \theta_m^\alpha(m') c(m',h) \langle f_s^{(1)}, hd\,\hat{\chi}_{m'}(x) e^{(\varphi(m)-\varphi(x))/h}\rangle.$$

Moreover, the function φ being constant on $\widehat{\mathcal{U}}_\alpha^{(0),\mathrm{II}}$, we can replace $\varphi(m)$ by $\varphi(m')$ in the above identity and it follows that

$$\langle f_s^{(1)}, d_{\varphi,h} f_m^{(0)}\rangle = \sum_{m' \in \widehat{\mathcal{U}}_\alpha^{(0)}} \theta_m^\alpha(m') \langle f_s^{(1)}, d_{\varphi,h} g_{m'}^{(0)}\rangle,$$

which is exactly the result to be proved. □

One of the crucial points of our analysis is to compute the coefficient $\hat{\ell}_{s,m}^\alpha$. Given $m \in \widehat{\mathcal{U}}_\alpha^{(0)}$, we define

$$h_\varphi(m) = \Bigg(\sum_{m' \in \widehat{H}_\alpha(m)} |\det \operatorname{Hess} \varphi(m)|^{-1/2}\Bigg)^{-1/2}, \tag{4-7}$$

with $\widehat{H}_\alpha(m)$ defined in (3-12). One has clearly $h_\varphi(m) = \pi^{d/4}\gamma_0(m)$, with γ_0 given by (3-13). Moreover, in the case where $H(m) = \{m\}$, one has $h_\varphi(m) = |\det \operatorname{Hess} \varphi(m)|^{1/4}$. Given $s \in \mathcal{V}^{(1)}$, we denote by $\hat{\lambda}_1(s)$ the unique negative eigenvalue of $\operatorname{Hess} \varphi(s)$. In order to keep uniform notation, we also extend the definition (4-7) to saddle points by

$$h_\varphi(s) = |\det \operatorname{Hess} \varphi(s)|^{1/4}.$$

Eventually, we introduce the diagonal matrix $\widehat{\Omega}^\alpha \in \mathscr{M}(\widehat{\mathcal{U}}_\alpha^{(0)}, \widehat{\mathcal{U}}_\alpha^{(0)})$ defined by

$$\widehat{\Omega}^\alpha f(m) = e^{-\widehat{S}(m)/h} f(m) \quad \text{for all } m \in \widehat{\mathcal{U}}_\alpha^{(0)}, \tag{4-8}$$

with $\widehat{S}(m) = \boldsymbol{\sigma}(\alpha) - \varphi(m)$. For $m \in \mathcal{U}_\alpha^{(0)}$, one has of course $\boldsymbol{\sigma}(\alpha) = \boldsymbol{\sigma}(m)$ and hence $\widehat{S}(m) = S(m)$ but this fails to be true for $m = \hat{m}(\alpha)$. We then define the rescaled matrix $\widetilde{\mathscr{L}}^\alpha = (\tilde{\ell}_{s,m}^\alpha) \in \mathscr{M}(\widehat{\mathcal{U}}_\alpha^{(0)}, \mathcal{V}_\alpha^{(1)})$ by

$$\widehat{\mathscr{L}}^\alpha = \widetilde{\mathscr{L}}^\alpha \widehat{\Omega}^\alpha;$$

i.e.,

$$\tilde{\ell}_{s,m}^\alpha = e^{\widehat{S}(m)/h} \hat{\ell}_{s,m}^\alpha \quad \text{for all } s \in \mathcal{V}_\alpha^{(1)},\ m \in \widehat{\mathcal{U}}_\alpha^{(0)}. \tag{4-9}$$

Going back to the matrix $\mathscr{L}^\alpha$, one has

$$\mathscr{L}^\alpha = \widetilde{\mathscr{L}}^\alpha \widehat{\Omega}^\alpha \mathscr{T}^\alpha.$$

Moreover, as already noticed below Definition 3.7, one has $\mathscr{T}^\alpha f(m) = f(m)$ for any f supported on $\mathcal{U}_\alpha^{(0),\mathrm{I}}$. Hence we get

$$\mathscr{L}^\alpha = \widetilde{\mathscr{L}}^\alpha \mathscr{T}^\alpha \Omega^\alpha, \tag{4-10}$$

with $\Omega^\alpha \in \mathscr{M}(\mathcal{U}_\alpha^{(0)}, \mathcal{U}_\alpha^{(0)})$ defined by $\Omega^\alpha f(m) = e^{-S(m)/h} f(m)$. The following lemma gives an asymptotic expansion of the matrix $\widetilde{\mathscr{L}}^\alpha$. We recall that $m_1(s)$ and $m_2(s)$ were defined in Lemma 3.3.

Lemma 4.4. *Let $\alpha \in \underline{\mathcal{A}}$ and $s \in \mathcal{V}_\alpha^{(1)}$, $m \in \widehat{\mathcal{U}}_\alpha^{(0)}$. The following hold true*:

(i) *If $m \notin \{m_1(s), m_2(s)\}$, then $\tilde{\ell}_{s,m}^\alpha = 0$.*

(ii) *The coefficients* $\tilde{\ell}^{\alpha}_{\boldsymbol{s},\boldsymbol{m}}$ *admit a classical expansion* $\tilde{\ell}^{\alpha}_{\boldsymbol{s},\boldsymbol{m}} \sim h^{1/2}\sum_{k\geq 0} h^k \tilde{\ell}^{\alpha,k}_{\boldsymbol{s},\boldsymbol{m}}$. *Moreover, one can choose* $\epsilon_0 = \pm 1$ *in* (3-26) *so that the leading terms satisfy*

$$\tilde{\ell}^{\alpha,0}_{\boldsymbol{s},\boldsymbol{m}_1(\boldsymbol{s})} = \pi^{-1/2}|\hat{\lambda}_1(\boldsymbol{s})|^{1/2}\frac{h_\varphi(\boldsymbol{m}_1(\boldsymbol{s}))}{h_\varphi(\boldsymbol{s})}, \tag{4-11}$$

and in the case where $\boldsymbol{m}_2(\boldsymbol{s}) \in \widehat{\mathcal{U}}^{(0)}_\alpha$,

$$\tilde{\ell}^{\alpha,0}_{\boldsymbol{s},\boldsymbol{m}_2(\boldsymbol{s})} = -\pi^{-1/2}|\hat{\lambda}_1(\boldsymbol{s})|^{1/2}\frac{h_\varphi(\boldsymbol{m}_2(\boldsymbol{s}))}{h_\varphi(\boldsymbol{s})}. \tag{4-12}$$

In particular, if $\boldsymbol{m}_2(\boldsymbol{s}) \in \widehat{\mathcal{U}}^{(0)}_\alpha$, *one has*

$$\frac{\tilde{\ell}^{\alpha,0}_{\boldsymbol{s},\boldsymbol{m}_1(\boldsymbol{s})}}{h_\varphi(\boldsymbol{m}_1(\boldsymbol{s}))} = -\frac{\tilde{\ell}^{\alpha,0}_{\boldsymbol{s},\boldsymbol{m}_2(\boldsymbol{s})}}{h_\varphi(\boldsymbol{m}_2(\boldsymbol{s}))} \tag{4-13}$$

for all $\boldsymbol{s} \in \mathcal{V}^{(1)}_\alpha$.

Proof. Suppose first that $\boldsymbol{m} \neq \boldsymbol{m}_1(\boldsymbol{s}), \boldsymbol{m}_2(\boldsymbol{s})$. Then, $\operatorname{supp}(d_{\varphi,h} g^{(0)}_{\boldsymbol{m}}) = \operatorname{supp}(d\hat{\chi}_{\boldsymbol{m}})$ is contained in a small neighborhood ω of $\Gamma(\boldsymbol{m})$. Since $\boldsymbol{m} \neq \boldsymbol{m}_1(\boldsymbol{s}), \boldsymbol{m}_2(\boldsymbol{s})$ it follows from Lemma 3.3 that $\boldsymbol{s} \notin \omega$ and hence $\tilde{\ell}^{\alpha}_{\boldsymbol{s},\boldsymbol{m}} = 0$ which proves (i).

Let us now compute the coefficients $\tilde{\ell}_{\boldsymbol{s},\boldsymbol{m}}$ for $\boldsymbol{m} \in \{\boldsymbol{m}_1(\boldsymbol{s}), \boldsymbol{m}_2(\boldsymbol{s})\} \cap \widehat{\mathcal{U}}^{(0)}_\alpha$ (observe that this set may be reduced to $\boldsymbol{m}_1(\boldsymbol{s})$). We compute these coefficients in the case where $\boldsymbol{m}_2(\boldsymbol{s}) \in \widehat{\mathcal{U}}^{(0)}_\alpha$. If it is not the case, the only nonzero coefficient is $\tilde{\ell}_{\boldsymbol{s},\boldsymbol{m}_1(\boldsymbol{s})}$, which is computed in the same way. Recall from (3-30), that the quasimodes on 1-forms are given by

$$f^{(1)}_{\boldsymbol{s}} = \epsilon_0 h^{-d/4}\psi_{\boldsymbol{s}}(x) b^{(1)}_{\boldsymbol{s}}(x,h) e^{-\varphi_{+,s}(x)/h}.$$

Summing up the construction of [Helffer, Klein and Nier 2004, Section 4.2], there exists an open neighborhood $V_{\boldsymbol{s}}$ of $\boldsymbol{s}$ on which one can find a system of local Morse coordinates $(y,z) \in \mathbb{R} \times \mathbb{R}^{d-1}$ in which $\boldsymbol{s}$ is the origin and such that the following properties hold true:

(1) In the above coordinate system one has

$$\varphi = \varphi(\boldsymbol{s}) + \frac{1}{2}\Big(\hat{\lambda}^1(\boldsymbol{s})y^2 + \sum_{j=2}^{d}\hat{\lambda}_j(\boldsymbol{s})z_j^2\Big),$$

$$\varphi_+ = \frac{1}{2}\Big(-\hat{\lambda}^1(\boldsymbol{s})y^2 + \sum_{j=2}^{d}\hat{\lambda}_j(\boldsymbol{s})z_j^2\Big),$$

where $(\hat{\lambda}_j(\boldsymbol{s}))_{j=1,\dots,d}$ are the eigenvalues of $\operatorname{Hess}(\varphi)$ at point $\boldsymbol{s}$.

(2) The amplitude $b^{(1)}_{\boldsymbol{s}}(x,h)$ admits a classical expansion

$$b^{(1)}_{\boldsymbol{s}} \sim \sum_{k=0}^{\infty} h^k w_{\boldsymbol{s},k} \tag{4-14}$$

with

$$w_{\boldsymbol{s},0} = (-1)^{d-1}\frac{|\det \operatorname{Hess}\varphi(\boldsymbol{s})|^{1/4}}{\pi^{d/4}}dy \quad \text{on } \{z=0\}. \tag{4-15}$$

(3) One can chose the orientation of the y-axis so that

$$E(\boldsymbol{m}_1(\boldsymbol{s}))\cap V_{\boldsymbol{s}}\subset\{y<0\}\cap V_{\boldsymbol{s}}\quad\text{and}\quad E(\boldsymbol{m}_2(\boldsymbol{s}))\cap V_{\boldsymbol{s}}\subset\{y>0\}\cap V_{\boldsymbol{s}}.$$

Moreover, the cut-off function $\chi_{\boldsymbol{m}}$ can be constructed so that:

(4) In $V_{\boldsymbol{s}}$ the functions $\hat{\chi}_{\boldsymbol{m}_j}$, $j=1,2$, depend only on the variable y.

Additionally, one can shrink $\omega_{\boldsymbol{s}}$ so that:

(5) $\operatorname{supp}(f_{\boldsymbol{s}}^{(1)})$ is contained in $V_{\boldsymbol{s}}$.

Observe that the only minor (but important) difference with [Helffer, Klein and Nier 2004] is the property (3), saying that each $\chi_{\boldsymbol{m}_j}$, $j=1,2$, is supported in one of the two different half-planes $\{y\lesseqgtr 0\}$. Let us now compute the first coefficient in the asymptotic expansion of $\tilde{\ell}^{p,\alpha}_{\boldsymbol{s},\boldsymbol{m}}$. Using the above properties, Proposition 3.5 and following the computations of [Helffer, Klein and Nier 2004, Section 6] we get

$$\begin{aligned}\hat{\ell}^{\alpha}_{\boldsymbol{s},\boldsymbol{m}}&=\langle f_{\boldsymbol{s}}^{(1)},d_{\varphi,h}g_{\boldsymbol{m}}^{(0)}\rangle\\&=h^{1-d/2}c(\boldsymbol{m},h)e(\boldsymbol{s},h)\int_{B(\boldsymbol{s},\epsilon)}e^{-(\varphi_+(x)+\varphi(x)-\varphi(\boldsymbol{m}))/h}(\hat{\chi}'_{\boldsymbol{m}}(y)+\mathcal{O}(h))\,dy\wedge dz_2\wedge\cdots\wedge dz_d\\&\qquad+\mathcal{O}_\epsilon(e^{-(\varphi(\boldsymbol{s})-\varphi(\boldsymbol{m})+c_\epsilon)/h}),\end{aligned}$$

with

$$e(\boldsymbol{s},h)=\epsilon_0(-1)^{d-1}\frac{|\det\operatorname{Hess}\varphi(\boldsymbol{s})|^{1/4}}{\pi^{d/4}}+\mathcal{O}(h)=\epsilon_0(-1)^{d-1}\pi^{-d/4}h_\varphi(\boldsymbol{s})+\mathcal{O}(h).$$

Using the local form of φ and φ_+, we get

$$\begin{aligned}\hat{\ell}^{\alpha}_{\boldsymbol{s},\boldsymbol{m}}&=h^{1-d/2}c(\boldsymbol{m},h)e(\boldsymbol{s},h)e^{-(\varphi(\boldsymbol{s})-\varphi(\boldsymbol{m}))/h}\int_{B(\boldsymbol{s},\epsilon)}e^{-g_-(z)/h}(\hat{\chi}'_{\boldsymbol{m}}(y)+\mathcal{O}(h))\,dy\wedge dz_2\wedge\cdots\wedge dz_d\\&\qquad+\mathcal{O}_\epsilon(e^{-(\varphi(\boldsymbol{s})-\varphi(\boldsymbol{m})+c_\epsilon)/h}),\end{aligned}$$

with $g_-(z)=\sum_{j=2}^{d}\hat{\lambda}_j(\boldsymbol{s})z_j^2$. Since $\hat{\chi}_{\boldsymbol{m}}$ depends only on y and $g_-\geq c\nu^2$ on $|z|_\infty\geq\nu$, the integration domain $B(\boldsymbol{s},\epsilon)$ can be replaced by a smaller one $W_{\boldsymbol{s}}=\{|y|<\epsilon,\ |z|_\infty\leq\nu_\epsilon\}$ modulo exponentially small error terms. Using also the identity $\widehat{S}(\boldsymbol{m})=\varphi(\boldsymbol{s})-\varphi(\boldsymbol{m})$, we get

$$\hat{\ell}^{\alpha}_{\boldsymbol{s},\boldsymbol{m}}=I_\epsilon(h)e^{-\widehat{S}(\boldsymbol{m})/h}+\mathcal{O}_\epsilon(e^{-(\widehat{S}(\boldsymbol{m})+c_\epsilon)/h}),$$

with

$$I_\epsilon(h)=h^{1-d/2}c(\boldsymbol{m},h)e(\boldsymbol{s},h)\int_{W_{\boldsymbol{s}}}e^{-g_-(z)/h}(\hat{\chi}'_{\boldsymbol{m}}(y)+\mathcal{O}(h))\,dy\wedge dz_2\wedge\cdots\wedge dz_d.$$

The integral on the right-hand side can be easily computed by means of Stoke's formula and the Laplace method. We get

$$\begin{aligned}I_\epsilon(h)&=h^{1-d/2}c(\boldsymbol{m},h)e(\boldsymbol{s},h)([\hat{\chi}_{\boldsymbol{m}}]^{\epsilon}_{-\epsilon}+\mathcal{O}(h))\int_{|z|_\infty\leq\nu_\epsilon}e^{-g_-(z)/h}\,dz_2\wedge\cdots\wedge dz_d\\&=h^{1/2}c(\boldsymbol{m},h)e(\boldsymbol{s},h)([\hat{\chi}_{\boldsymbol{m}}]^{\epsilon}_{-\epsilon}+\mathcal{O}(h))\Big(\frac{\pi^{(d-1)/2}}{|\hat{\lambda}_2(\boldsymbol{s})\cdots\hat{\lambda}_d(\boldsymbol{s})|^{1/2}}\Big).\end{aligned}$$

Combining this with the expressions of $c(\boldsymbol{m},h)$ and $e(\boldsymbol{s},h)$, we obtain

$$\tilde{\ell}^{\alpha,0}_{\boldsymbol{s},\boldsymbol{m}} = \epsilon_0(-1)^{d-1}[\hat{\chi}_{\boldsymbol{m}}]^{\epsilon}_{-\epsilon}\pi^{-1/2}|\hat{\lambda}_1(\boldsymbol{s})|^{1/2}\frac{h_\varphi(\boldsymbol{m})}{h_\varphi(\boldsymbol{s})}.$$

We now remark that with our choice of $\hat{\chi}_m$, one has $[\hat{\chi}_{\boldsymbol{m}_1}]^{\epsilon}_{-\epsilon} = -1$ and $[\hat{\chi}_{\boldsymbol{m}_2}]^{\epsilon}_{-\epsilon} = 1$. Taking $\epsilon_0 = (-1)^d$, we get immediately the formula of (ii). □

5. Computation of the approximated singular values

From Lemma A.2, we know that the singular values of a block-diagonal matrix are given by the singular values of each block. Hence, in view of the results of the preceding section, we study the matrices $\mathscr{L}^{\boldsymbol{\alpha}}$. The first step in the analysis is to prove that $\mathscr{L}^{\alpha}$ is injective except for $\alpha = \underline{\alpha}$.

5A. *Injectivity of the matrix $\mathscr{L}^{\boldsymbol{\alpha}}$.* We first compute the kernel of the matrix $\widetilde{\mathscr{L}}^{\alpha}$.

Lemma 5.1. *Let $\alpha \in \underline{A}$. Then*:

- *If α is of type I (that is, $\mathcal{U}^{(0),\,\mathrm{II}}_\alpha = \varnothing$), then $\widetilde{\mathscr{L}}^{\alpha,0}$ is injective.*
- *If α is of type II, then* $\mathrm{Ker}(\widetilde{\mathscr{L}}^{\alpha,0}) = \mathbb{R}\xi_0$, *where $\xi_0 \in \mathbb{R}^{\hat{q}_\alpha} \simeq \mathcal{F}_\alpha$ is defined by*

$$\xi_0(\boldsymbol{m}) = h_\varphi(\boldsymbol{m})^{-1}$$

for all $\boldsymbol{m} \in \widehat{\mathcal{U}}^{(0)}_\alpha$.

Proof. Suppose first that α is of type II. Let $x \in \mathscr{F}_\alpha = \mathscr{F}(\widehat{\mathcal{U}}^{(0)}_\alpha)$ be such that $\widetilde{\mathscr{L}}^{\alpha,0}x = 0$. Then

$$\sum_{\boldsymbol{m}\in\widehat{\mathcal{U}}^{(0)}_\alpha} \tilde{\ell}^{\alpha,0}_{\boldsymbol{s},\boldsymbol{m}} x_{\boldsymbol{m}} = 0 \quad \text{for all } \boldsymbol{s} \in \mathcal{V}^{(1)}_\alpha. \tag{5-1}$$

From (i) of Lemma 4.4 it follows that

$$\tilde{\ell}^{\alpha,0}_{\boldsymbol{s},\boldsymbol{m}_1(\boldsymbol{s})} x_{\boldsymbol{m}_1(\boldsymbol{s})} = -\tilde{\ell}^{\alpha,0}_{\boldsymbol{s},\boldsymbol{m}_2(\boldsymbol{s})} x_{\boldsymbol{m}_2(\boldsymbol{s})} \quad \text{for all } \boldsymbol{s} \in \mathcal{V}^{(1)}_\alpha.$$

Moreover, since α is of type II, we know $\boldsymbol{m}_2(\boldsymbol{s}) \in \widehat{\mathcal{U}}^{(0)}_\alpha$ for any $\boldsymbol{s} \in \mathcal{V}^{(1)}_\alpha$ and thanks to (4-13) we get

$$x_{\boldsymbol{m}_1(\boldsymbol{s})} h_\varphi(\boldsymbol{m}_1(\boldsymbol{s})) = x_{\boldsymbol{m}_2(\boldsymbol{s})} h_\varphi(\boldsymbol{m}_2(\boldsymbol{s})) \quad \text{for all } \boldsymbol{s} \in \mathcal{V}^{(1)}_\alpha. \tag{5-2}$$

Now, we recall that for any $\boldsymbol{s} \in \mathcal{V}^{(1)}_\alpha$, $\boldsymbol{m}_1(\boldsymbol{s})$ and $\boldsymbol{m}_2(\boldsymbol{s})$ are exactly the two minima such that $\boldsymbol{s} = \Gamma_\alpha(\boldsymbol{m}_1) \cap \Gamma_\alpha(\boldsymbol{m}_2)$. Therefore, we deduce from (5-2) that

$$\text{for all } \boldsymbol{m}, \boldsymbol{m}' \in \widehat{\mathcal{U}}^{(0)}_\alpha, \quad (\Gamma_\alpha(\boldsymbol{m}) \cap \Gamma_\alpha(\boldsymbol{m}') \neq \varnothing \implies h_\varphi(\boldsymbol{m})x_{\boldsymbol{m}} = h_\varphi(\boldsymbol{m}')x_{\boldsymbol{m}'}).$$

By the definition of the equivalence relation $\mathcal{R}$, this implies that $x_{\boldsymbol{m}} h_\varphi(\boldsymbol{m})$ is constant on $\widehat{\mathcal{U}}^{(0)}_\alpha$, which means exactly that $x \in \mathbb{R}\xi_0$.

Suppose now that α is of type I and let $x \in \mathscr{F}(\mathcal{U}^{(0)}_\alpha)$ such that $\widetilde{\mathscr{L}}^{\alpha,0}x = 0$. As before, one shows that there exists a constant c such that for all $\boldsymbol{m} \in \mathcal{U}^{(0)}_\alpha$, $h_\varphi(\boldsymbol{m})x_{\boldsymbol{m}} = c$. Recall that the nonempty set $\mathcal{V}^{(1),b}_\alpha$

was defined in Lemma 3.4. Given $s_b \in \mathcal{V}_\alpha^{(1),\boldsymbol{b}}$, since $\boldsymbol{m}_2(s_b) = \hat{\boldsymbol{m}}(\alpha) \notin \widehat{\mathcal{U}}_\alpha^{(0)}$, one has $\tilde{\ell}^{\alpha,0}_{s_b,\boldsymbol{m}} = 0$ for any $\boldsymbol{m} \neq \boldsymbol{m}_1(s_b)$ and

$$\tilde{\ell}^{\alpha,0}_{s_b,\boldsymbol{m}_1(s_b)} = \pi^{-1/2}|\hat{\lambda}_1(s_b)|^{1/2} \neq 0.$$

Combined with (5-1) this shows that $x_{\boldsymbol{m}_1(s_b)} = 0$ and hence $c = 0$, which proves that $\mathrm{Ker}(\widetilde{\mathscr{L}}^{\alpha,0}) = 0$. □

Proposition 5.2. *Let $\alpha \in \underline{\mathcal{A}}$, then the matrix $\widehat{\mathscr{L}}^\alpha := \widetilde{\mathscr{L}}^\alpha \mathscr{T}^\alpha$ admits a classical expansion $\widehat{\mathscr{L}}^\alpha \sim h^{1/2}\sum_j h^j \widehat{\mathscr{L}}^{\alpha,j}$ and the matrix $\widehat{\mathscr{L}}^{\alpha,0}$ is injective.*

Proof. By Lemmas 3.6 and 4.4 the matrices $\widetilde{\mathscr{L}}^\alpha$ and $\mathscr{T}^\alpha$ admit classical expansions $\widetilde{\mathscr{L}}^\alpha \sim h^{1/2}\sum h^j \widetilde{\mathscr{L}}^{\alpha,j}$ and $\mathscr{T}^\alpha \sim \sum h^j \mathscr{T}^{\alpha,j}$. Therefore, $\widehat{\mathscr{L}}^\alpha$ admits a classical expansion $\widehat{\mathscr{L}}^\alpha \sim h^{1/2}\sum_j h^j \widehat{\mathscr{L}}^{\alpha,j}$ with $\widehat{\mathscr{L}}^{\alpha,0} = \widetilde{\mathscr{L}}^{\alpha,0}\mathscr{T}^{\alpha,0}$.

Let us now prove that $\widehat{\mathscr{L}}^{\alpha,0}$ is injective.

Suppose first that α is of type I. Then $\mathscr{T}^\alpha = \mathscr{T}^{\alpha,0} = \mathrm{Id}$ and the result follows immediately from the first part of Lemma 5.1.

Suppose now that α is of type II and let $x \in \mathscr{F}(\mathcal{U}^{(0)})$ be such that $\widetilde{\mathscr{L}}^{\alpha,0}\mathscr{T}^{\alpha,0}x = 0$. We have the decomposition $x = x^{\mathrm{I}} + x^{\mathrm{II}}$, with $x^\bullet$ supported in $\widehat{\mathcal{U}}^{(0),\bullet}$. Thanks to (3-20), we have

$$\mathscr{T}^{\alpha,0}x(\boldsymbol{m}) = x^{\mathrm{I}}(\boldsymbol{m}) + (\widehat{\mathscr{T}}^{\alpha,0}x^{\mathrm{II}})(\boldsymbol{m}),$$

with $\widehat{\mathscr{T}}^{\alpha,0} : \mathscr{F}(\mathcal{U}^{(0),\mathrm{II}}) \to \mathscr{F}(\widehat{\mathcal{U}}^{(0),\mathrm{II}})$ such that $\mathrm{Ran}\,\widehat{\mathscr{T}}^{\alpha,0} = (\mathbb{R}\theta_0^\alpha)^\perp$, where the function θ_0^α is defined by (3-11). On the other hand, we have $\ker\widetilde{\mathscr{L}}^{\alpha,0} = \mathbb{R}\xi_0$ and we have the decomposition $\xi_0 = \xi_0^{\mathrm{I}} + \xi_0^{\mathrm{II}}$, with $\xi_0^{\mathrm{II}} = \theta^{\alpha,0}$. The equation $\widetilde{\mathscr{L}}^{\alpha,0}\mathscr{T}^{\alpha,0}x = 0$ implies that there exists $\lambda \in \mathbb{R}$ such that $\mathscr{T}^{\alpha,0}x = \lambda\xi_0$ and hence $\widehat{\mathscr{T}}^{\alpha,0}x^{\mathrm{II}} = \lambda\xi_0^{\mathrm{II}}$. On the other hand, by construction, $\mathrm{Ran}\,\widehat{\mathscr{T}}^{\alpha,0} = (\xi_0^{\mathrm{II}})^\perp$. This implies that $\lambda = 0$ and proves the result. □

Corollary 5.3. *For all $\alpha \in \underline{\mathcal{A}}$ the matrix $\mathscr{L}^\alpha$ is injective.*

Proof. This follows directly from the above proposition and the fact that

$$\mathscr{L}^\alpha = \widehat{\mathscr{L}}^\alpha \mathscr{T}^\alpha = \widetilde{\mathscr{L}}^\alpha \widehat{\Omega}^\alpha \mathscr{T}^\alpha = \widehat{\mathscr{L}}^\alpha \Omega^\alpha, \tag{5-3}$$

with Ω^α defined below (4-10) which is invertible. □

5B. ***Graded structure of the matrices $\mathscr{L}^\alpha$.*** Throughout this section, we assume that $\alpha \in \mathcal{A}$ is fixed. Recall that we defined $\mathcal{S}_\alpha = S(\mathcal{U}_\alpha^{(0)})$, $p(\alpha) = \#\mathcal{S}_\alpha$ and some integers $\nu_1^\alpha < \cdots < \nu_{p(\alpha)}^\alpha$ such that

$$\mathcal{S}_\alpha = \{S_{\nu_1^\alpha}, \dots, S_{\nu_{p(\alpha)}^\alpha}\},$$

with the convention $S_{\nu_1^\alpha} > \cdots > S_{\nu_{p(\alpha)}^\alpha}$. In order to lighten the notation we will drop the indices α and write from now $p = p(\alpha)$, $\nu_j = \nu_j^\alpha$. To the set of heights $\mathcal{S}_\alpha$, we can associate a natural partition

$$\widehat{\mathcal{U}}_\alpha^{(0)} = \bigsqcup_{n=1}^{p} \widehat{\mathcal{U}}_{\alpha,n}^{(0)} \tag{5-4}$$

with $\widehat{\mathcal{U}}_{\alpha,n}^{(0)} = \{\boldsymbol{m} \in \widehat{\mathcal{U}}_\alpha^{(0)} : \varphi(\boldsymbol{m}) = \boldsymbol{\sigma}(\alpha) - S_{\nu_n}\}$. We order this partition by deciding that $\widehat{\mathcal{U}}_{\alpha,n+1}^{(0)} \prec \widehat{\mathcal{U}}_{\alpha,n}^{(0)}$. On the other hand, we recall that $\mathscr{L}^\alpha = \widehat{\mathscr{L}}^\alpha \Omega^\alpha$ with $\widehat{\mathscr{L}}^\alpha = \widetilde{\mathscr{L}}^\alpha \mathscr{T}^\alpha$. Let us compute the matrices $\widehat{\mathscr{L}}^\alpha$

and Ω^α in the basis given by the above partition of $\widehat{\mathcal{U}}_\alpha^{(0)}$. With a slight abuse of notation we still denote by $\widehat{\mathscr{L}}^\alpha$ and Ω^α the resulting matrices. Since $\widehat{S}(\boldsymbol{m}) = \boldsymbol{\sigma}(\alpha) - S_{\nu_k}$ on $\mathcal{U}_{\alpha,k}^{(0)}$, it follows from (4-8) that in the above partition, the matrix Ω^α can be written

$$\Omega^\alpha = \begin{pmatrix} e^{-S_{\nu_p}/h} I_{r_p} & 0 & \cdots & \cdots & 0 \\ 0 & e^{-S_{\nu_{p-1}}/h} I_{r_{p-1}} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & 0 & e^{-S_{\nu_1}/h} I_{r_1} \end{pmatrix}, \tag{5-5}$$

where the $r_j = \#\mathcal{U}_{\alpha,j}^{(0)}$ are such that $r_1 + \cdots + r_p = \#\mathcal{U}_\alpha^{(0)}$. Factorizing by $e^{-S_{\nu_p}/h}$, we get $\Omega^\alpha = e^{-S_{\nu_p}/h}\widehat{\Omega}^\alpha(\tau)$, with

$$\widehat{\Omega}^\alpha(\tau) = \begin{pmatrix} I_{r_p} & 0 & \cdots & \cdots & 0 \\ 0 & \tau_2 I_{r_{p-1}} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & 0 & \tau_2\tau_3\cdots\tau_p I_{r_1} \end{pmatrix}, \tag{5-6}$$

where $\tau = (\tau_2, \dots, \tau_p) \in (\mathbb{R}_+^*)^p$ is defined by $\tau_j = e^{(S_{\nu_{p-(j-2)}} - S_{\nu_{p-(j-1)}})/h}$ for any $j = 2, \dots, p$. With this new notation, one deduces from (5-3), that $\mathscr{L}^{\alpha,*}\mathscr{L}^\alpha = he^{-2S_{\nu_p}/h}\widehat{\mathcal{M}}^\alpha(\tau)$, with

$$\widehat{\mathcal{M}}^\alpha(\tau) = \widehat{\Omega}^\alpha(\tau)(h^{-1}\widehat{\mathscr{L}}^{\alpha,*}\widehat{\mathscr{L}}^\alpha)\widehat{\Omega}^\alpha(\tau). \tag{5-7}$$

It turns out that such matrices can be described in a slightly more general setting that is useful to compute their spectrum. We introduce this setting now. Throughout, we denote by $\mathscr{S}^+(E)$ the set of symmetric positive definite matrices on a vector space E. We will denote by $\mathscr{S}_{\mathrm{cl}}^+(E)$ the set of h-dependent matrices $M(h) \in \mathscr{S}^+(E)$ admitting a classical expansion $M(h) \sim \sum_j h^j M_j$ with $M_0 \in \mathscr{S}^+(E)$. We will sometimes drop E and write for short $\mathscr{S}^+$, $\mathscr{S}_{\mathrm{cl}}^+$.

Definition 5.4. Let $\mathscr{E} = (E_j)_{j=1,\dots,p}$ be a sequence of finite-dimensional vector spaces E_j of dimension $r_j > 0$, let $E = \bigoplus_{j=1,\dots,p} E_j$ and let $\tau = (\tau_2, \dots, \tau_p) \in (\mathbb{R}_+^*)^{p-1}$. Suppose that $\tau \mapsto \mathcal{M}(\tau)$ is a smooth map from $(\mathbb{R}_+^*)^{p-1}$ into the set of matrices $\mathscr{M}(E)$:

- We say that $\mathcal{M}(\tau)$ is an $(\mathscr{E}, \tau)$-graded matrix if there exists $\mathcal{M}' \in \mathscr{S}^+(E)$ independent of τ such that $\mathcal{M}(\tau) = \Omega(\tau)\mathcal{M}'\Omega(\tau)$, with $\Omega(\tau) \in \mathscr{M}(E)$ of the form (5-6); that is, $\Omega = \operatorname{diag}(\epsilon_j(\tau) I_{r_j},\ j = 1, \dots, p)$, where $\epsilon_1(\tau) = 1$ and $\epsilon_j(\tau) = \left(\prod_{k=2}^j \tau_k\right)$ for all $j \geq 2$.
- We say that a family of $(\mathscr{E}, \tau)$-graded matrices $\mathcal{M}_h(\tau),\ h \in]0, h_0]$ is classical if one has $\mathcal{M}_h(\tau) = \Omega(\tau)\mathcal{M}'(h)\Omega(\tau)$ for some matrix $\mathcal{M}'(h) \in \mathscr{S}_{\mathrm{cl}}^+(E)$.

Throughout, we denote by $\mathscr{G}(\mathscr{E}, \tau)$ the set of $(\mathscr{E}, \tau)$-graded matrices and by $\mathscr{G}_{\mathrm{cl}}(\mathscr{E}, \tau)$ the set of classical $(\mathscr{E}, \tau)$-graded matrices.

Let us remark that for $p = 1$, a graded matrix is simply a τ-independent symmetric positive definite matrix.

Lemma 5.5. *Suppose that $\mathcal{M}_h(\tau)$ is a classical $(\mathscr{E},\tau)$-graded family of matrices and that $p \geq 2$. Then one has*

$$\mathcal{M}_h(\tau) = \begin{pmatrix} J(h) & \tau_2 B_h(\tau')^* \\ \tau_2 B_h(\tau') & \tau_2^2 \mathcal{N}_h(\tau') \end{pmatrix}, \tag{5-8}$$

with

- $J(h) \in \mathscr{S}_{\mathrm{cl}}^{+}(E_1)$,
- $\mathcal{N}_h(\tau') \in \mathscr{G}_{\mathrm{cl}}(\mathscr{E}',\tau')$, *with* $\tau' = (\tau_3,\dots,\tau_p)$ *and* $\mathscr{E}' = (E_j)_{j=2,\dots,p}$,
- $B_h(\tau') \in \mathscr{M}\big(E_1, \bigoplus_{j=2}^{p} E_j\big)$ *satisfying*

  $$B_h(\tau')^* = (b_2(h)^*, \tau_3 b_3(h)^*, \tau_3\tau_4 b_4(h)^*, \dots, \tau_3\cdots\tau_p b_p(h)^*),$$

  with $b_j(h) : E_1 \to E_j$ *independent of* τ *admitting a classical expansion.*

Moreover, the matrix $\mathcal{N}_h(\tau') - B_h(\tau')J(h)^{-1}B_h(\tau')^*$ *belongs to* $\mathscr{G}_{\mathrm{cl}}(\mathscr{E}',\tau')$.

Proof. Assume that $\mathcal{M}_h(\tau) = \Omega(\tau)\mathcal{M}'(h)\Omega(\tau)$, with $\Omega(\tau)$ of the form (5-6). First observe that

$$\Omega(\tau) = \begin{pmatrix} I_{r_p} & 0 \\ 0 & \tau_2\Omega'(\tau'), \end{pmatrix},$$

with

$$\Omega'(\tau') = \begin{pmatrix} I_{r_{p-1}} & 0 & \cdots & \cdots & 0 \\ 0 & \tau_3 I_{r_{p-2}} & 0 & \cdots & 0 \\ \vdots & 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & 0 & \tau_3\tau_4\cdots\tau_p I_{r_1} \end{pmatrix}.$$

On the other hand, we can write

$$\mathcal{M}'(h) = \begin{pmatrix} J(h) & B'(h)^* \\ B'(h) & \mathcal{N}'(h) \end{pmatrix},$$

with $J(h), \mathcal{N}'(h) \in \mathscr{S}_{\mathrm{cl}}^{+}$ and $B'(h)$ admitting a classical expansion. Therefore,

$$\Omega(\tau)\mathcal{M}'_h\Omega(\tau) = \begin{pmatrix} J(h) & \tau_2 B'(h)^*\Omega'(\tau') \\ \tau_2\Omega'(\tau')B'(h) & \tau_2^2\Omega'(\tau')\mathcal{N}'(h)\Omega'(\tau') \end{pmatrix},$$

which has exactly the form (5-8) with $B_h(\tau') = \Omega'(\tau')B'(h)$ and $\mathcal{N}_h(\tau') = \Omega'(\tau')\mathcal{N}'(h)\Omega'(\tau')$. By construction, $\mathcal{N}_h(\tau')$ belongs to $\mathscr{G}_{\mathrm{cl}}(\mathscr{E}',\tau')$ and $B_h(\tau')$ has the required form.

It remains to prove that

$$\mathcal{R}_h := \mathcal{N}_h(\tau') - B_h(\tau')J(h)^{-1}B_h(\tau')^*$$

belongs to $\mathscr{G}_{\mathrm{cl}}(\mathscr{E}',\tau')$. First observe that since $J(h)$ is symmetric positive definite, this quantity is well-defined. Moreover, one has by construction

$$\begin{aligned} \mathcal{R}_h &= \Omega'(\tau')\mathcal{N}'(h)\Omega'(\tau') - \Omega'(\tau')B'(h)J(h)^{-1}B'(h)^*\Omega'(\tau') \\ &= \Omega'(\tau')\mathcal{R}'(h)\Omega'(\tau'), \end{aligned}$$

with $\mathcal{R}'(h) = \mathcal{N}'(h) - B'(h)J(h)^{-1}B'(h)^*$. Since $J(h) \in \mathscr{S}^+_{\mathrm{cl}}$, we have $J(h)^{-1} \in \mathscr{S}^+_{\mathrm{cl}}$ and $\mathcal{R}'(h)$ admits a classical expansion $\mathcal{R}'(h) \sim \sum_j h^j \mathcal{R}'_j$ with

$$\mathcal{R}'_0 = J_0 - B'_0 J_0^{-1}(B'_0)^*.$$

Moreover, since $\mathcal{M}'(h) \in \mathscr{S}^+_{\mathrm{cl}}$, the matrix

$$\mathcal{M}'_0 = \begin{pmatrix} J_0 & (B'_0)^* \\ B'_0 & \mathcal{N}'_0 \end{pmatrix}$$

is symmetric definite positive. Hence, it follows directly from Lemma A.5 that $\mathcal{R}'_0 \in \mathscr{S}^+$. □

5C. *The spectrum of graded matrices.* Using Lemma 5.5, we define an application $\mathcal{R} : \mathscr{G}_{\mathrm{cl}}(\mathscr{E}, \tau) \to \mathscr{G}_{\mathrm{cl}}(\mathscr{E}', \tau')$, with $\tau' = (\tau_3, \dots, \tau_p)$ and $\mathscr{E}' = \bigoplus_{j=2}^p E_j$, by

$$\mathcal{R}(\mathcal{M}_h(\tau)) = \mathcal{N}_h(\tau') - B_h(\tau')J(h)^{-1}B_h^*(\tau') \tag{5-9}$$

for any $\mathcal{M}_h(\tau) \in \mathscr{G}_{\mathrm{cl}}(\mathscr{E}, \tau)$. Of course, the map $\mathcal{R}$ depends on $\mathscr{E}$ and τ, but we omit this dependence since the set on which $\mathcal{R}$ is acting will be obvious in the sequel. By a slight abuse of notation we will write $\mathcal{R}^k = \mathcal{R} \circ \cdots \circ \mathcal{R}$ (k times). Obviously, $\mathcal{R}^k$ acts from $\mathscr{G}(\mathscr{E}, \tau)$ into $\mathscr{G}(\mathscr{E}^{(k)}, \tau^{(k)})$ with $\mathscr{E}^{(k)} = \bigoplus_{j=k+1}^p E_j$ and $\tau^{(k)} = (\tau_{k+2}, \dots, \tau_p)$. In the same way, we defined $\mathcal{R}$, we can define a map $\mathcal{J} : \mathscr{G}_{\mathrm{cl}}(\mathscr{E}, \tau) \to \mathscr{S}^+_{\mathrm{cl}}(E_1)$ by $\mathcal{J}(\mathcal{M}_h(\tau)) = \mathcal{M}_h$ if $p = 1$ and $\mathcal{J}(\mathcal{M}_h(\tau)) = J(h)$ for any $\mathcal{M}_h(\tau)$ having the form (5-8) if $p \geq 2$.

Theorem 5.6. *Let $\mathscr{E} = (E_j)_{j=1,\dots,p}$ be a finite sequence of vector spaces E_j of finite dimension $n_j = \dim E_j$ and let $\tau = (\tau_2, \dots, \tau_p) \in (\mathbb{R}_+^*)^{p-1}$. Suppose that $\mathcal{M}_h(\tau)$ is classical $(\mathscr{E}, \tau)$-graded. There exists $h_0 > 0$ and $\delta > 0$ such that uniformly with respect to $h \in \,]0, h_0]$ and $|\tau|_\infty < \delta$, one has*

$$\sigma(\mathcal{M}_h(\tau)) = \bigsqcup_{j=1}^{p} \epsilon_j \sigma(\mathcal{J} \circ \mathcal{R}^{j-1}(\mathcal{M}_h(\tau)))(1 + \mathcal{O}(|\tau|_\infty^2)), \tag{5-10}$$

with $\epsilon_j = \epsilon_j(\tau)$ given in Definition 5.4.

Remark 5.7. In the above theorem, the matrix $\mathcal{J} \circ \mathcal{R}^{j-1}(\mathcal{M}_h(\tau))$ is always independent of the parameter τ. Let us define $\{\lambda_1^j \leq \cdots \leq \lambda_{n_j}^j\} = \sigma(\mathcal{J} \circ \mathcal{R}^{j-1}(\mathcal{M}_h(\tau)))$. The identity (5-10) means that there exists $a, b > 0$ independent of τ, h such that

$$\sigma(\mathcal{M}_h(\tau)) \subset \bigsqcup_{j=1}^{p} \epsilon_j [a, b]$$

and that, for all $j = 1, \dots, p$, $\mathcal{M}_h(\tau)$ has exactly n_j eigenvalues $\mu_1^j \leq \cdots \leq \mu_{n_j}^j$ in $\epsilon_j[a, b]$ and

$$\mu_n^j = \epsilon_j(\lambda_n^j + \mathcal{O}(|\tau|_\infty^2)).$$

Proof. We prove the theorem by induction on p. Throughout the proof the notation $\mathcal{O}(\cdot)$ is uniform with respect to the parameters h and τ. For $p = 1$, $\mathcal{M}_h(\tau) = \mathcal{M}_h \in \mathscr{S}^+_{\mathrm{cl}}(E_1)$ is independent of τ and $\mathcal{J}\mathcal{R}^0(\mathcal{M}_h(\tau)) = \mathcal{J}\mathcal{M}_h(\tau) = \mathcal{M}_h$, which proves the statement.

Suppose now that $p \geq 2$ and let $\mathcal{M}_h(\tau) \in \mathscr{G}_{\mathrm{cl}}(\mathscr{E}, \tau)$. We have

$$\mathcal{M}_h(\tau) = \begin{pmatrix} J(h) & \tau_2 B_h(\tau')^* \\ \tau_2 B_h(\tau') & \tau_2^2 \mathcal{N}_h(\tau') \end{pmatrix},$$

with $J(h)$, $B_h(\tau')$ and $\mathcal{N}_h(\tau')$ as in Lemma 5.5. In order to lighten the notation we will drop the variables τ, τ' in the proof below. For $\lambda \in \mathbb{C}$, let

$$\mathcal{P}(\lambda) := \mathcal{M}_h - \lambda = \begin{pmatrix} J(h) - \lambda & \tau_2 B_h^* \\ \tau_2 B_h & \tau_2^2 \mathcal{N}_h - \lambda \end{pmatrix}. \tag{5-11}$$

This is an holomorphic function, and since it is nontrivial, its inverse is well-defined except for a finite number of values of λ which are exactly the eigenvalues of $\mathcal{M}_h$. Moreover $\lambda \in \mathbb{C} \mapsto \mathcal{P}(\lambda)^{-1}$ is meromorphic with poles in $\sigma(\mathcal{M}_h)$ and for any μ in $\sigma(\mathcal{M}_h)$, the rank of the residue of $\mathcal{P}(\lambda)^{-1}$ at μ is exactly the multiplicity of μ as an eigenvalue.

Let us first prove that $\mathcal{M}_h$ admits at least n_1 eigenvalues of size 1. Let $\lambda_n^1 = \lambda_n^1(h)$, $n = 1, \dots, n_1$, denote the increasing sequence of eigenvalues of the positive definite matrix $J(h)$. Since $J(h) = J_0 + \mathcal{O}(h)$ with $J_0 \in \mathscr{S}^+$, the $\lambda_n^1(h)$ satisfy $\lambda_n^1(h) = \lambda_{n,0}^1 + \mathcal{O}(h)$, with $\lambda_{n,0}^1$ an eigenvalue of J_0. In particular $\lambda_{n,0}^1 > 0$ for all $n = 1, \dots, n_1$ and hence there exists $c_1, d_1 > 0$ and $h_0 > 0$ such that for $h \in]0, h_0]$ and all $n = 1, \dots, n_1$, one has $\lambda_n^1(h) \in [c_1, d_1]$. Let $n \in \{1, \dots, n_1\}$ be fixed and consider $D_n = D_n(h, \tau_2) = \{z \in \mathbb{C} : |z - \lambda_n^1| \leq M\tau_2^2\}$ for some $M > 0$ that will be chosen large enough later and $\widetilde{D}_n = \{z \in \mathbb{C} : |z - \lambda_n^1| \leq 2M\tau_2^2\}$. Observe that for $h, \tau_2 > 0$ small enough, the disks $\widetilde{D}_n$ are disjoint. By definition, one has $\mathcal{N}_h(\tau') = \mathcal{O}(1)$ and since $\lambda_n^1 \geq c_1 > 0$, this implies that for $\tau_2 > 0$ small enough with respect to c and $\lambda \in \widetilde{D}_n$, the matrix $\tau_2^2 \mathcal{N}_h(\tau') - \lambda$ is invertible, and $(\tau_2^2 \mathcal{N}_h(\tau') - \lambda)^{-1} = \mathcal{O}(1)$. Moreover, for $\lambda \in \widetilde{D}_n \setminus D_n$, $J(h) - \lambda$ is invertible and $(J(h) - \lambda)^{-1} = \mathcal{O}(\tau_2^{-2} M^{-1})$. This implies that for $M > 0$ large enough, $J(h) - \lambda - \tau_2^2 B_h^* (\tau_2^2 \mathcal{N}_h - \lambda)^{-1} B_h$ is invertible with

$$\begin{aligned} (J(h) - \lambda - \tau_2^2 B_h^* (\tau_2^2 \mathcal{N}_h - \lambda)^{-1} B_h)^{-1} &= (J(h) - \lambda)^{-1} \big(I - \tau_2^2 B_h^* (\tau_2^2 \mathcal{N}_h - \lambda)^{-1} B_h (J(h) - \lambda)^{-1}\big)^{-1} \\ &= (J(h) - \lambda)^{-1} (1 + \mathcal{O}(M^{-1})). \end{aligned} \tag{5-12}$$

Hence, the standard Schur complement procedure shows that for $\lambda \in \widetilde{D}_n \setminus D_n$, $\mathcal{P}(\lambda)$ is invertible with inverse $\mathcal{E}(\lambda)$ given by

$$\mathcal{E}(\lambda) = \begin{pmatrix} E(\lambda) & -\tau_2 E(\lambda) B_h^* (\tau_2^2 \mathcal{N}_h - \lambda)^{-1} \\ -\tau_2 (\tau_2^2 \mathcal{N}_h - \lambda)^{-1} B_h E(\lambda) & E_0(\lambda) \end{pmatrix}, \tag{5-13}$$

with

$$\begin{aligned} E(\lambda) &= (J(h) - \lambda - \tau_2^2 B_h^* (\tau_2^2 \mathcal{N}_h - \lambda)^{-1} B_h)^{-1}, \\ E_0(\lambda) &= (\tau_2^2 \mathcal{N}_h - \lambda)^{-1} + \tau_2^2 (\tau_2^2 \mathcal{N}_h - \lambda)^{-1} B_h E(\lambda) B_h^* (\tau_2^2 \mathcal{N}_h - \lambda)^{-1}. \end{aligned}$$

By functional calculus and the Cauchy formula, the number of eigenvalues of $\mathcal{M}_h$ (counted with multiplicity) in D_n is equal to the rank of the projector

$$\Pi_n = \frac{1}{2i\pi} \int_{\partial D_n} \mathcal{E}(\lambda) \, d\lambda.$$

One has $\mathrm{rk}(\pi_n) \ge \mathrm{rk}(\widetilde{\Pi}_n)$, where we set

$$\widetilde{\Pi}_n = \begin{pmatrix} \mathrm{Id} & 0 \\ 0 & 0 \end{pmatrix} \Pi_n \begin{pmatrix} \mathrm{Id} & 0 \\ 0 & 0 \end{pmatrix}.$$

On the other hand, an elementary computation shows that

$$\widetilde{\Pi}_n = \frac{1}{2i\pi} \int_{\partial D_n} \begin{pmatrix} E(\lambda) & 0 \\ 0 & 0 \end{pmatrix} d\lambda = \begin{pmatrix} E_n & 0 \\ 0 & 0 \end{pmatrix},$$

with

$$E_n = \frac{1}{2i\pi} \int_{\partial D_n} (J(h) - \lambda - \tau_2^2 B_h^* (\tau_2^2 \mathcal{N}_h - \lambda)^{-1} B_h)^{-1} \, d\lambda.$$

As a consequence we get $\mathrm{rk}(\Pi_n) \ge \mathrm{rk}(E_n)$. Moreover, for M large enough independent of (h, τ), the matrix $(I - \tau_2^2 B_h^* (\tau_2^2 \mathcal{N}_h - \lambda)^{-1} B_h (J(h) - \lambda)^{-1})^{-1}$ is holomorphic in $\widetilde{D}_n$. It follows from (5-12) that the rank of E_n is exactly the multiplicity of λ_n^1 and hence the rank of Π_n is bounded from below by the multiplicity of λ_n^1. Therefore, $\mathcal{M}_h$ admits at least n_1 eigenvalues $\mu_1^1 \le \cdots \le \mu_{n_1}^1$ in the interval $[c_1 - M\tau_2^2, d_1 + M\tau_2^2]$ and these eigenvalues satisfy

$$\mu_n^1 = \lambda_n^1 + \mathcal{O}(\tau_2^2) \quad \text{for all } n = 1, \dots, n_1. \tag{5-14}$$

Let us now study the eigenvalues below τ_2^2. Throughout the proof, we let $t = |\tau'|_\infty$. Thanks to the last part of Lemma 5.5, the matrix $\mathcal{Z}_h(\tau') := \mathcal{R}(\mathcal{M}_h(\tau)) = \mathcal{N}_h - B_h J(h)^{-1} B_h^*$ is classical $(\mathscr{E}', \tau')$-graded. Hence, it follows from the induction hypothesis that uniformly with respect to h, one has

$$\sigma(\mathcal{Z}_h(\tau')) = \bigsqcup_{j=2}^{p} \tilde{\epsilon}_j \sigma(\mathcal{J} \circ \mathcal{R}^{j-2}(\mathcal{Z}_h(\tau')))(1 + \mathcal{O}(|\tau'|_\infty^2)), \tag{5-15}$$

with $\tilde{\epsilon}_j = \left(\prod_{l=3}^{j} \tau_l\right)^2$ for $j \ge 3$ and $\tilde{\epsilon}_2 = 1$. Moreover, by definition, one has $\mathcal{Z}_h = \mathcal{R}(\mathcal{M}_h(\tau))$; hence (5-15) can be rewritten as

$$\sigma(\mathcal{Z}_h(\tau')) = \bigsqcup_{j=2}^{p} \tilde{\epsilon}_j \sigma(\mathcal{J} \circ \mathcal{R}^{j-1}(\mathcal{M}_h(\tau)))(1 + \mathcal{O}(|\tau'|_\infty^2)). \tag{5-16}$$

Since $\mathcal{M}_h(\tau') \in \mathscr{G}_{\mathrm{cl}}(\mathscr{E}, \tau)$, for all $j = 2, \dots, p$ the matrix $\mathcal{J} \circ \mathcal{R}^{j-1}(\mathcal{M}_h(\tau))$ belongs to $\mathscr{S}_{\mathrm{cl}}^{+}(E_j)$. For $j = 2, \dots, p$, let $\lambda_1^j(h) \le \cdots \le \lambda_{n_j}^j(h)$ denote the eigenvalues of the symmetric matrix $\mathcal{J} \circ \mathcal{R}^{j-1}(\mathcal{M}_h(\tau))$. As above, this implies that there exist $c_j, d_j > 0$ and $h_0 > 0$ such that for all $h \in]0, h_0]$ the eigenvalues $\lambda_n^j(h)$ satisfy $\lambda_n^j(h) \in [c_j, d_j]$ for all $n = 1, \dots, n_j$. Suppose now that $j \in \{2, \dots, p\}$ and $n \in \{1, \dots, n_j\}$ are fixed and consider $D'_{j,n} = \{z \in \mathbb{C} : |z - \epsilon_j \lambda_n^j| \le M t^2 \epsilon_j\}$ for some $M > 0$ to be chosen large enough and $\widetilde{D}'_{j,n} = \{z \in \mathbb{C} : |z - \epsilon_j \lambda_n^j| \le 2M t^2 \epsilon_j\}$. As above, we introduce also the corresponding projector

$$\Pi'_{j,n} = \frac{1}{2i\pi} \int_{\partial D'_{j,n}} \mathcal{E}(\lambda) \, d\lambda.$$

Since J_0 is invertible, we know that for λ in $\widetilde{D}'_{j,n}$ and h, t small enough, $J(h)-\lambda$ is invertible and once again the Schur complement formula permits us to write the inverse of $\mathcal{P}(\lambda)$,

$$\mathcal{E}(\lambda) = \begin{pmatrix} E_0(\lambda) & -\tau_2(J(h)-\lambda)^{-1}B_h^*E(\lambda) \\ -\tau_2 E(\lambda)B_h(J(h)-\lambda)^{-1} & E(\lambda) \end{pmatrix}, \tag{5-17}$$

with

$$E(\lambda) = (\tau_2^2\mathcal{N}_h - \lambda - \tau_2^2 B_h(J(h)-\lambda)^{-1}B_h^*)^{-1},$$
$$E_0(\lambda) = (J(h)-\lambda)^{-1} + \tau_2^2(J(h)-\lambda)^{-1}B_h^*E(\lambda)B_h(J(h)-\lambda)^{-1}.$$

Setting $\lambda = \tau_2^2 z$, we get (using the relation $\epsilon_j = \tau_2^2\tilde{\epsilon}_j$)

$$\Pi'_{j,n} = \frac{\tau_2^2}{2i\pi}\int_{\partial\widehat{D}'_{j,n}} \mathcal{E}(\tau_2^2 z)\,dz,$$

with $\widehat{D}'_n = \{z \in \mathbb{C} : |z - \tilde{\epsilon}_j\lambda_n^j| \le Mt^2\tilde{\epsilon}_j\}$. Moreover, for $|z-\tilde{\epsilon}_j\lambda_n^j| = Mt^2\tilde{\epsilon}_j$, the matrix $J(h)$ is invertible with $J(h)^{-1} = \mathcal{O}(1)$; hence we have

$$\begin{aligned} E(\tau_2^2 z) &= \tau_2^{-2}(\mathcal{N}_h - z - B_h(J(h)-\tau_2^2 z)^{-1}B_h^*)^{-1} \\ &= \tau_2^{-2}(\mathcal{Z}_h - z + \mathcal{O}(\tau_2^2|z|))^{-1} \\ &= \tau_2^{-2}(\mathcal{Z}_h - z)^{-1}(I + \mathcal{O}(\tau_2^2\tilde{\epsilon}_j\|(\mathcal{Z}_h - z)^{-1}\|)). \end{aligned}$$

Moreover, by the definition of $\widehat{D}'_{j,n}$ and thanks to (5-15), one has $\operatorname{dist}(z, \sigma(\mathcal{Z}_h)) \ge \frac{1}{2}Mt^2\tilde{\epsilon}_j$ for any $z \in \partial\widehat{D}'_{j,n}$. Hence $\|(\mathcal{Z}_h - z)^{-1}\| \le 2(Mt^2\tilde{\epsilon}_j)^{-1}$ and since $t \ge \tau_2$, it follows that

$$E(\tau_2^2 z) = \tau_2^{-2}(\mathcal{Z}_h - z)^{-1}(I + \mathcal{O}(M^{-1})).$$

Integrating along $\partial\widetilde{D}'_{j,n}$ and working as above, we get

$$\Pi'_{j,n} = \frac{1}{2i\pi}\int_{\partial D'_{j,n}} \begin{pmatrix} E_0(\lambda) & R^{\dagger}_{\tau_2}E(\lambda) \\ E(\lambda)R_{\tau_2} & E(\lambda) \end{pmatrix} d\lambda,$$

with $R_{\tau_2}(\lambda) = -\tau_2(\tau_2^2\mathcal{N}_h - \lambda)^{-1}B_h$ and $R^{\dagger}_{\tau_2}(\lambda) = -\tau_2 B_h^*(\tau_2^2\mathcal{N}_h - \lambda)^{-1}$. The same argument as above shows that $\operatorname{rk}(\Pi_n) \ge \operatorname{rk}(E'_n)$ with

$$E'_n = \frac{\tau_2^2}{2i\pi}\int_{\partial\widehat{D}'_{j,n}} E(\tau_2^2 z)\,dz = \frac{1}{2i\pi}\int_{\partial\widehat{D}'_{j,n}} (\mathcal{Z}_h - z)^{-1}(I + \mathcal{O}(M^{-1}))^{-1}\,dz.$$

By the induction hypothesis, this shows that the rank of E'_n is exactly the multiplicity of λ_n^j and hence the rank of $\Pi'_{j,n}$ is bounded from below by this multiplicity. Therefore, for any $j = 2, \dots, p$, $\mathcal{M}_h$ admits at least n_j eigenvalues $\mu_1^1 \le \cdots \le \mu_{n_1}^1$ in the interval $\epsilon_j[c_j - Mt^2, d_j + Mt^2]$ and these eigenvalues satisfy

$$\mu_n^j = \epsilon_j(\lambda_n^j + \mathcal{O}(|\tau|_\infty^2)) \quad \text{for all } n = 1, \dots, n_j. \tag{5-18}$$

Combining this estimate with (5-14) and using the fact the $\dim(E) = \sum_{j=1}^p r_j$, we obtain the μ_n^j are the only eigenvalues of $\mathcal{M}_h$. ☐

5D. ***The singular values of $\mathscr{L}^{\alpha}$.*** Given $\boldsymbol{m}, \boldsymbol{m}_1, \boldsymbol{m}_2 \in \mathcal{U}^{(0)}$ and $\boldsymbol{s} \in \mathcal{V}^{(1)}$, we define

$$\upsilon_2(\boldsymbol{s}, \boldsymbol{m}, \boldsymbol{m}_1, \boldsymbol{m}_2) = \pi^{-1/2} |\hat{\lambda}_1(\boldsymbol{s})|^{1/2} \left(\frac{h_\varphi(\boldsymbol{m}_1)}{h_\varphi(\boldsymbol{s})} \delta_{\boldsymbol{m},\boldsymbol{m}_1} - \frac{h_\varphi(\boldsymbol{m}_2)}{h_\varphi(\boldsymbol{s})} \delta_{\boldsymbol{m},\boldsymbol{m}_2} \right), \tag{5-19}$$

$$\upsilon_1(\boldsymbol{s}, \boldsymbol{m}, \boldsymbol{m}_1) = \pi^{-1/2} |\hat{\lambda}_1(\boldsymbol{s})|^{1/2} \frac{h_\varphi(\boldsymbol{m}_1)}{h_\varphi(\boldsymbol{s})} \delta_{\boldsymbol{m},\boldsymbol{m}_1}. \tag{5-20}$$

Let us define the matrix $\Upsilon^\alpha \in \mathscr{M}(\widehat{\mathcal{U}}_\alpha^{(0)}, \mathcal{V}_\alpha^{(1)})$ by

$$\Upsilon^\alpha(\boldsymbol{s}, \boldsymbol{m}) = \begin{cases} \upsilon_2(\boldsymbol{s}, \boldsymbol{m}, \boldsymbol{m}_1(\boldsymbol{s}), \boldsymbol{m}_2(\boldsymbol{s})) & \text{if } \boldsymbol{m}_2(\boldsymbol{s}) \in \widehat{\mathcal{U}}_\alpha^{(0)}, \\ \upsilon_1(\boldsymbol{s}, \boldsymbol{m}, \boldsymbol{m}_1(\boldsymbol{s})) & \text{if } \boldsymbol{m}_2(\boldsymbol{s}) \notin \widehat{\mathcal{U}}_\alpha^{(0)}, \end{cases} \tag{5-21}$$

where the indices $\boldsymbol{m}, \boldsymbol{s}$ are enumerated according to the partitions of Section 5B. Observe that with this notation, the conclusion of Lemma 4.4 can be written as $\widetilde{\mathscr{L}}^{\alpha,0} = \Upsilon$. Moreover, the above expression can be simplified according to the type of α. More precisely,

- if α is of type I, then $\boldsymbol{m}_2(\boldsymbol{s}) \in \widehat{\mathcal{U}}_\alpha^{(0)}$ if and only if $\boldsymbol{s} \in \mathcal{V}_\alpha^{(1),i}$,
- if α is of type II, then $\boldsymbol{m}_2(\boldsymbol{s})$ is always in $\widehat{\mathcal{U}}_\alpha^{(0)}$.

Theorem 5.8. *Let $\mathcal{M}^\alpha = \mathscr{L}^{\alpha,*}\mathscr{L}^\alpha$. There exists $c > 0$ such that, counted with multiplicity, one has*

$$\sigma(\mathcal{M}^\alpha) = \bigsqcup_{j=1}^{p(\alpha)} h e^{-2h^{-1} S_{\nu_j^\alpha}} \sigma(M^{\alpha,j})(1 + \mathcal{O}(e^{-c/h})),$$

where the matrices $M^{\alpha,j}$ have a classical expansion $M^{\alpha,j} \sim \sum h^k M_k^{\alpha,j}$ whose leading term is given by

$$M_0^{\alpha,j} = \mathcal{J}\mathcal{R}^{j-1}(\mathcal{Z}^\alpha),$$

where $\mathcal{Z}^\alpha = \Omega^\alpha \mathscr{T}^{\alpha,0} \Upsilon^{\alpha,*} \Upsilon^\alpha \mathscr{T}^{\alpha,0} \Omega^\alpha$ belongs to $\mathscr{G}(\mathscr{E}, \tau)$ with $\mathscr{E} = (\mathscr{F}(\widehat{\mathcal{U}}_{\alpha,j}^{(0)}))_{j=1,\dots,p}$ and $\tau = (\tau_j)_{j=1,\dots,p}$, with $\tau_j = e^{(S_{\nu_{p-(j-2)}} - S_{\nu_{p-(j-1)}})/h}$.

Proof. One has

$$\mathcal{M}^\alpha = \mathscr{L}^{\alpha,*}\mathscr{L}^\alpha = h e^{-2S_{p_1}/h} \widehat{\mathcal{M}}^\alpha,$$

with $\widehat{\mathcal{M}}^\alpha$ given by (5-7),

$$\widehat{\mathcal{M}}^\alpha(\tau) = \hat{\Omega}^\alpha(\tau)^* \widehat{\mathcal{M}}^{\alpha,\prime} \hat{\Omega}^\alpha(\tau),$$

with $\widehat{\mathcal{M}}^{\alpha,\prime} = (h^{-1} \widehat{\mathscr{L}}^{\alpha,*} \widehat{\mathscr{L}}^\alpha)$. Of course, this matrix is symmetric positive and thanks to Proposition 5.2, it admits a classical expansion

$$\widehat{\mathcal{M}}^{\alpha,\prime} \sim \sum_k h^k \widehat{\mathcal{M}}_k^{\alpha,\prime}$$

with $\widehat{\mathcal{M}}_0^{\alpha,\prime} = (\widehat{\mathscr{L}}^{\alpha,0})^* \widehat{\mathscr{L}}^{\alpha,0} = \mathscr{T}^{\alpha,0} \Upsilon^{\alpha,*} \Upsilon^\alpha \mathscr{T}^{\alpha,0} \in \mathscr{S}^+$. This shows that $\widehat{\mathcal{M}}^{\alpha,\prime}$ belongs to $\mathscr{S}_{\mathrm{cl}}^+$. Hence $\widehat{\mathcal{M}}^\alpha$ is classical $(\mathscr{E}, \tau)$-graded with $\mathscr{E} = (\mathscr{F}(\widehat{\mathcal{U}}_{\alpha,j}^{(0)}))_{j=1,\dots,p}$ and $\tau = (\tau_2, \dots, \tau_p)$, with $\tau_j = e^{(S_{\nu_{p-(j-2)}} - S_{\nu_{p-(j-1)}})/h}$ and the conclusion follows directly from Theorem 5.6. ☐

6. Proof of the main theorem

In this section we explain how one can deduce Theorem 2.8 from Theorem 5.8. As in [Helffer, Klein and Nier 2004], the general idea is to compare the singular values of the successive reduced matrix by a mean of Fan inequalities. As preparation, we shall compare the matrices $\mathcal{L}^{\pi,\prime}$ and $\mathcal{L}^{\mathrm{bkw},\prime}$ defined in Section 3. First, observe that thanks to (4-4), (4-5), (4-10), one has

$$\mathcal{L}^{\mathrm{bkw},\prime} = \mathscr{J}\mathcal{L}^{\mathrm{bkw},\prime\prime} = \mathscr{J}\mathscr{L} = \mathscr{J}\tilde{\mathscr{L}}\mathscr{T}\Omega, \tag{6-1}$$

with $\mathscr{J} : \mathscr{F}(\mathcal{V}^{(1)}) \to \mathscr{F}(\mathcal{U}^{(1)})$ defined by $\mathscr{J}_{\boldsymbol{s},\boldsymbol{s}'} = \delta_{\boldsymbol{s},\boldsymbol{s}'}$, $\tilde{\mathscr{L}} = \mathrm{diag}(\tilde{\mathscr{L}}^{\alpha}, \alpha \in \underline{\mathcal{A}})$, $\mathscr{T} = \mathrm{diag}(\mathscr{T}^{\alpha}, \alpha \in \underline{\mathcal{A}})$ and $\Omega = \mathrm{diag}(\Omega^{\alpha}, \alpha \in \underline{\mathcal{A}})$.

Lemma 6.1. *There exists $\gamma > 0$ such that*

$$\mathcal{L}^{\pi,\prime} = (\mathscr{J} + \mathcal{O}(e^{-\gamma/h}))\mathscr{L}.$$

Proof. First observe that thanks to Lemma 4.1, one has

$$\mathcal{L}^{\pi,\prime} = \mathcal{L}^{\mathrm{bkw},\prime} + \mathcal{R}, \tag{6-2}$$

with $\mathcal{R} : \mathscr{F}(\underline{\mathcal{U}}^{(0)}) \to \mathscr{F}(\mathcal{U}^{(1)})$ satisfying

$$\mathcal{R}_{\boldsymbol{s},\boldsymbol{m}} = \mathcal{O}(e^{-(S(\boldsymbol{m})+\gamma)/h}) \quad \text{for all } \boldsymbol{m} \in \underline{\mathcal{U}}^{(0)}, \tag{6-3}$$

for some $\gamma > 0$. Using (6-1), we get

$$\mathcal{L}^{\pi,\prime} = \mathscr{J}\tilde{\mathscr{L}}\mathscr{T}\Omega + \tilde{\mathcal{R}}\Omega,$$

with $\tilde{\mathcal{R}} = \mathcal{O}(e^{-\gamma/h})$. Hence, we have to prove that there exists $\overline{\mathcal{R}} : \mathscr{F}(\mathcal{V}^{(1)}) \to \mathscr{F}(\mathcal{U}^{(1)})$ such that $\tilde{\mathcal{R}} = \overline{\mathcal{R}}\tilde{\mathscr{L}}\mathscr{T}$ and $\overline{\mathcal{R}} = \mathcal{O}(e^{-\gamma/h})$. From Proposition 5.2, we know that the matrix $\mathscr{W} := (\tilde{\mathscr{L}}\mathscr{T})^*\tilde{\mathscr{L}}\mathscr{T}$ is invertible with inverse uniformly bounded with respect to h. This allows us to define $\overline{\mathcal{R}} := \tilde{\mathcal{R}}\mathscr{W}^{-1}(\tilde{\mathscr{L}}\mathscr{T})^*$. Thanks to the above remarks, we have $\overline{\mathcal{R}} = \mathcal{O}(e^{-\gamma/h})$ and by construction

$$\overline{\mathcal{R}}\tilde{\mathscr{L}}\mathscr{T} = \tilde{\mathcal{R}}\mathscr{W}^{-1}(\tilde{\mathscr{L}}\mathscr{T})^*\tilde{\mathscr{L}}\mathscr{T} = \tilde{\mathcal{R}},$$

which completes the proof. □

We are now ready to prove Theorem 2.8. Until the end of this section, $\gamma > 0$ denotes a constant independent of h that may change from line to line. We shall also denote by $\mathrm{SV}(M)$ the singular values of any matrix M.

From Section 2C, we know that the n_0 exponentially small eigenvalues of $\Delta_\varphi^{(0)}$ are the square of the singular values of the matrix $\mathcal{L}$. Thanks to Lemmas 3.12 and 3.13, we have

$$\mathcal{L} = (\mathrm{Id} + \mathcal{O}(e^{-\gamma/h}))\mathcal{L}^{\pi}(\mathrm{Id} + \mathcal{O}(e^{-\gamma/h}))$$

and it follows from the Fan inequality (Lemma A.1) that

$$\mathrm{SV}(\mathcal{L}) = \mathrm{SV}(\mathcal{L}^{\pi})(1 + \mathcal{O}(e^{-\gamma/h})).$$

Hence, we are reduced to computing the singular values of $\mathcal{L}^{\pi}$. Since the first column of $\mathcal{L}^{\pi}$ is the null vector, it follows that the nonzero singular values of $\mathcal{L}^{\pi}$ are the singular values of $\mathcal{L}^{\pi,\prime}$. From Lemma 6.1, we know that

$$\mathcal{L}^{\pi,\prime} = (\mathscr{J} + \mathcal{O}(e^{-\gamma/h}))\mathscr{L}, \tag{6-4}$$

and since $\mathscr{J}^*\mathscr{J} = \mathrm{Id}$ this implies for h small enough

$$\mathscr{L} = (\mathscr{J}^* + \mathcal{O}(e^{-\gamma/h}))\mathcal{L}^{\pi,\prime}. \tag{6-5}$$

Using the fact that $\|\mathscr{J}\| = \|\mathscr{J}^*\| = 1$, (6-4) and (6-5) combined with Lemma A.1 show that

$$\mathrm{SV}(\mathcal{L}^{\pi,\prime}) = (1 + \mathcal{O}(e^{-\gamma/h}))\,\mathrm{SV}(\mathscr{L}).$$

Combined with Theorem 5.8 this proves Theorem 2.8.

7. Some particular cases and examples

In this section, we rephrase Theorem 5.8 in the particular situations $p(\alpha) = 1$ and $p(\alpha) = 2$.

7A. *The case $p(\alpha) = 1$.* In this section we assume that $p(\alpha) = 1$. Then, the set $\mathcal{S}_\alpha$ is reduced to a singleton $\mathcal{S}_\alpha = \{S_{\nu_1^\alpha}\}$. Moreover, the points of $\mathcal{U}_\alpha^{(0)}$ are either all of type I, or all of type II.

7A1. *The case where α is of type II.* We first assume that α is of type II. Then all the points $\boldsymbol{m} \in \mathcal{U}_\alpha^{(0)}$ are of type II and Theorem 5.8 takes the following form.

Theorem 7.1. *Let $\alpha \in \mathcal{A}$ be such that $p(\alpha) = 1$ and all the points of $\mathcal{U}_\alpha^{(0)}$ are of type II. Then the matrix $\mathscr{L}^\alpha$ has exactly $q_\alpha = \#\mathcal{U}_\alpha^{(0)}$ singular values counted with multiplicity $\rho_{\alpha,\mu}(h)$, $\mu = 1, \dots, q_\alpha$. They have the form*

$$\rho_{\alpha,\mu}(h) = h^{1/2}\zeta_{\alpha,\mu}(h)e^{-S_{\nu_1^\alpha}/h},$$

where $\zeta_{\alpha,\mu} \sim \sum_{r=0}^{\infty} h^r \zeta_{\alpha,\mu,r}$ is a classical symbol such that the $\zeta_{\alpha,\mu,0}$, $\mu = 1, \dots, q_\alpha$, are the nonzero singular values of the matrix $\Upsilon^\alpha \in \mathscr{M}(\widehat{\mathcal{U}}_\alpha^{(0)}, \mathcal{V}_\alpha^{(1)})$ given by

$$\Upsilon^\alpha_{\boldsymbol{s},\boldsymbol{m}} = \pi^{-1/2}|\hat{\lambda}_1(\boldsymbol{s})|^{1/2}\left(\frac{h_\varphi(\boldsymbol{m}_1(\boldsymbol{s}))}{h_\varphi(\boldsymbol{s})}\delta_{\boldsymbol{m},\boldsymbol{m}_1(\boldsymbol{s})} - \frac{h_\varphi(\boldsymbol{m}_2(\boldsymbol{s}))}{h_\varphi(\boldsymbol{s})}\delta_{\boldsymbol{m},\boldsymbol{m}_2(\boldsymbol{s})}\right) \quad \textit{for all } \boldsymbol{s} \in \mathcal{V}_\alpha^{(1)},\ \boldsymbol{m} \in \widehat{\mathcal{U}}_\alpha^{(0)},$$

with $\boldsymbol{m}_1(\boldsymbol{s}), \boldsymbol{m}_2(\boldsymbol{s})$ defined in Lemma 3.3.

Observe that the description of the approximated small eigenvalues of Δ_φ in the above theorem is very close in spirit to that obtained in nondegenerate situations. Though, the different eigenvalues $\rho_{\alpha,\mu}$ are linked to one another, the only minima involved in the computation of the prefactors $\zeta_{\alpha,\mu}$ are associated to the typical height $S_{\nu_1^\alpha}$. In that sense, we can say that the above formula is a generalized Eyring–Kramers formula.

As already mentioned in the Introduction, the matrix Υ^α enjoys a nice interpretation in terms of graph theory. In order to simplify, suppose that the function φ is such that the coefficients of Υ^α are either 1 or -1. Define a graph $\mathcal{G}_\alpha$ associated to the equivalence class α in the following way. The vertices of the graph are the minima $\boldsymbol{m} \in \widehat{\mathcal{U}}_\alpha^{(0)}$ and the edges are the saddle points $\boldsymbol{s} \in \mathcal{V}_\alpha^{(1)}$. The two vertices associated to the edge $s \in \mathcal{V}_\alpha^{(1)}$ are just $m_1(s)$ and $m_2(s)$. With this definition it turns out that the matrix Υ^α is the transpose of the incidence matrix of a certain oriented version of the graph $\mathcal{G}_a$. As a consequence, the $|\zeta_{\alpha,\mu,0}|^2$ are the eigenvalues of the corresponding graph Laplacian $\Delta_{\mathcal{G}} = (\delta_{m,m'})_{m,m' \in \widehat{\mathcal{U}}^{(0)}}$ defined by

$$\delta_{m,m'} = \begin{cases} \mathrm{d}(m) & \text{if } m = m', \\ -1 & \text{if } m \neq m' \text{ and there is an edge between } m \text{ and } m', \\ 0 & \text{otherwise,} \end{cases} \tag{7-1}$$

where the degree $\mathrm{d}(m)$ is the number of edges incident to the vertex m.

Figure 2 in the Introduction presents an example of a potential φ having one unique saddle value σ and such that all local minima are absolute minima. We represent also in Figure 2 the graph associated to the nontrivial equivalence class (that is, the one which is not reduced to one element).

In the case where the coefficients of Υ^α are not necessarily equal to ± 1, the same interpretation is available with weighted graphs. We refer to [Cvetković, Doob and Sachs 1995] for definitions and standard results on graph theory.

7A2. *The case where α is of type I.* In this section, we compute explicitly the singular values of $\mathscr{L}^\alpha$, when α is of type I.

Theorem 7.2. *Let $\alpha \in \mathcal{A}$ be such that $p(\alpha) = 1$ and all the points of $\mathcal{U}_\alpha^{(0)}$ are of type I. Then, the matrix $\mathscr{L}^\alpha$ has exactly $q_\alpha := \#\mathcal{U}_\alpha^{(0)}$ singular values counted with multiplicity. These singular values $\rho_{\alpha,\mu}(h)$, $\mu = 1, \dots, q_\alpha$, have the form*

$$\rho_{\alpha,\mu}(h) = \zeta_{\alpha,\mu}(h) e^{-S_{\nu_1^\alpha}/h},$$

where $\zeta_{\alpha,\mu} \sim h^{1/2} \sum_{r=0}^{\infty} h^r \zeta_{\alpha,\mu,r}$ has a classical expansion such that $\zeta_{\alpha,\mu,0}$ are the q_α singular values of the matrix Υ^α given by

$$\Upsilon_{s,m} = \pi^{-1/2} |\hat{\lambda}_1(s)|^{1/2} \left(\frac{h_\varphi(m_1(s))}{h_\varphi(s)} \delta_{m,m_1(s)} - \frac{h_\varphi(m_2(s))}{h_\varphi(s)} \delta_{m,m_2(s)} \right)$$

if $s \in \mathcal{V}_\alpha^{(1),i}$ and

$$\Upsilon_{s,m} = \pi^{-1/2} |\hat{\lambda}_1(s)|^{1/2} \frac{h_\varphi(m_1(s))}{h_\varphi(s)} \delta_{m,m_1(s)}$$

if $s \in \mathcal{V}_\alpha^{(1),b}$. Moreover, these singular values are nonzero.

As in the case of points of type II we can interpret the matrix $\widetilde{\mathscr{L}}^{\alpha,0}$ in terms of graphs. However, some saddle points are now associated to only one minimum. In terms of the graph, this leads to some edges having only one vertex, which means that we are dealing with hypergraphs.

7B. ***The case $p(\alpha) = 2$.*** Throughout this section we assume that $p(\alpha) = 2$. Then φ takes two different values $\varphi_- < \varphi_+$ on $\mathcal{U}_\alpha^{(0)}$. One has $\mathcal{S}_\alpha = \{S_{\nu_+^\alpha} < S_{\nu_-^\alpha}\}$ with $S_{\nu_\pm^\alpha} = \sigma(\alpha) - \varphi_\pm$.

7B1. *The case where α is of type II.* The partition (5-4) takes the form $\widehat{\mathcal{U}}_\alpha^{(0)} = \widehat{\mathcal{U}}_{\alpha,+}^{(0)} \sqcup \widehat{\mathcal{U}}_{\alpha,-}^{(0)}$ with $\widehat{\mathcal{U}}_{\alpha,\pm}^{(0)} = \{\boldsymbol{m} \in \mathcal{U}_\alpha^{(0)} : \varphi(\boldsymbol{m}) = \varphi_\pm\}$. Since α is of type II, $\boldsymbol{m}_2(\boldsymbol{s}) \in \widehat{\mathcal{U}}_\alpha^{(0)}$ for all $\boldsymbol{s}$. It is then convenient to introduce the partition of $\mathcal{V}_\alpha^{(1)}$ given by

$$\mathcal{V}_\alpha^{(1)} = \mathcal{V}_{\alpha,+}^{(1)} \sqcup \mathcal{V}_{\alpha,+-}^{(1)} \cup \mathcal{V}_{\alpha,-}^{(1)}, \tag{7-2}$$

with $\mathcal{V}_{\alpha,+}^{(1)} = \{\boldsymbol{s} \in \mathcal{V}_\alpha^{(1)} : \boldsymbol{m}_1(\boldsymbol{s}), \boldsymbol{m}_2(\boldsymbol{s}) \in \widehat{\mathcal{U}}_{\alpha,+}^{(0)}\}$ and $\mathcal{V}_{\alpha,-}^{(1)} = \{\boldsymbol{s} \in \mathcal{V}_\alpha^{(1)} : \boldsymbol{m}_1(\boldsymbol{s}), \boldsymbol{m}_2(\boldsymbol{s}) \in \widehat{\mathcal{U}}_{\alpha,-}^{(0)}\}$, where the functions $\boldsymbol{m}_1, \boldsymbol{m}_2$ are defined by Lemma 3.3. In the case $\boldsymbol{s} \in \mathcal{V}_{\alpha,+-}^{(1)}$, it follows from the choice of Lemma 3.3 that $\boldsymbol{m}_1(\boldsymbol{s}) \in \widehat{\mathcal{U}}_{\alpha,+}^{(0)}$ and $\boldsymbol{m}_2(\boldsymbol{s}) \in \widehat{\mathcal{U}}_{\alpha,-}^{(0)}$. We order the above partitions by deciding $\widehat{\mathcal{U}}_{\alpha,+}^{(0)} \prec \widehat{\mathcal{U}}_{\alpha,-}^{(0)}$ and $\mathcal{V}_{\alpha,+}^{(1)} \prec \mathcal{V}_{\alpha,+-}^{(1)} \prec \mathcal{V}_{\alpha,-}^{(1)}$. Then, the matrix $\mathscr{Y}^\alpha := h^{-1/2} e^{-S_{\nu_+^\alpha}/h} \widehat{\mathscr{L}}^\alpha$ has the form

$$\mathscr{Y}^\alpha = \begin{pmatrix} \iota & 0 \\ b_{+-} & \tau b_{-+} \\ 0 & \tau a \end{pmatrix},$$

where $\tau = e^{(S_{\nu_+^\alpha} - S_{\nu_-^\alpha})/h}$ and the matrices ι, b_{+-}, b_{-+} admit a classical expansion whose principal terms are given by the formula

- for all $\boldsymbol{s} \in \mathcal{V}_{\alpha,+}^{(1)}$ and $\boldsymbol{m} \in \widehat{\mathcal{U}}_{\alpha,+}^{(0)}$ one has $\iota_{\boldsymbol{s},\boldsymbol{m}}^0 = \upsilon_2(\boldsymbol{s}, \boldsymbol{m}, \boldsymbol{m}_1(\boldsymbol{s}), \boldsymbol{m}_2(\boldsymbol{s}))$,
- for all $\boldsymbol{s} \in \mathcal{V}_{\alpha,-}^{(1)}$ and $\boldsymbol{m} \in \widehat{\mathcal{U}}_{\alpha,-}^{(0)}$ one has $a_{\boldsymbol{s},\boldsymbol{m}}^0 = \upsilon_2(\boldsymbol{s}, \boldsymbol{m}, \boldsymbol{m}_1(\boldsymbol{s}), \boldsymbol{m}_2(\boldsymbol{s}))$,
- for all $\boldsymbol{s} \in \mathcal{V}_{\alpha,+-}^{(1)}$, $\boldsymbol{m} \in \widehat{\mathcal{U}}_{\alpha,+}^{(0)}$ and $\boldsymbol{m}' \in \widehat{\mathcal{U}}_{\alpha,-}^{(0)}$ one has $(b_{+-}^0)_{\boldsymbol{s},\boldsymbol{m}} = \upsilon_1(\boldsymbol{s}, \boldsymbol{m}, \boldsymbol{m}_1(\boldsymbol{s}))$ and $(b_{-+}^0)_{\boldsymbol{s},\boldsymbol{m}'} = -\upsilon_1(\boldsymbol{s}, \boldsymbol{m}', \boldsymbol{m}_2(\boldsymbol{s}))$,

with υ_2, υ_1 given by (5-19), (5-20). By a standard block-matrix computation one has

$$(\mathscr{Y}^\alpha)^* \mathscr{Y}^\alpha = \begin{pmatrix} J & \tau \widehat{B} \\ \tau \widehat{B}^* & \tau^2 \widehat{A} \end{pmatrix}, \tag{7-3}$$

with $J = \iota^* \iota + b_{+-}^* b_{+-}$, $\widehat{B} = b_{+-}^* b_{-+}$ and $\widehat{A} = a^* a + b_{-+}^* b_{-+}$. All these matrices admit a classical expansion, $\widehat{A} \simeq \sum_{k \geq 0} h^k \widehat{A}^k$, $\widehat{B} \simeq \sum_{k \geq 0} h^k \widehat{B}^k$, $J = \sum_{k \geq 0} h^k J^k$ and one has $J^0 = \iota^{0,*} \iota^0 + b_{+-}^{0,*} b_{+-}^0$, $\widehat{B}^0 = b_{+-}^{0,*} b_{-+}^0$ and $\widehat{A}^0 = a^{0,*} a^0 + b_{-+}^{0,*} b_{-+}^0$, where we use the notation $(c^j)^* = c^{j,*}$.

Theorem 7.3. *The matrix $\mathscr{L}^\alpha$ has exactly $q_{\alpha,\pm} = \#\mathcal{U}_{\alpha,\pm}^{(0)}$ singular values $\lambda_{\alpha,\mu}^\pm(h)$, $\mu = 1, \ldots, q_{\alpha,\pm}$, counted with multiplicity which are of order $h^{1/2} e^{-S_{\nu_\pm^\alpha}/h}$. These singular values have the form*

$$\lambda_{\alpha,\mu}^\pm(h) = \zeta_{\alpha,\mu}^\pm(h) e^{-S_{\nu_\pm^\alpha}/h},$$

where

$$\zeta_{\alpha,\mu}^\pm \sim h^{1/2} \sum_k h^k \zeta_{\alpha,\mu,k}^\pm$$

is a classical symbol such that $(\zeta_{\alpha,\mu,0}^\pm)^2$ are the $q_{\alpha,\pm}$ nonzero eigenvalues of the matrices $G^\pm$ given by $G^+ = J^0$ and

$$G^- = \widehat{A}^0 - (\widehat{B}^0)^* (J^0)^{-1} \widehat{B}^0,$$

where $\widehat{A}^0$, J^0 and $\widehat{B}^0$ are defined below (7-3).

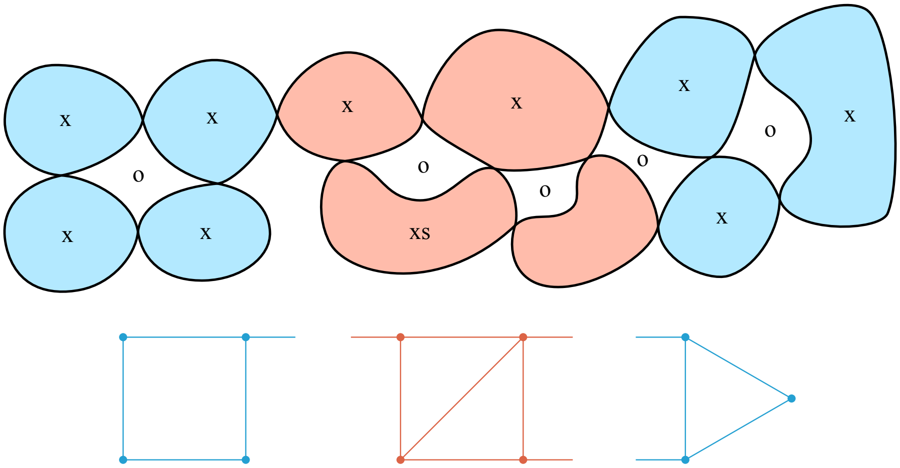

Figure 9. Top: the sublevel set $\{\varphi < \sigma\}$ associated to a potential φ having a unique saddle value and two minimal values. Bottom: the associated hypergraphs.

Let us make a few comments on this theorem. First, observe that the prefactor $\zeta^{\pm} = \zeta^{\pm}_{\alpha,\mu}$ obeys two different laws whether we are in the "+" or "−" case. In the "+" case, ζ^{+} is determined by the matrix J^0 which depends only on the minima $\boldsymbol{m} \in \mathcal{U}^{(0)}_{\alpha}$ such that $S(\boldsymbol{m}) = S_{\nu_+}$. In that sense, the behavior of ζ^{+} obeys a law similar to the generalized Eyring–Kramers law of Theorem 7.1. In the "−" case, the situation is different since the matrix G^{-} involves values of φ on all minima and not only those for which $S(\boldsymbol{m}) = S_{\nu_-}$. Hence the term $(\widehat{B}^0)^*(J^0)^{-1}\widehat{B}^0$ in the definition of G^{-} can be understood as a tunneling term between minima associated to both heights.

This interpretation is confirmed by the following example. Suppose that φ has two distinct minimal values and one saddle value. Figure 9 below represents such a potential. The blue wells correspond to the absolute minimal value and the red one to the other minimal value. All the saddle points are supposed to be at the same level. Then, the matrices $\widehat{A}^0$ and J^0 can be viewed as the Laplacians of the hypergraphs built as follows. First we consider the graph $\mathcal{G}$ associated to all the minima whose vertex are the minima and edges are the saddle points between two minima (without distinction on the level of the minima). The blue and red hypergraphs $\mathcal{G}_b$ and $\mathcal{G}_r$ are obtained by cutting the graph $\mathcal{G}$ on edges between a blue and a red minimum. Eventually, the matrix B links blue and red minima.

7B2. *The case where α is of type I.* In this section we assume that α is of type I. The partition (5-4) takes the form $\mathcal{U}^{(0)}_{\alpha} = \mathcal{U}^{(0)}_{\alpha,-} \sqcup \mathcal{U}^{(0)}_{\alpha,+}$ with

$$\mathcal{U}^{(0)}_{\alpha,\pm} = \{\boldsymbol{m} \in \mathcal{U}^{(0)}_{\alpha} : \varphi(\boldsymbol{m}) = \varphi_{\pm}\}.$$

We order the two elements of $\mathscr{P}^{(0)}_{\alpha}$ by deciding $\mathcal{U}^{(0)}_{\alpha,+} \prec \mathcal{U}^{(0)}_{\alpha,-}$. In order to deal with the saddle points, we introduce the partition $\mathscr{P}^{(1)}_{\alpha}$ which is a mix of partitions used in Lemma 3.4 and Section 7B1:

$$\mathcal{V}^{(1)}_{\alpha} = \mathcal{V}^{(1)}_{\alpha,+,b} \sqcup \mathcal{V}^{(1)}_{\alpha,+,i} \sqcup \mathcal{V}^{(1)}_{\alpha,+-} \sqcup \mathcal{V}^{(1)}_{\alpha,-,b} \sqcup \mathcal{V}^{(1)}_{\alpha,-,i}$$

with

$$\begin{aligned}
\mathcal{V}^{(1)}_{\alpha,+,-} &= \{\boldsymbol{s} \in \mathcal{V}^{(1),i}_{\alpha} : \boldsymbol{m}_1(\boldsymbol{s}) \in \mathcal{U}^{(0)}_{\alpha,+}, \boldsymbol{m}_2(\boldsymbol{s}) \in \mathcal{U}^{(0)}_{\alpha,-}\},\\
\mathcal{V}^{(1)}_{\alpha,+,i} &= \{\boldsymbol{s} \in \mathcal{V}^{(1),i}_{\alpha} : \boldsymbol{m}_1(\boldsymbol{s}), \boldsymbol{m}_2(\boldsymbol{s}) \in \mathcal{U}^{(0)}_{\alpha,+}\},\\
\mathcal{V}^{(1)}_{\alpha,+,b} &= \{s \in \mathcal{V}^{(1),b}_{\alpha} : \boldsymbol{m}_1(s) \in \mathcal{U}^{(0)}_{\alpha,+}\},\\
\mathcal{V}^{(1)}_{\alpha,-,i} &= \{\boldsymbol{s} \in \mathcal{V}^{(1),i}_{\alpha} : \boldsymbol{m}_1(\boldsymbol{s}), \boldsymbol{m}_2(\boldsymbol{s}) \in \mathcal{U}^{(0)}_{\alpha,-}\},\\
\mathcal{V}^{(1)}_{\alpha,-,b} &= \{s \in \mathcal{V}^{(1),b}_{\alpha} : \boldsymbol{m}_1(s) \in \mathcal{U}^{(0)}_{\alpha,-}\}.
\end{aligned} \tag{7-4}$$

Here the functions $\boldsymbol{m}_1$, $\boldsymbol{m}_2$ are defined by Lemma 3.3. One has the following

Theorem 7.4. *Assume that $p(\alpha) = 2$ and α is of type I. The matrix $\mathscr{L}^\alpha$ has exactly $q_{\alpha,\pm} = \#\mathcal{U}^{(0)}_{\alpha,\pm}$ singular values $\lambda^\pm_{\alpha,\mu}(h)$, $\mu = 1, \dots, q_{\alpha,\pm}$, counted with multiplicity which are of order $h^{1/2}e^{-S_{\nu^\alpha_\pm}/h}$. These singular values have the form*

$$\lambda^\pm_{\alpha,\mu}(h) = \zeta^\pm_{\alpha,\mu}(h)e^{-S_{\nu^\alpha_\pm}/h}$$

where $\zeta^\pm_{\alpha,\mu} \sim h^{1/2}\sum_k h^k \zeta^\pm_{\alpha,\mu,k}$ is a classical symbol such that $(\zeta^\pm_{\alpha,\mu,0})^2$ are the $q_{\alpha,\pm}$ eigenvalues (which are nonzero) of the matrices $G^\pm$ given by $G^+ = J^0$ and $G^- = A^0 - (B^0)^*(J^0)^{-1}B^0$, where A^0, B^0 and J^0 are defined by

$$J^0 = \iota^{0,*}\iota^0 + b^{0,*}_{+-}b^0_{+-}, \quad B^0 = b^{0,*}_{+-}b^0_{-+}, \quad A^0 = a^{0,*}a^0 + b^{0,*}_{-+}b^0_{-+},$$

with the matrices a^0, b^0_{+-}, b^0_{-+} and ι^0 defined by

- *for all $\boldsymbol{s} \in \mathcal{V}^{(1)}_{\alpha,+,i}$ and $\boldsymbol{m} \in \mathcal{U}^{(0)}_{\alpha,+}$ one has $\iota^0_{\boldsymbol{s},\boldsymbol{m}} = \Upsilon_2(\boldsymbol{s}, \boldsymbol{m}, \boldsymbol{m}_1(\boldsymbol{s}), \boldsymbol{m}_2(\boldsymbol{s}))$,*
- *for all $\boldsymbol{s} \in \mathcal{V}^{(1)}_{\alpha,+,b}$ and $\boldsymbol{m} \in \mathcal{U}^{(0)}_{\alpha,+}$ one has $\iota^0_{\boldsymbol{s},\boldsymbol{m}} = \Upsilon_1(\boldsymbol{s}, \boldsymbol{m}, \boldsymbol{m}_1(\boldsymbol{s}))$,*
- *for all $\boldsymbol{s} \in \mathcal{V}^{(1)}_{\alpha,-,i}$ and $\boldsymbol{m} \in \mathcal{U}^{(0)}_{\alpha,-}$ one has $a^0_{\boldsymbol{s},\boldsymbol{m}} = \Upsilon_2(\boldsymbol{s}, \boldsymbol{m}, \boldsymbol{m}_1(\boldsymbol{s}), \boldsymbol{m}_2(\boldsymbol{s}))$,*
- *for all $\boldsymbol{s} \in \mathcal{V}^{(1)}_{\alpha,-,b}$ and $\boldsymbol{m} \in \mathcal{U}^{(0)}_{\alpha,-}$ one has $a^0_{\boldsymbol{s},\boldsymbol{m}} = \Upsilon_1(\boldsymbol{s}, \boldsymbol{m}, \boldsymbol{m}_1(\boldsymbol{s}))$,*
- *for all $\boldsymbol{s} \in \mathcal{V}^{(1)}_{\alpha,+-}$, $\boldsymbol{m} \in \mathcal{U}^{(0)}_{\alpha,+}$ and $\boldsymbol{m}' \in \mathcal{U}^{(0)}_{\alpha,-}$ one has $(b^0_{+-})_{\boldsymbol{s},\boldsymbol{m}} = \Upsilon_1(\boldsymbol{s}, \boldsymbol{m}, \boldsymbol{m}_1(\boldsymbol{s}))$ and $(b^0_{-+})_{\boldsymbol{s},\boldsymbol{m}'} = -\Upsilon_1(\boldsymbol{s}, \boldsymbol{m}', \boldsymbol{m}_2(\boldsymbol{s}))$.*

7C. *Some examples.*

7C1. *Computations in dimension 1 with $p(\alpha) = 1$.* Let us compute the small eigenvalues of the potential φ represented in Figure 10.

As already noticed in the discussion below Theorem 2.8, there are exactly three equivalence classes for $\mathcal{R}$ in that case: $\mathcal{U}^{(0)}_1 = \{\boldsymbol{m}_{1,1}\}$, $\mathcal{U}^{(0)}_2 = \{\boldsymbol{m}_{2,1}, \boldsymbol{m}_{2,2}\}$ and $\mathcal{U}^{(0)}_3 = \{\boldsymbol{m}_{2,3}\}$. Let us denote by $\boldsymbol{s}_1$ the saddle point between $\boldsymbol{m}_{2,1}$ and $\boldsymbol{m}_{2,2}$, by $\boldsymbol{s}_2$ the saddle point between $\boldsymbol{m}_{2,2}$ and $\boldsymbol{m}_{1,1}$ and by $\boldsymbol{s}_3$ the saddle point between $\boldsymbol{m}_{1,1}$ and $\boldsymbol{m}_{2,3}$. Define also $S_2 = \varphi(\boldsymbol{s}_1) - \varphi(\boldsymbol{m}_{2,1}) = \varphi(\boldsymbol{s}_1) - \varphi(\boldsymbol{m}_{2,2})$ and $S_3 = \varphi(\boldsymbol{s}_3) - \varphi(\boldsymbol{m}_{2,3})$. Observe also that for all $\boldsymbol{m} \in \mathcal{U}^{(0)}$, one has $H(\boldsymbol{m}) = \{\boldsymbol{m}\}$. Then the matrix $\mathcal{L}^{\mathrm{bkw}}$ defined by (4-2), admits the form

$$\mathcal{L}^{\mathrm{bkw}} = \left(\frac{h}{\pi}\right)^{1/2} \begin{pmatrix} 0 & d^2_{1,1} & d^2_{1,2} & 0 \\ 0 & d^2_{2,1} & d^2_{2,2} & 0 \\ 0 & 0 & 0 & d^3 \end{pmatrix},$$

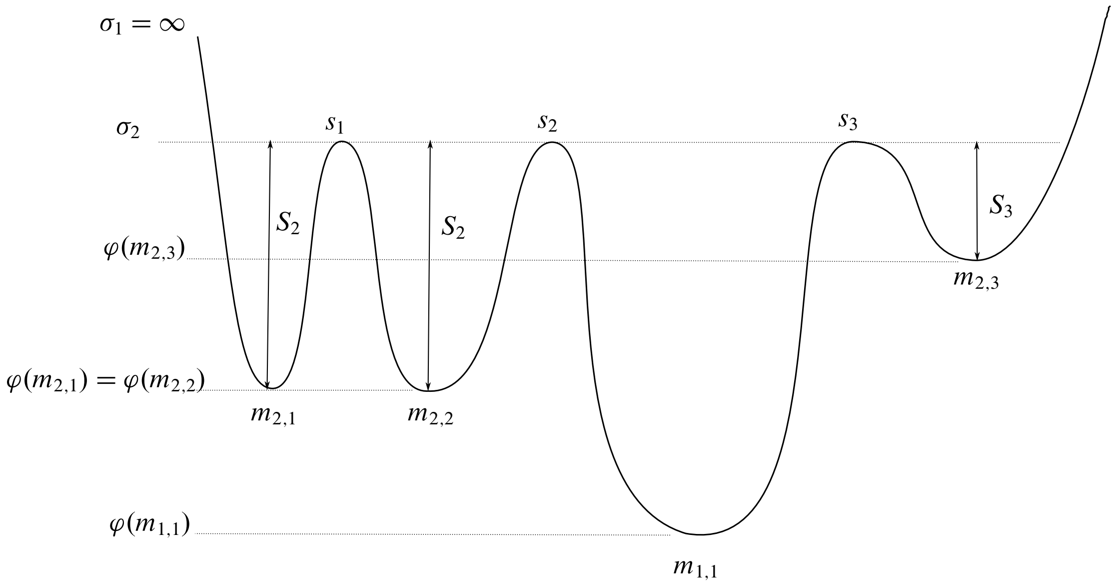

Figure 10. A potential with $p(\alpha) = 1$ for all α.

with the coefficients given by

$$d_{1,1}^2 = (|\varphi''(\boldsymbol{s}_1)\varphi''(\boldsymbol{m}_{2,1})|^{1/4} + \mathcal{O}(h))e^{-S_2/h}, \quad d_{1,2}^2 = -(|\varphi''(\boldsymbol{s}_1)\varphi''(\boldsymbol{m}_{2,2})|^{1/4} + \mathcal{O}(h))e^{-S_2/h},$$

$$d_{2,1}^2 = 0, \quad d_{2,2}^2 = (|\varphi''(\boldsymbol{s}_2)\varphi''(\boldsymbol{m}_{2,2})|^{1/4} + \mathcal{O}(h))e^{-S_2/h}, \quad d^3 = (|\varphi''(\boldsymbol{s}_3)\varphi''(\boldsymbol{m}_{2,3})|^{1/4} + \mathcal{O}(h))e^{-S_3/h}.$$

The corresponding squares of singular values are then

$$\lambda_0 = 0, \quad \lambda_3 = \frac{h}{\pi}(|\varphi''(\boldsymbol{s}_3)\varphi''(\boldsymbol{m}_{2,3})|^{1/2} + \mathcal{O}(h))e^{-2S_3/h} \quad \text{and} \quad \lambda_2^{\pm} = \frac{h}{\pi}(\mu_2^{\pm} + \mathcal{O}(h))e^{-2S_2/h},$$

where $\mu_2^{\pm}$ are the squares of the singular values of the matrix

$$\widetilde{\mathcal{D}}^2 = \begin{pmatrix} a & -b \\ 0 & c \end{pmatrix},$$

with $a = |\varphi''(\boldsymbol{s}_1)\varphi''(\boldsymbol{m}_{2,1})|^{1/4}$, $b = |\varphi''(\boldsymbol{s}_1)\varphi''(\boldsymbol{m}_{2,2})|^{1/4}$ and $c = |\varphi''(\boldsymbol{s}_2)\varphi''(\boldsymbol{m}_{2,2})|^{1/4}$. It follows that

$$(\widetilde{\mathcal{D}}^2)^*\widetilde{\mathcal{D}}^2 = \begin{pmatrix} a^2 & -ab \\ -ab & b^2+c^2 \end{pmatrix},$$

whose eigenvalues can be computed handily. For instance, if $|\varphi''(\boldsymbol{s})| = |\varphi''(\boldsymbol{m})| = 1$ for all $\boldsymbol{s} \in \mathcal{U}^{(1)}$ and $\boldsymbol{m} \in \mathcal{U}^{(0)}$, one has

$$(\widetilde{\mathcal{D}}^2)^*\widetilde{\mathcal{D}}^2 = \begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix},$$

whose eigenvalues are $\mu_2^{\pm} = \frac{3}{2} \pm \frac{\sqrt{5}}{2}$.

We would like to conclude this example by noticing that one has necessarily $\mu_2^+ \neq \mu_2^-$. Indeed, if one computes the characteristic polynomial of the above matrix, one finds $P(x) = x^2 - (a^2+b^2+c^2)x + a^2c^2$, whose discriminant is given by

$$\Delta = (a^2+b^2+c^2)^2 - 4a^2c^2 = ((a-c)^2+b^2)((a+c)^2+b^2).$$

Since φ is a Morse function, one has $b \neq 0$ and hence $\Delta > 0$.

7C2. *Computations in dimension 1 with* $p(\alpha) = 2$. Suppose now that the potential φ is as represented in Figure 7. As already noticed there are exactly two equivalence classes for $\mathcal{R}$ in that case, $\mathcal{U}_1^{(0)} = \{\boldsymbol{m}_{1,1}\}$ and $\mathcal{U}_2^{(0)} = \{\boldsymbol{m}_{2,1}, \boldsymbol{m}_{2,2}, \boldsymbol{m}_{2,3}\}$, and again, one has $H(\boldsymbol{m}) = \{\boldsymbol{m}\}$ for all $\boldsymbol{m} \in \mathcal{U}^{(0)}$. Let us denote by $\boldsymbol{s}_1$ the saddle point between $\boldsymbol{m}_{2,1}$ and $\boldsymbol{m}_{2,2}$, by $\boldsymbol{s}_2$ the saddle point between $\boldsymbol{m}_{2,2}$ and $\boldsymbol{m}_{2,3}$ and by $\boldsymbol{s}_3$ the saddle point between $\boldsymbol{m}_{2,3}$ and $\boldsymbol{m}_{1,1}$. Define also $S_2 = \varphi(\boldsymbol{s}_1) - \varphi(\boldsymbol{m}_{2,1}) = \varphi(\boldsymbol{s}_1) - \varphi(\boldsymbol{m}_{2,2})$ and $S_3 = \varphi(\boldsymbol{s}_2) - \varphi(\boldsymbol{m}_{2,3})$. Then the matrix $\mathcal{L}^{\mathrm{bkw},\prime\prime}$ admits the following form in the basis $(f^{(0)}_{\boldsymbol{m}_{2,3}}, f^{(0)}_{\boldsymbol{m}_{2,1}}, f^{(0)}_{\boldsymbol{m}_{2,2}})$ and $(f^{(1)}_{\boldsymbol{s}_3}, f^{(1)}_{\boldsymbol{s}_2}, f^{(1)}_{\boldsymbol{s}_1})$:

$$\mathcal{L}^{\mathrm{bkw},\prime\prime} = \left(\frac{h}{\pi}\right)^{1/2} e^{-S_3/h} \begin{pmatrix} \iota & 0 & 0 \\ b_1 & 0 & b_2 e^{-(S_2-S_3)/h} \\ 0 & a_1 e^{-(S_2-S_3)/h} & a_2 e^{-(S_2-S_3)/h} \end{pmatrix},$$

with the leading terms of the coefficients given by

$$\iota^0 = -|\varphi''(\boldsymbol{s}_3)\varphi''(\boldsymbol{m}_{2,3})|^{1/4}, \quad b_1^0 = |\varphi''(\boldsymbol{s}_2)\varphi''(\boldsymbol{m}_{2,3})|^{1/4}, \quad b_2^0 = |\varphi''(\boldsymbol{s}_2)\varphi''(\boldsymbol{m}_{2,2})|^{1/4}$$

and

$$a_1^0 = |\varphi''(\boldsymbol{s}_1)\varphi''(\boldsymbol{m}_{2,1})|^{1/4}, \quad a_2^0 = -|\varphi''(\boldsymbol{s}_1)\varphi''(\boldsymbol{m}_{2,2})|^{1/4}.$$

In order to simplify the computation, assume that $\varphi''(\boldsymbol{m}) = 1$ for all $\boldsymbol{m} \in \mathcal{U}^{(0)}$ and $\varphi''(\boldsymbol{s}_1) = \varphi''(\boldsymbol{s}_2) = -1$. Define $\theta = |\varphi''(\boldsymbol{s}_3)|$ and $\tau = e^{-(S_2-S_3)/h}$. Then

$$\mathcal{L}^{\mathrm{bkw},\prime\prime} = \left(\frac{h}{\pi}\right)^{1/2} e^{-S_3/h} \left(\begin{pmatrix} -\theta & 0 & 0 \\ 1 & 0 & \tau \\ 0 & \tau & -\tau \end{pmatrix} + \mathcal{O}(h)\right).$$

Hence, we can apply Theorem 7.4 with

$$a^0 = (1 \ -1), \quad \iota_0 = -\theta, \quad b^0_{+-} = 1, \quad b^0_{-+} = (0 \ 1).$$

It follows that the singular values of order $e^{-S_2/h}$ are

$$\mu_\pm(h) = \left(\frac{h}{\pi}\right)^{1/2} e^{-S_2/h}(\sqrt{\lambda_\pm} + \mathcal{O}(h)),$$

with $\lambda_\pm$ eigenvalues of $M^0 := A^0 - (B^0)^*(J^0)^{-1}B^0$, with

$$A^0 = \begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix}, \quad B^0 = (0 \ -1), \quad J^0 = 1 + \theta^2.$$

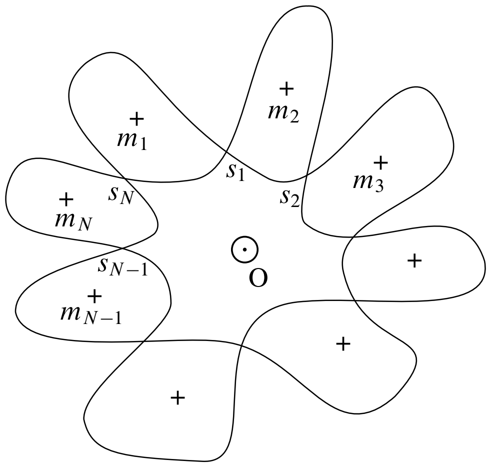

Figure 11. N wells in dimension 2.

Hence

$$M^0 = \begin{pmatrix} 1 & -1 \\ -1 & 2-\nu \end{pmatrix},$$

with $\nu = 1/(1+\theta^2) \in]0,1[$. The eigenvalues of this matrix are

$$\lambda_\pm = \frac{3-\nu}{2} \pm \frac{\sqrt{(3-\nu)^2 - 4(1-\nu)}}{2}.$$

This can be seen as perturbations by the well of height S_3 of the eigenvalues $\lambda_\pm$ computed in the previous example (obtained by taking $\nu = 0$ in the above formula).

7C3. *Computations in higher dimensions.* Consider the case of the potential φ having $N \geq 3$ minima $\boldsymbol{m}_1, \dots, \boldsymbol{m}_N$ and one local maximum at the origin as presented in Figure 11. Assume also that there are exactly N saddle points $\boldsymbol{s}_1, \dots, \boldsymbol{s}_N$, all at the same height $\varphi(\boldsymbol{s}_j) = \sigma_2$ and that the set $\{\varphi < \sigma_2\}$ has exactly N connected components $E_1, \dots, E_N$, each E_j containing the minimum m_j, and that for all $j = 1, \dots, N$, $\{\boldsymbol{s}_j\} = \overline{E}_j \cap \overline{E}_{j+1}$ with the convention $E_{N+1} = E_1$. Assume in addition that all the $\varphi(\boldsymbol{m}_j)$ are equal and write $S = \sigma_2 - \varphi(\boldsymbol{m}_1)$. Let us choose $\boldsymbol{m}_1$ as the global minimum associated to $\sigma_1 = \infty$. Then all the other minima are associated to the saddle value σ_2. It is clear that they all belong to the same equivalence class and that they are all of type II. Moreover, for all $\boldsymbol{m} \in \mathcal{U}^{(0)} \setminus \{\boldsymbol{m}_1\}$, one has $H(\boldsymbol{m}) = \{\boldsymbol{m}\}$. Then, we can apply Theorem 7.1 to get the spectrum of the Witten Laplacian associated to φ. It follows that the eigenvalues are given by $\lambda_1 = 0$ and for all $n = 2, \dots, N$

$$\lambda_n(h) = b_n(h) e^{-2S/h}(1 + \mathcal{O}(e^{-\alpha/h})), \tag{7-5}$$

where b_n admits a classical expansion

$$b_n(h) \simeq \frac{h}{\pi} \sum_{k \geq 0} b_{n,k} h^k.$$

Moreover, one has $b_{n,0} = \mu_n^2$, where the $\mu_n,\ n = 2, \dots, N$, are the nonzero singular values of the matrix

$$\mathcal{L} := \begin{pmatrix} \alpha_1\beta_1 & -\alpha_2\beta_1 & 0 & \cdots & \cdots & 0 \\ 0 & \alpha_2\beta_2 & -\alpha_3\beta_2 & 0 & \cdots & 0 \\ 0 & 0 & \alpha_3\beta_3 & \ddots & \cdots & 0 \\ \vdots & & & & & \vdots \\ 0 & \cdots & \cdots & 0 & \alpha_{N-1}\beta_{N-1} & -\alpha_N\beta_{N-1} \\ -\alpha_1\beta_N & 0 & \cdots & \cdots & 0 & \alpha_N\beta_N \end{pmatrix},$$

where we set $\alpha_j = \varphi''(\boldsymbol{m}_j)^{1/4}$ and $\beta_j = (-\varphi''(\boldsymbol{s}_j))^{1/4}$.

If one assumes additionally that α_j and β_j are independent of j, let say $\alpha_j = \alpha$ and $\beta_j = \beta$, then $\mathcal{L} = \alpha\beta\mathcal{A}$ with

$$\mathscr{A} = \begin{pmatrix} 1 & -1 & 0 & \cdots & \cdots & 0 & 0 \\ 0 & 1 & -1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 1 & -1 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \cdots & \cdots & 0 & 1 & -1 \\ -1 & 0 & \cdots & \cdots & 0 & 0 & 1 \end{pmatrix}.$$

The singular values of $\mathscr{A}$ are the square roots of the eigenvalues of

$$\mathscr{A}^*\mathscr{A} = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & -1 \\ -1 & 2 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 \\ \vdots & & & & & \vdots \\ 0 & 0 & \cdots & -1 & 2 & -1 \\ -1 & 0 & 0 & 0 & -1 & 2 \end{pmatrix},$$

which are known to be $\nu_k = 2(1 - \cos(2k\pi/N)),\ k = 0, \dots, N-1$. In particular, for all $2 \le k < N/2$, ν_k has multiplicity 2 since $\nu_k = \nu_{N-k}$.

Suppose now that the potential φ is invariant by a rotation of angle $2\pi/N$; then (7-5) still holds true with $b_n(h)$ being the singular values of a matrix of the form

$$\mathscr{A} = \theta(h)\begin{pmatrix} 1 & -1 & 0 & \cdots & \cdots & 0 & 0 \\ 0 & 1 & -1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 1 & -1 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \cdots & \cdots & 0 & 1 & -1 \\ -1 & 0 & \cdots & \cdots & 0 & 0 & 1 \end{pmatrix},$$

with $\theta(h) \simeq \sum_{k\ge 0} h^k \theta_k$. Hence, the above computation is still valid and it follows that for $2 \le k < N/2$, $b_k(h) = b_{N-k}(h)$. This permits us to recover the results of [Hérau, Hitrik and Sjöstrand 2011, Section 7.4].

Appendix A: Some results in linear algebra

We collect here some helpful results from linear algebra.

Lemma A.1 (Fan inequalities). *Let A, B be two matrices and denote by $\mu_n(X)$ the singular values of X. Then*

$$\mu_n(AB) \le \|B\|\mu_n(A),$$
$$\mu_n(AB) \le \|A\|\mu_n(B),$$

where $\|C\|$ denotes the norm of $C : \mathbb{R}^p \to \mathbb{R}^q$ with $\mathbb{R}^\bullet$ endowed with ℓ^2 norms.

Proof. See [Simon 1979]. □

Lemma A.2. *Let $A = \operatorname{diag}(A_1, \dots, A_N)$ be a block diagonal matrix. Then the singular values of A are the singular values of the A_n counted with multiplicities.*

Proof. It is straightforward, since $A^*A = \operatorname{diag}(A_1^*A_1, \dots, A_N^*A_N)$. □

Lemma A.3. *Let E, F be two finite-dimensional vector spaces and $A(h) : E \to F$ be a family of linear operators depending on a parameter $h \in]0, 1]$. Assume that $A(h)$ admits a classical expansion $A(h) \sim \sum_{k\ge 0} h^k A_k$ and that the matrix A_0 has nonzero singular values. Then, for $h > 0$ small enough the singular values $\mu_n(h)$ of $A(h)$ admit a classical expansion*

$$\mu_n(h) \sim \sum_{k\ge 0} h^k \mu_n^k,$$

where the μ_n^0 are the singular values of A_0.

Proof. Since the singular values of $A(h)$ are the eigenvalues of A^*A, which is selfadjoint, the result follows easily from Kato's perturbation theory of analytic families of selfadjoint operators [Kato 1966, Chapter 2, Section 1] applied to the expansion of A^*A in h powers cut at finite rank. □

Lemma A.4. *Let A be a $p \times (q + 1)$ matrix and T a $(q + 1) \times q$ matrix. Assume that $T^*T = \mathrm{Id}$ and that $\ker A = \operatorname{Ran}(T)^\perp$. Then the singular values of A are $\{0, z_1, \dots, z_q\}$, where $z_1, \dots, z_q$ are the singular values of AT.*

Proof. First observe that since $\ker A = \operatorname{Ran}(T)^\perp$, 0 is a singular value of multiplicity 1 of A. Let us denote by $\tilde{\xi}_0$ a unit vector such that $\ker A = \mathbb{R}\tilde{\xi}_0$. By definition, there exists an orthonormal basis $\xi_1, \dots, \xi_q$ of $\mathbb{R}^q$ such that

$$T^*A^*AT\xi_k = z_k^2\xi_k \tag{A-1}$$

for all $k = 1, \dots, q$. Let us set $\tilde{\xi}_k = T\xi_k$. Since $T^*T = \mathrm{Id}$; then the set of $\tilde{\xi}_k$ is an orthonormal family of $\mathbb{R}^{q+1}$. Moreover, since $\ker A = \operatorname{Ran}(T)^\perp$, we have $\Xi = \{\tilde{\xi}_0, \dots, \tilde{\xi}_q\}$ is an orthonormal basis of $\mathbb{R}^{q+1}$. Moreover, for all $k = 1, \dots, q$, it follows from (A-1) that

$$|A\tilde{\xi}_k|^2 = |AT\xi_k|^2 = z_k^2.$$

This shows that the matrix A^*A in the basis Ξ is exactly $\operatorname{diag}(0, z_1^2, \dots, z_q^2)$ and proves the result. □

Lemma A.5. *Let $\mathcal{M}$ be a real matrix. Assume that $\mathcal{M}$ is symmetric definite positive and that it admits a block decomposition*

$$\mathcal{M} = \begin{pmatrix} J & B^* \\ B & N \end{pmatrix}.$$

Then J and $N - B^* J^{-1} B$ are symmetric definite positive.

Proof. This is quite standard, but we recall the proof for the reader's convenience. Of course J and $N - B^* J^{-1} B$ are symmetric. Moreover, since $\mathcal{M}$ is positive definite,

$$\langle Jx, x\rangle = \left\langle \mathcal{M}\begin{pmatrix} x \\ 0 \end{pmatrix}, \begin{pmatrix} x \\ 0 \end{pmatrix}\right\rangle \geq c|x|^2$$

for some $c > 0$. This shows that J is definite positive. On the other hand, setting

$$\Omega = \begin{pmatrix} I & -J^{-1}B^* \\ 0 & I \end{pmatrix},$$

one has

$$\Omega^* \mathcal{M} \Omega = \begin{pmatrix} J & 0 \\ 0 & N - BJ^{-1}B^* \end{pmatrix}.$$

Since $\mathcal{M}$ is positive definite, this implies that $N - BJ^{-1}B^*$ is positive definite. □

Appendix B: Link between $\mathcal{R}$ and the Generic Assumption

Proposition B.1. *Suppose that the Generic Assumption is satisfied; that is, for all $\boldsymbol{m} \in \mathcal{U}^{(0)}$ one has the following:*

- *$\varphi_{|E(\boldsymbol{m})}$ has a unique minimum point.*
- *If E is a connected component of $\{\varphi < \sigma(\boldsymbol{m})\}$ such that $E \cap \mathcal{V}^{(1)} \neq \varnothing$, there exists a unique $\boldsymbol{s} \in \mathcal{V}^{(1)}$ such that $\varphi(\boldsymbol{s}) = \sup E \cap \mathcal{V}^{(1)}$. In particular, $E \cap \varphi^{-1}(]-\infty, \varphi(\boldsymbol{s})[)$ is the union of exactly two different connected components.*

Then for all $\boldsymbol{m} \in \mathcal{U}^{(0)}$, Cl$(\boldsymbol{m})$ *is reduced to $\{\boldsymbol{m}\}$.*

Proof. If $\boldsymbol{m} = \underline{\boldsymbol{m}}$ there is nothing to prove. Suppose that $\boldsymbol{m} \in \underline{\mathcal{U}}^{0)}$ and apply assumption (ii) to $E_-(\boldsymbol{m})$. One has evidently $\mathcal{V}^{(1)} \cap E_-(\boldsymbol{m}) \neq \varnothing$ since it contains $\overline{E(\boldsymbol{m})} \subset E_-(\boldsymbol{m})$ and $E(\boldsymbol{m})$ is a critical component. Hence, $E_-(\boldsymbol{m}) \cap \{\varphi < \sigma(\boldsymbol{m})\}$ has exactly two connected components which are necessarily $\widehat{E}(\boldsymbol{m})$ and $E(\boldsymbol{m})$. Suppose now that $\boldsymbol{m}'\mathcal{R}\boldsymbol{m}$. Then $\sigma(\boldsymbol{m}') = \sigma(\boldsymbol{m})$ and hence $\boldsymbol{m}' \notin \widehat{E}(\boldsymbol{m})$. Therefore $\boldsymbol{m}' \in E(\boldsymbol{m})$, which implies $\boldsymbol{m} = \boldsymbol{m}'$. □

Remark B.2. There exist functions φ such that Cl$(\boldsymbol{m}) = \{\boldsymbol{m}\}$ for all $\boldsymbol{m} \in \mathcal{U}^{(0)}$ and that do not satisfy the Generic Assumption. Take for instance $\varphi : \mathbb{R}^2 \to \mathbb{R}$ with two minima $\boldsymbol{m}_1, \boldsymbol{m}_2$ and two saddle points $\boldsymbol{s}_1, \boldsymbol{s}_2$ such that

$$\varphi(\boldsymbol{m}_1) < \varphi(\boldsymbol{m}_2) < \varphi(\boldsymbol{s}_1) = \varphi(\boldsymbol{s}_2).$$

Then, of course Cl$(\boldsymbol{m}_j) = \{\boldsymbol{m}_j\}$ for $j = 1, 2$. On the other hand, since $\boldsymbol{s}_1, \boldsymbol{s}_2$ are two saddle points at the same height (which turns out to be the maximal height of saddle points), (ii) of (GA) is not satisfied.

Appendix C: List of symbols

We list the notation used in the paper and give the first place each appears:

$\mathcal{U}^{(0)}, \mathcal{U}^{(1)}$	page 155
n_0, n_1	page 155
$\mathscr{F}(\cdot)$	page 155
$\mathcal{V}^{(1)}$	Definition 2.1
$\mathscr{C}, \underline{\Sigma}, \Sigma$	Definition 2.1
$S, \boldsymbol{\sigma}$	above (2-3)
$\mathcal{S}$	(2-3)
$\underline{\mathcal{U}}^{(0)}$	(2-4)
E	(2-5)
$\Gamma(\boldsymbol{m})$	below (2-5)
$H(\boldsymbol{m})$	(2-6)
E_-	(2-7)
$\widehat{E}$	(2-9)
$\hat{\boldsymbol{m}}$	(2-10)
$\mathcal{U}^{(0),\mathrm{I}}, \mathcal{U}^{(0),\mathrm{II}}$	Definition 2.3
$\mathcal{R}$	Definition 2.5
$\mathcal{U}_\alpha^{(0)}$	(2-14)
$\mathcal{A}, \underline{\mathcal{A}}$	below (2-14)
q_α	below (2-14)
$\mathcal{U}_\alpha^{(0),\mathrm{I}}, \mathcal{U}_\alpha^{(0),\mathrm{II}}$	below (2-14)
$\mathcal{S}_\alpha$	(2-16)
$p(\alpha)$	(2-16)
ν_j^α	below (2-16)
$\mathcal{V}_\alpha^{(1)}$	(3-2)
$\widehat{\mathcal{U}}_\alpha^{(0)}$	(3-3)
Γ_α	(3-4)
$\mathcal{V}_\alpha^{(1),b}, \mathcal{V}_\alpha^{(1),i}$	Lemma 3.4
$\widehat{\mathcal{U}}_\alpha^{(0),\mathrm{II}}$	(3-10)
$\theta_0^\alpha(\boldsymbol{m})$	(3-11)
$\widehat{H}_\alpha(\boldsymbol{m})$	(3-12)
$\widehat{\mathcal{U}}_\alpha^{(0)}$	(3-15)
$\mathscr{T}^\alpha$	Definition 3.7
$\mathcal{L}^\pi$	(4-1)
$\mathcal{L}^{\pi,\prime}$	below (4-1)
$\mathcal{L}^{\mathrm{bkw}}$	(4-2)
$\mathcal{L}^{\mathrm{bkw},\prime}$	(4-3)
$\mathcal{L}^{\mathrm{bkw},\prime\prime}$	(4-5)
$\mathscr{L}$	above Lemma 4.2
$\mathscr{L}^\alpha$	(4-6)
$\widehat{\mathscr{L}}^\alpha$	Lemma 4.3
$h_\varphi(\boldsymbol{m})$	(4-7)
$\widetilde{\mathscr{L}}^\alpha$	(4-9)
$\widehat{\mathscr{L}}^\alpha$	(5-3)
$\mathscr{S}^+, \mathscr{S}^+_{\mathrm{cl}}$	above Definition 5.4
$\mathscr{G}(\mathscr{E}, \tau), \mathscr{G}_{\mathrm{cl}}(\mathscr{E}, \tau)$	Definition 5.4
υ_2	(5-19)
υ_1	(5-20)

Acknowledgement

The author would like to thank D. Le Peutrec for numerous discussions; in particular for pointing out a fundamental argument in the induction step of the proof of the main result. This paper was written while the author was on leave at Stanford University and UC Berkeley. He was supported by the European Research Council, ERC-2012-ADG, project number 320845, “Semi-Classical Analysis of Partial Differential Equations”, by the Stanford Mathematics Department and by the France-Berkeley Fund, FBF 2016-0071, “Semiclassical Study of Randomness and Dynamics”.

References

[Bony, Hérau and Michel 2015] J.-F. Bony, F. Hérau, and L. Michel, “Tunnel effect for semiclassical random walks”, *Anal. PDE* **8**:2 (2015), 289–332. MR Zbl

[Bovier, Gayrard and Klein 2005] A. Bovier, V. Gayrard, and M. Klein, "Metastability in reversible diffusion processes, II: Precise asymptotics for small eigenvalues", *J. Eur. Math. Soc.* (*JEMS*) **7**:1 (2005), 69–99. MR Zbl

[Cvetković, Doob and Sachs 1995] D. M. Cvetković, M. Doob, and H. Sachs, *Spectra of graphs: theory and applications*, 3rd ed., Johann Ambrosius Barth, Heidelberg, 1995. MR Zbl

[Cycon, Froese, Kirsch and Simon 1987] H. L. Cycon, R. G. Froese, W. Kirsch, and B. Simon, *Schrödinger operators with application to quantum mechanics and global geometry*, Springer, 1987. MR Zbl

[Dang and Rivière 2017] N. V. Dang and G. Rivière, "Pollicott–Ruelle spectrum and Witten Laplacians", preprint, 2017. arXiv

[Di Gesù, Lelièvre, Le Peutrec and Nectoux 2017] G. Di Gesù, T. Lelièvre, D. Le Peutrec, and B. Nectoux, "Sharp asymptotics of the first exit point density", preprint, 2017. arXiv

[Dimassi and Sjöstrand 1999] M. Dimassi and J. Sjöstrand, *Spectral asymptotics in the semi-classical limit*, London Mathematical Society Lecture Note Series **268**, Cambridge University Press, 1999. MR Zbl

[Evans and Tabrizian 2016] L. C. Evans and P. R. Tabrizian, "Asymptotics for scaled Kramers–Smoluchowski equations", *SIAM J. Math. Anal.* **48**:4 (2016), 2944–2961. MR Zbl

[Helffer 1988] B. Helffer, *Semi-classical analysis for the Schrödinger operator and applications*, Lecture Notes in Mathematics **1336**, Springer, 1988. MR Zbl

[Helffer and Nier 2006] B. Helffer and F. Nier, *Quantitative analysis of metastability in reversible diffusion processes via a Witten complex approach: the case with boundary*, Mém. Soc. Math. Fr. (N.S.) **105**, Société Mathématique de France, Paris, 2006. MR Zbl

[Helffer and Sjöstrand 1985] B. Helffer and J. Sjöstrand, "Puits multiples en mécanique semi-classique, IV: Étude du complexe de Witten", *Comm. Partial Differential Equations* **10**:3 (1985), 245–340. MR Zbl

[Helffer, Klein and Nier 2004] B. Helffer, M. Klein, and F. Nier, "Quantitative analysis of metastability in reversible diffusion processes via a Witten complex approach", *Mat. Contemp.* **26** (2004), 41–85. MR Zbl

[Hérau and Nier 2004] F. Hérau and F. Nier, "Isotropic hypoellipticity and trend to equilibrium for the Fokker–Planck equation with a high-degree potential", *Arch. Ration. Mech. Anal.* **171**:2 (2004), 151–218. MR Zbl

[Hérau, Hitrik and Sjöstrand 2011] F. Hérau, M. Hitrik, and J. Sjöstrand, "Tunnel effect and symmetries for Kramers–Fokker–Planck type operators", *J. Inst. Math. Jussieu* **10**:3 (2011), 567–634. MR Zbl

[Herrmann and Niethammer 2011] M. Herrmann and B. Niethammer, "Kramers' formula for chemical reactions in the context of Wasserstein gradient flows", *Commun. Math. Sci.* **9**:2 (2011), 623–635. MR Zbl

[Kato 1966] T. Kato, *Perturbation theory for linear operators*, Die Grundlehren der mathematischen Wissenschaften **132**, Springer, 1966. MR Zbl

[Kramers 1940] H. A. Kramers, "Brownian motion in a field of force and the diffusion model of chemical reactions", *Physica* **7** (1940), 284–304. MR Zbl

[Landim, Misturini and Tsunoda 2015] C. Landim, R. Misturini, and K. Tsunoda, "Metastability of reversible random walks in potential fields", *J. Stat. Phys.* **160**:6 (2015), 1449–1482. MR

[Le Peutrec 2010] D. Le Peutrec, "Small eigenvalues of the Neumann realization of the semiclassical Witten Laplacian", *Ann. Fac. Sci. Toulouse Math.* (6) **19**:3-4 (2010), 735–809. MR Zbl

[Le Peutrec, Nier and Viterbo 2013] D. Le Peutrec, F. Nier, and C. Viterbo, "Precise Arrhenius law for p-forms: the Witten Laplacian and Morse–Barannikov complex", *Ann. Henri Poincaré* **14**:3 (2013), 567–610. MR Zbl

[Lelièvre, Rousset and Stoltz 2010] T. Lelièvre, M. Rousset, and G. Stoltz, *Free energy computations: a mathematical perspective*, Imperial College Press, London, 2010. MR Zbl

[Michel and Zworski 2018] L. Michel and M. Zworski, "A semiclassical approach to the Kramers–Smoluchowski equation", *SIAM J. Math. Anal.* **50**:5 (2018), 5362–5379. MR Zbl

[Peletier, Savaré and Veneroni 2012] M. A. Peletier, G. Savaré, and M. Veneroni, "Chemical reactions as Γ-limit of diffusion", *SIAM Rev.* **54**:2 (2012), 327–352. MR Zbl

[Simon 1979] B. Simon, *Trace ideals and their applications*, London Mathematical Society Lecture Note Series **35**, Cambridge University Press, 1979. MR Zbl

[Wales 2006] D. Wales, “Energy landscapes: calculating pathways and rates”, *Int. Rev. Phys. Chem.* **25**:1-2 (2006), 237–282.

[Witten 1982] E. Witten, “Supersymmetry and Morse theory”, *J. Differential Geom.* **17**:4 (1982), 661–692. MR Zbl

Received 31 Mar 2018. Revised 4 Feb 2019. Accepted 6 Mar 2019.

LAURENT MICHEL: laurent.michel@math.u-bordeaux.fr
Université de Bordeaux, Institut Mathématiques de Bordeaux, Talence, France

PURE and APPLIED ANALYSIS

Vol. 1, No. 2, 2019
dx.doi.org/10.2140/paa.2019.1.207

SEMICLASSICAL RESOLVENT ESTIMATES FOR SHORT-RANGE L^∞ POTENTIALS

GEORGI VODEV

We prove semiclassical resolvent estimates for real-valued potentials $V \in L^\infty(\mathbb{R}^n)$, $n \geq 3$, satisfying $V(x) = \mathcal{O}(\langle x\rangle^{-\delta})$ with $\delta > 3$.

1. Introduction and statement of results

Our goal in this note is to study the resolvent of the Schrödinger operator

$$P(h) = -h^2\Delta + V(x),$$

where $0 < h \ll 1$ is a semiclassical parameter, Δ is the negative Laplacian in $\mathbb{R}^n$, $n \geq 3$, and $V \in L^\infty(\mathbb{R}^n)$ is a real-valued potential satisfying

$$|V(x)| \leq C\langle x\rangle^{-\delta}, \tag{1-1}$$

with some constants $C > 0$ and $\delta > 3$. More precisely, we are interested in bounding from above the quantity

$$g_s^{\pm}(h,\varepsilon) := \log \|\langle x\rangle^{-s}(P(h) - E \pm i\varepsilon)^{-1}\langle x\rangle^{-s}\|_{L^2\to L^2},$$

where $L^2 := L^2(\mathbb{R}^n)$, $0 < \varepsilon < 1$, $s > \frac{1}{2}$ and $E > 0$ is a fixed energy level independent of h. Such bounds are known in various situations. For example, for long-range real-valued C^1 potentials it is proved in [Datchev 2014] when $n \geq 3$ and in [Shapiro 2019] when $n = 2$ that

$$g_s^{\pm}(h,\varepsilon) \leq Ch^{-1}, \tag{1-2}$$

with some constant $C > 0$ independent of h and ε. Previously, the bound (1-2) was proved for smooth potentials in [Burq 2002] and an analog of (1-2) for Hölder potentials was proved in [Vodev 2014b]. A high-frequency analog of (1-2) on more complex Riemannian manifolds was also proved in [Burq 1998; Cardoso and Vodev 2002]. In all these papers the regularity of the potential (and of the perturbation in general) plays an essential role. Without any regularity, the problem of bounding $g_s^{\pm}$ from above by an explicit function of h gets quite tough. Nevertheless, it was recently shown in [Shapiro 2018] that for real-valued compactly supported L^∞ potentials one has the bound

$$g_s^{\pm}(h,\varepsilon) \leq Ch^{-4/3}\log(h^{-1}), \tag{1-3}$$

MSC2010: 35P25.
Keywords: resolvent estimates.

with some constant $C > 0$ independent of h and ε. The bound (1-3) was also proved in [Klopp and Vogel 2019], still for real-valued compactly supported L^∞ potentials but with the weight $\langle x\rangle^{-s}$ replaced by a cut-off function. When $n = 1$ it was shown in [Dyatlov and Zworski 2019] that we have the better bound (1-2) instead of (1-3). When $n \geq 2$, however, the bound (1-3) seems hard to improve without extra conditions on the potential. The problem of showing that the bound (1-3) is optimal is largely open. In contrast, it is well known that the bound (1-2) cannot be improved in general; e.g., see [Datchev et al. 2015].

In this note we show that the bound (1-3) still holds for noncompactly supported L^∞ potentials when $n \geq 3$. Our main result is the following.

Theorem 1.1. *Under the condition* (1-1), *there exists* $h_0 > 0$ *such that for all* $0 < h \leq h_0$ *the bound* (1-3) *holds true.*

Remark. It is easy to see from the proof, see the inequality (4-2), that the bound (1-3) holds also for a complex-valued potential V satisfying (1-1), provided that its imaginary part satisfies the condition

$$\mp \operatorname{Im} V(x) \geq 0 \quad \text{for all } x \in \mathbb{R}^n.$$

To prove this theorem we adapt the Carleman estimates proved in [Shapiro 2018] simplifying some key arguments as, for example, the construction of the phase function φ. This is made possible by defining the key function F in Section 3 differently, without involving the second derivative φ''. The consequence is that we do not need to seek φ' as a solution to a differential equation as done in [Shapiro 2018], but it suffices to define it explicitly. Note also that similar (but simpler) Carleman estimates were used in [Vodev 2014a] to prove high-frequency resolvent estimates for the magnetic Schrödinger operator with large L^∞ magnetic potentials.

2. Construction of the phase and weight functions

We will first construct the weight function. We begin by introducing the continuous function

$$\mu(r) = \begin{cases} (r+1)^2 - 1 & \text{for } 0 \leq r \leq a, \\ (a+1)^2 - 1 + (a+1)^{-2s+1} - (r+1)^{-2s+1} & \text{for } r \geq a, \end{cases}$$

where

$$\tfrac{1}{2} < s < \tfrac{1}{2}(\delta - 2) \tag{2-1}$$

and $a = h^{-m}$ with some parameter $m > 0$ to be fixed in the proof of Lemma 2.3 below depending only on δ and s. Clearly, the first derivative (in sense of distributions) of μ satisfies

$$\mu'(r) = \begin{cases} 2(r+1) & \text{for } 0 \leq r < a, \\ (2s-1)(r+1)^{-2s} & \text{for } r > a. \end{cases}$$

The main properties of the functions μ and μ' are given in the following.

Lemma 2.1. *For all $r > 0$, $r \neq a$, we have the inequalities*

$$2r^{-1}\mu(r) - \mu'(r) \geq 0, \tag{2-2}$$

$$\mu'(r) \geq C_1(r+1)^{-2s}, \tag{2-3}$$

$$\frac{\mu(r)^2}{\mu'(r)} \leq C_2 a^4 (r+1)^{2s} \tag{2-4}$$

with some constants $C_1, C_2 > 0$.

Proof. For $r < a$ the left-hand side of (2-2) is equal to 2, while for $r > a$ it is bounded from below by

$$2r^{-1}(a^2 + 2a - s) > 2a^2 r^{-1} > 0,$$

provided a is taken large enough. Furthermore, we clearly have (2-3) for $r < a$ with $C_1 = 2$, while for $r > a$ it holds with $C_1 = 2s - 1$. Therefore, (2-3) holds with $C_1 = \min\{2, 2s-1\}$. The bound (2-4) follows with $C_2 = 2C_1^{-1}$ from (2-3) and the observation that $\mu(r)^2 \leq (a+1)^4 \leq 2a^4$ for all r. □

We now turn to the construction of the 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

$$\varphi'(r) = \begin{cases} \tau(r+1)^{-1} - \tau(a+1)^{-1} & \text{for } 0 \leq r \leq a, \\ 0 & \text{for } r \geq a, \end{cases}$$

where

$$\tau = \tau_0 h^{-1/3}, \tag{2-5}$$

with some parameter $\tau_0 \gg 1$ independent of h to be fixed in Lemma 2.3 below. Clearly, the first derivative of φ' satisfies

$$\varphi''(r) = \begin{cases} -\tau(r+1)^{-2} & \text{for } 0 \leq r < a, \\ 0 & \text{for } r > a. \end{cases}$$

Lemma 2.2. *For all $r \geq 0$ we have the bound*

$$h^{-1}\varphi(r) \lesssim h^{-4/3} \log \frac{1}{h}. \tag{2-6}$$

Proof. We have

$$\max \varphi = \int_0^a \varphi'(r)\, dr \leq \tau \int_0^a (r+1)^{-1}\, dr = \tau \log(a+1),$$

which clearly implies (2-6) in view of the choice of τ and a. □

For $r \neq a$, set

$$A(r) = (\mu \varphi'^2)'(r),$$

$$B(r) = \frac{\big(\mu(r)(h^{-1}(r+1)^{-\delta} + |\varphi''(r)|)\big)^2}{h^{-1}\varphi'(r)\mu(r) + \mu'(r)}.$$

The following lemma will play a crucial role in the proof of the Carleman estimates in the next section.

Lemma 2.3. *Given any $C > 0$ independent of the variable r and the parameters h, τ and a, there exist $\tau_0 = \tau_0(C) > 0$ and $h_0 = h_0(C) > 0$ so that for τ satisfying* (2-5) *and for all $0 < h \le h_0$ we have the inequality*

$$A(r) - CB(r) \ge -\tfrac{1}{2} E\mu'(r) \tag{2-7}$$

for all $r > 0,\ r \ne a$.

Proof. For $r < a$ we have

$$\begin{aligned} A(r) &= -(\varphi'^2)'(r) + \tau^2 \partial_r (1 - (r+1)(a+1)^{-1})^2 \\ &= -2\varphi'(r)\varphi''(r) - 2\tau^2 (a+1)^{-1}(1 - (r+1)(a+1)^{-1}) \\ &\ge 2\tau (r+1)^{-2}\varphi'(r) - 2\tau^2 (a+1)^{-1} \\ &\ge 2\tau (r+1)^{-2}\varphi'(r) - \tau^2 a^{-1}\mu'(r) \\ &\ge 2\tau (r+1)^{-2}\varphi'(r) - \mathcal{O}(h^{m-1})\mu'(r), \end{aligned}$$

where we have used that $\mu'(r) \ge 2$. Taking $m > 2$ we get

$$A(r) \ge 2\tau (r+1)^{-2}\varphi'(r) - \mathcal{O}(h)\mu'(r) \tag{2-8}$$

for all $r < a$. We will now bound the function B from above. Let first $0 < r \le \frac{1}{2}a$. Since in this case we have

$$\varphi'(r) \ge \tfrac{1}{3}\tau (r+1)^{-1},$$

we obtain

$$\begin{aligned} B(r) &\lesssim \frac{\mu(r)(h^{-2}(r+1)^{-2\delta} + \varphi''(r)^2)}{h^{-1}\varphi'(r)} \\ &\lesssim (\tau h)^{-1} \frac{\mu(r)(r+1)^{2-2\delta}}{\varphi'(r)^2} \tau (r+1)^{-2}\varphi'(r) + h\frac{\mu(r)\varphi''(r)^2}{\mu'(r)\varphi'(r)}\mu'(r) \\ &\lesssim \tau^{-3}h^{-1}(r+1)^{6-2\delta}\tau (r+1)^{-2}\varphi'(r) + \tau h\mu'(r) \\ &\lesssim \tau_0^{-3}\tau (r+1)^{-2}\varphi'(r) + \tau_0 h^{2/3}\mu'(r), \end{aligned}$$

where we have used that $\delta > 3$. This bound, together with (2-8), clearly implies (2-7), provided τ_0^{-1} and h are taken small enough depending on C.

Let now $\frac{1}{2}a < r < a$. Then we have the bound

$$\begin{aligned} B(r) &\le \left(\frac{\mu(r)}{\mu'(r)}\right)^2 (h^{-1}(r+1)^{-\delta} + |\varphi''(r)|)^2 \mu'(r) \\ &\lesssim (h^{-2}(r+1)^{2-2\delta} + \tau^2 (r+1)^{-2})\mu'(r) \\ &\lesssim (h^{-2}a^{2-2\delta} + \tau^2 a^{-2})\mu'(r) \\ &\lesssim (h^{2m(\delta-1)-2} + h^{2m-2/3})\mu'(r) \lesssim h\mu'(r), \end{aligned}$$

provided m is taken large enough. Again, this bound, together with (2-8), implies (2-7).

It remains to consider the case $r > a$. Using that $\mu = \mathcal{O}(a^2)$, together with (2-3), and taking into account that s satisfies (2-1), we get

$$\begin{aligned} B(r) &= \frac{\big(\mu(r)(h^{-1}(r+1)^{-\delta})\big)^2}{\mu'(r)} \\ &\lesssim h^{-2}a^4(r+1)^{4s-2\delta}\mu'(r) \lesssim h^{-2}a^{4+4s-2\delta}\mu'(r) \\ &\lesssim h^{2m(\delta-2-2s)-2}\mu'(r) \lesssim h\mu'(r), \end{aligned}$$

provided that m is taken large enough. Since in this case $A(r) = 0$, the above bound clearly implies (2-7). □

3. Carleman estimates

Our goal in this section is to prove the following:

Theorem 3.1. *Suppose* (1-1) *holds and let s satisfy* (2-1). *Then, for all functions $f \in H^2(\mathbb{R}^n)$ such that $\langle x\rangle^s(P(h)-E\pm i\varepsilon)f \in L^2$ and for all $0 < h \ll 1$, $0 < \varepsilon \le ha^{-2}$, we have the estimate*

$$\|\langle x\rangle^{-s}e^{\varphi/h}f\|_{L^2} \le Ca^2h^{-1}\|\langle x\rangle^{s}e^{\varphi/h}(P(h)-E\pm i\varepsilon)f\|_{L^2} + Ca\tau(\varepsilon/h)^{1/2}\|e^{\varphi/h}f\|_{L^2}, \tag{3-1}$$

with a constant $C > 0$ independent of h, ε and f.

Proof. We pass to the polar coordinates $(r, w) \in \mathbb{R}^+ \times \mathbb{S}^{n-1}$, $r = |x|$, $w = x/|x|$, and recall that $L^2(\mathbb{R}^n) = L^2(\mathbb{R}^+ \times \mathbb{S}^{n-1}, r^{n-1}dr\,dw)$. In what follows we denote by $\|\cdot\|$ and $\langle\cdot,\cdot\rangle$ the norm and the scalar product in $L^2(\mathbb{S}^{n-1})$. We will make use of the identity

$$r^{(n-1)/2}\Delta r^{-(n-1)/2} = \partial_r^2 + \frac{\tilde{\Delta}_w}{r^2}, \tag{3-2}$$

where $\tilde{\Delta}_w = \Delta_w - \frac{1}{4}(n-1)(n-3)$ and Δ_w denotes the negative Laplace–Beltrami operator on $\mathbb{S}^{n-1}$. Set $u = r^{(n-1)/2}e^{\varphi/h}f$ and

$$\begin{aligned} \mathcal{P}^\pm(h) &= r^{(n-1)/2}(P(h)-E\pm i\varepsilon)r^{-(n-1)/2}, \\ \mathcal{P}^\pm_\varphi(h) &= e^{\varphi/h}\mathcal{P}^\pm(h)e^{-\varphi/h}. \end{aligned}$$

Using (3-2) we can write the operator $\mathcal{P}^\pm(h)$ in the coordinates (r, w) as

$$\mathcal{P}^\pm(h) = \mathcal{D}_r^2 + \frac{\Lambda_w}{r^2} - E \pm i\varepsilon + V,$$

where we have put $\mathcal{D}_r = -ih\partial_r$ and $\Lambda_w = -h^2\tilde{\Delta}_w$. Since the function φ depends only on the variable r, this implies

$$\mathcal{P}^\pm_\varphi(h) = \mathcal{D}_r^2 + \frac{\Lambda_w}{r^2} - E \pm i\varepsilon - \varphi'^2 + h\varphi'' + 2i\varphi'\mathcal{D}_r + V.$$

For $r > 0$, $r \ne a$, introduce the function

$$F(r) = -\langle(r^{-2}\Lambda_w - E - \varphi'(r)^2)u(r,\cdot), u(r,\cdot)\rangle + \|\mathcal{D}_r u(r,\cdot)\|^2$$

and observe that its first derivative is given by

$$F'(r)=\frac{2}{r}\langle r^{-2}\Lambda_w u(r,\cdot),u(r,\cdot)\rangle+((\varphi')^2)'\|u(r,\cdot)\|^2-2h^{-1}\operatorname{Im}\langle\mathcal{P}_\varphi^\pm(h)u(r,\cdot),\mathcal{D}_r u(r,\cdot)\rangle$$
$$\pm 2\varepsilon h^{-1}\operatorname{Re}\langle u(r,\cdot),\mathcal{D}_r u(r,\cdot)\rangle+4h^{-1}\varphi'\|\mathcal{D}_r u(r,\cdot)\|^2+2h^{-1}\operatorname{Im}\langle(V+h\varphi'')u(r,\cdot),\mathcal{D}_r u(r,\cdot)\rangle.$$

Thus, if μ is the function defined in the previous section, we obtain the identity

$$\mu'F+\mu F'=(2r^{-1}\mu-\mu')\langle r^{-2}\Lambda_w u(r,\cdot),u(r,\cdot)\rangle+(E\mu'+(\mu(\varphi')^2)')\|u(r,\cdot)\|^2$$
$$-2h^{-1}\mu\operatorname{Im}\langle\mathcal{P}_\varphi^\pm(h)u(r,\cdot),\mathcal{D}_r u(r,\cdot)\rangle\pm 2\varepsilon h^{-1}\mu\operatorname{Re}\langle u(r,\cdot),\mathcal{D}_r u(r,\cdot)\rangle$$
$$+(\mu'+4h^{-1}\varphi'\mu)\|\mathcal{D}_r u(r,\cdot)\|^2+2h^{-1}\mu\operatorname{Im}\langle(V+h\varphi'')u(r,\cdot),\mathcal{D}_r u(r,\cdot)\rangle.$$

Using that $\Lambda_w\ge 0$, together with (2-2), we get the inequality

$$\begin{aligned}\mu'F+\mu F'&\ge(E\mu'+(\mu(\varphi')^2)')\|u(r,\cdot)\|^2+(\mu'+4h^{-1}\varphi'\mu)\|\mathcal{D}_r u(r,\cdot)\|^2\\&\quad-\frac{3h^{-2}\mu^2}{\mu'}\|\mathcal{P}_\varphi^\pm(h)u(r,\cdot)\|^2-\tfrac{1}{3}\mu'\|\mathcal{D}_r u(r,\cdot)\|^2-\varepsilon h^{-1}\mu(\|u(r,\cdot)\|^2+\|\mathcal{D}_r u(r,\cdot)\|^2)\\&\quad-3h^{-2}\mu^2(\mu'+4h^{-1}\varphi'\mu)^{-1}\|(V+h\varphi'')u(r,\cdot)\|^2-\tfrac{1}{3}(\mu'+4h^{-1}\varphi'\mu)\|\mathcal{D}_r u(r,\cdot)\|^2\\&\ge\big(E\mu'+(\mu(\varphi')^2)'-C\mu^2(\mu'+h^{-1}\varphi'\mu)^{-1}(h^{-1}(r+1)^{-\delta}+|\varphi''|)^2\big)\|u(r,\cdot)\|^2\\&\quad-\frac{3h^{-2}\mu^2}{\mu'}\|\mathcal{P}_\varphi^\pm(h)u(r,\cdot)\|^2-\varepsilon h^{-1}\mu(\|u(r,\cdot)\|^2+\|\mathcal{D}_r u(r,\cdot)\|^2),\end{aligned}$$

with some constant $C>0$. Now we use Lemma 2.3 to conclude that

$$\mu'F+\mu F'\ge\tfrac{1}{2}E\mu'\|u(r,\cdot)\|^2-\frac{3h^{-2}\mu^2}{\mu'}\|\mathcal{P}_\varphi^\pm(h)u(r,\cdot)\|^2-\varepsilon h^{-1}\mu(\|u(r,\cdot)\|^2+\|\mathcal{D}_r u(r,\cdot)\|^2).$$

We now integrate this inequality with respect to r and use that, since $\mu(0)=0$, we have

$$\int_0^\infty(\mu'F+\mu F')\,dr=0.$$

Thus we obtain the estimate

$$\begin{aligned}&\tfrac{1}{2}E\int_0^\infty\mu'\|u(r,\cdot)\|^2\,dr\\&\qquad\le 3h^{-2}\int_0^\infty\frac{\mu^2}{\mu'}\|\mathcal{P}_\varphi^\pm(h)u(r,\cdot)\|^2\,dr+\varepsilon h^{-1}\int_0^\infty\mu(\|u(r,\cdot)\|^2+\|\mathcal{D}_r u(r,\cdot)\|^2)\,dr.\end{aligned}\tag{3-3}$$

Using that $\mu=\mathcal{O}(a^2)$ together with (2-3) and (2-4) we get from (3-3)

$$\begin{aligned}&\int_0^\infty(r+1)^{-2s}\|u(r,\cdot)\|^2\,dr\\&\quad\le Ca^4h^{-2}\int_0^\infty(r+1)^{2s}\|\mathcal{P}_\varphi^\pm(h)u(r,\cdot)\|^2\,dr+C\varepsilon h^{-1}a^2\int_0^\infty(\|u(r,\cdot)\|^2+\|\mathcal{D}_r u(r,\cdot)\|^2)\,dr,\end{aligned}\tag{3-4}$$

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

$$\begin{aligned}\operatorname{Re}\int_0^\infty \langle \mathcal{P}_\varphi^\pm(h)u(r,\cdot), u(r,\cdot)\rangle\, dr &= \int_0^\infty \|\mathcal{D}_r u(r,\cdot)\|^2\, dr + \int_0^\infty \langle r^{-2}\Lambda_w u(r,\cdot), u(r,\cdot)\rangle\, dr \\ &\quad - \int_0^\infty (E+\varphi'^2)\|u(r,\cdot)\|^2\, dr + \int_0^\infty \langle V u(r,\cdot), u(r,\cdot)\rangle\, dr.\end{aligned}$$

This implies

$$\begin{aligned}\int_0^\infty \|\mathcal{D}_r u(r,\cdot)\|^2\, dr &\le \mathcal{O}(\tau^2)\int_0^\infty \|u(r,\cdot)\|^2\, dr \\ &\quad + \gamma\int_0^\infty (r+1)^{-2s}\|u(r,\cdot)\|^2\, dr + \gamma^{-1}\int_0^\infty (r+1)^{2s}\|\mathcal{P}_\varphi^\pm(h)u(r,\cdot)\|^2\, dr \qquad (3\text{-}5)\end{aligned}$$

for every $\gamma > 0$. We take now γ small enough, independent of h, and recall that $\varepsilon h^{-1}a^2 \le 1$. Thus, combining the estimates (3-4) and (3-5), we get

$$\begin{aligned}&\int_0^\infty (r+1)^{-2s}\|u(r,\cdot)\|^2\, dr \\ &\qquad \le Ca^4h^{-2}\int_0^\infty (r+1)^{2s}\|\mathcal{P}_\varphi^\pm(h)u(r,\cdot)\|^2\, dr + C\varepsilon h^{-1}a^2\tau^2\int_0^\infty \|u(r,\cdot)\|^2\, dr, \qquad (3\text{-}6)\end{aligned}$$

with a new constant $C > 0$ independent of h and ε. It is an easy observation now that the estimate (3-6) implies (3-1). □

4. Resolvent estimates

In this section we will derive the bound (1-3) from Theorem 3.1. Indeed, it follows from the estimate (3-1) and Lemma 2.2 that for $0 < h \ll 1$, $0 < \varepsilon \le ha^{-2}$ and s satisfying (2-1) we have

$$\|\langle x\rangle^{-s} f\|_{L^2} \le M\|\langle x\rangle^{s}(P(h) - E \pm i\varepsilon)f\|_{L^2} + M\varepsilon^{1/2}\|f\|_{L^2}, \qquad (4\text{-}1)$$

where

$$M = \exp(Ch^{-4/3}\log(h^{-1})),$$

with a constant $C > 0$ independent of h and ε. On the other hand, since the operator $P(h)$ is symmetric, we have

$$\begin{aligned}\varepsilon\|f\|_{L^2}^2 &= \pm\operatorname{Im}\langle (P(h)-E\pm i\varepsilon)f, f\rangle_{L^2} \\ &\le (2M)^{-2}\|\langle x\rangle^{-s} f\|_{L^2}^2 + (2M)^2\|\langle x\rangle^{s}(P(h)-E\pm i\varepsilon)f\|_{L^2}^2. \qquad (4\text{-}2)\end{aligned}$$

We rewrite (4-2) in the form

$$M\varepsilon^{1/2}\|f\|_{L^2} \le \tfrac{1}{2}\|\langle x\rangle^{-s} f\|_{L^2} + 2M^2\|\langle x\rangle^{s}(P(h)-E\pm i\varepsilon)f\|_{L^2}. \qquad (4\text{-}3)$$

We now combine (4-1) and (4-3) to get

$$\|\langle x\rangle^{-s} f\|_{L^2} \le 4M^2 \|\langle x\rangle^{s}(P(h)-E\pm i\varepsilon) f\|_{L^2}. \tag{4-4}$$

It follows from (4-4) that the resolvent estimate

$$\|\langle x\rangle^{-s}(P(h)-E\pm i\varepsilon)^{-1}\langle x\rangle^{-s}\|_{L^2\to L^2} \le 4M^2 \tag{4-5}$$

holds for all $0<h\ll 1,\ 0<\varepsilon\le ha^{-2}$ and s satisfying (2-1). On the other hand, for $\varepsilon\ge ha^{-2}$ the estimate (4-5) holds in a trivial way. Indeed, in this case, since the operator $P(h)$ is symmetric, the norm of the resolvent is bounded above by $\varepsilon^{-1}=\mathcal{O}(h^{-2m-1})$. Finally, observe that if (4-5) holds for s satisfying (2-1), it holds for all $s>\frac{1}{2}$.

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

[Datchev et al. 2015] K. Datchev, S. Dyatlov, and M. Zworski, "Resonances and lower resolvent bounds", *J. Spectr. Theory* **5**:3 (2015), 599–615. MR Zbl

[Dyatlov and Zworski 2019] S. Dyatlov and M. Zworski, "Mathematical theory of scattering resonances", unpublished book, 2019, available at http://math.mit.edu/~dyatlov/res/res_final.pdf.

[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

[Shapiro 2018] J. Shapiro, "Semiclassical resolvent bound for compactly supported L^∞ potentials", preprint, 2018. To appear in *J. Spectr. Theory*. arXiv

[Shapiro 2019] J. Shapiro, "Semiclassical resolvent bounds in dimension two", *Proc. Amer. Math. Soc.* (online publication February 2019).

[Vodev 2014a] G. Vodev, "Resolvent estimates for the magnetic Schrödinger operator", *Anal. PDE* **7**:7 (2014), 1639–1648. MR Zbl

[Vodev 2014b] G. Vodev, "Semi-classical resolvent estimates and regions free of resonances", *Math. Nachr.* **287**:7 (2014), 825–835. MR Zbl

Received 12 Sep 2018. Revised 23 Oct 2018. Accepted 6 Dec 2018.

GEORGI VODEV: `georgi.vodev@univ-nantes.fr`
Université de Nantes, Laboratoire de Mathématiques Jean Leray, Nantes, France

PURE and APPLIED
ANALYSIS

Vol. 1, No. 2, 2019
dx.doi.org/10.2140/paa.2019.1.215

AN EVOLUTION EQUATION APPROACH TO THE KLEIN–GORDON OPERATOR ON CURVED SPACETIME

JAN DEREZIŃSKI AND DANIEL SIEMSSEN

We develop a theory of the Klein–Gordon equation on curved spacetimes. Our main tool is the method of (nonautonomous) evolution equations on Hilbert spaces. This approach allows us to treat low regularity of the metric, of the electromagnetic potential and of the scalar potential. Our main goal is a construction of various kinds of propagators needed in quantum field theory.

1. Introduction

We consider the *Klein–Gordon operator on a Lorentzian manifold* (M, g) *minimally coupled to an electromagnetic potential* A *and with a scalar potential* Y. In local coordinates it can be written as

$$K := \Box_A + Y = |g|^{-1/2}(D_\mu - A_\mu)|g|^{1/2} g^{\mu\nu}(D_\nu - A_\nu) + Y, \tag{1-1}$$

where $|g| = |\det[g_{\mu\nu}]|$ and $D_\mu = -\mathrm{i}\partial_\mu$. As in our recent work [Dereziński and Siemssen 2018], we are interested in inverses and bisolutions of the Klein–Gordon operator K.

MSC2010: primary 35L05, 47D06; secondary 58J45, 81Q10, 81T20.

Keywords: Klein–Gordon equation, Klein–Gordon operator, propagator, evolution equation, quantum field theory, quantum field theory in curved spacetimes.

Heuristically, they are defined as follows:

- An operator G is a *bisolution* of K if it satisfies

$$KG = 0 \quad \text{and} \quad GK = 0.$$

- An operator G is an *inverse* of K if it satisfies

$$KG = \mathbb{1} \quad \text{and} \quad GK = \mathbb{1}.$$

To make these statements rigorous, one needs to specify the spaces between which these operators act, making sure that the composition of K and G is well-defined. Often, G can be understood as an operator from $C_{\mathrm{c}}^{\infty}(M)$ to $C^{\infty}(M)$.

The Klein–Gordon operator has several distinguished inverses and bisolutions. They are known by many names, e.g., "propagator" or "two-point function". Inverses are often also called "Green's functions".

The most well-known propagators are probably the *forward* (*retarded*) *propagator* $G^{\vee}$ and the *backward* (*advanced*) *propagator* $G^{\wedge}$. Their difference $G^{\mathrm{PJ}} := G^{\vee} - G^{\wedge}$ is sometimes called the *Pauli–Jordan propagator*, which is the name we use. In the literature one can also find other names, such as "commutator function" or "causal propagator".[1] These three propagators are important in the Cauchy problem of the classical theory. Therefore, we will call them jointly *classical propagators*. It is well known that on globally hyperbolic spacetimes the classical propagators exist and are unique.

In quantum field theory, one needs also other propagators: two inverses, the *Feynman propagator* G^{F} and the *anti-Feynman propagator* $G^{\overline{\mathrm{F}}}$, as well as the *positive*- and *negative-frequency bisolutions* $G^{(\pm)}$. We will call them jointly *nonclassical propagators*. A positive-frequency bisolution yields the two-point function of a vacuum state — a pure quasifree state whose Gelfand–Naimark–Segal (GNS) representation yields a Hilbert space for the quantum field theory. The integral kernel of the Feynman propagator coincides with the expectation value of time-ordered products of quantum fields. It is used to evaluate Feynman diagrams.

The analysis of the Klein–Gordon equation is especially simple if the spacetime is stationary and the Hamiltonian is positive. On the mathematical side, if in addition the Hamiltonian is bounded away from zero (the "positive-mass case"), we have a natural Hilbert space structure for the Cauchy data. The most obvious choice is the so-called *energy Hilbert space*. It is also natural to consider a whole scale of Hilbert spaces, which includes the energy space. The generator of the dynamics is self-adjoint on all of these spaces. Thus the functional analytic setting for stationary spacetimes in the "positive-mass case" is rather clean and simple. If we assume that the Hamiltonian is only positive, without a positive lower bound, (the "zero-mass case"), then the functional-analytic setup becomes slightly more technically involved, but the general picture remains the same.

[1] We try to use as much as possible the terminology from classic textbooks on quantum field theory. For instance, "Pauli–Jordan function" is the name used for G^{PJ} already in [Bogoliubov and Shirkov 1980]. The same authors call G^{F} the "causal Green's function", since the choice of G^{F} for the evaluation of Feynman diagrams expresses causality in quantum field theory. Therefore, using the name "causal propagator" for G^{PJ} clashes with the traditional terminology and, we believe, should be discouraged.

On the physical side, on a stationary spacetime with a positive Hamiltonian, it is clear how to define the nonclassical propagators. The positive- and negative-frequency bisolutions, as well as the Feynman and anti-Feynman propagators, are constructed from the spectral projections of the generator of the dynamics. These constructions, at least implicitly, can be found in various works devoted to quantum field theory on curved spacetimes. In a systematic way the static case has been worked out recently in [Dereziński and Siemssen 2018]; see also [Dereziński and Gérard 2013, Chapter 18]. In [Dereziński and Siemssen 2018], we assumed in addition the "positive-mass condition", and the results of that paper can be easily generalized to stationary spacetimes (using, e.g., the stationary special case of Sections 2.1 and 2.2 as a starting point).

The positivity of the Hamiltonian plays an important role in the construction of nonclassical propagators. This is related to the fact that nonpositive Hamiltonians lead to problems in quantum field theory, which are often collectively called the *Klein paradox*. The original paper by Klein involved fermions and the Dirac equation with a large step potential causing spontaneous *pair creation*. One can easily resolve the fermionic Klein paradox in the second quantized theory. Splitting the Hilbert space into the particle and antiparticle subspaces and applying second quantization makes the quantum Hamiltonian positive definite. The corresponding problem for bosons is much more serious. If the classical Hamiltonian is not positive, it will not become positive by quantization. Besides, in this case there is no positive scalar product preserved by the evolution, as is the case for Dirac fermions. This typically leads to the so-called *superradiance*. In mathematical terms it means that the scattering operator has a norm greater than 1, or it does not exist at all because the norm of the evolution grows all the time.

This paper is devoted to the study of the Klein–Gordon equation on rather general (possibly, nonstationary) spacetimes. We construct both the classical propagators and certain families of nonclassical propagators. Let us first describe the basic steps of our construction of the classical propagators:

(1) We assume that there is a manifold Σ such that the spacetime M is diffeomorphic to $\mathbb{R} \times \Sigma$. This diffeomorphism provides a global time function t whose level sets Σ_t are assumed to be spacelike. It also defines a flow whose generator ∂_t is assumed to be timelike.

(2) We rewrite the Klein–Gordon equation as a (nonautonomous) first-order equation for the Cauchy data on Σ_t. Thus the generator of the evolution can be written as a 2×2 matrix.

(3) We make various assumptions on the metric, electromagnetic and scalar potentials. The assumptions on their regularity are rather weak; however, they are global in spacetime. We assume that the positive-mass condition holds for all times; that is, all instantaneous Hamiltonians have a strictly positive lower bound.

(4) We apply functional-analytic methods from the theory of *nonautonomous evolution equations*, as developed in [Kato 1970]. Note that, unlike in [Dereziński and Siemssen 2018], in the nonstationary case we do not have a unique distinguished energy space. Instead, we have a whole time-dependent family of instantaneous-energy Hilbert spaces describing the Cauchy data at each time. Under the assumptions we impose, these spaces can be identified with one another. They have a variable scalar product, but a common topology — thus the Cauchy data at each time belong to a single *Hilbertizable space*.

(5) The Pauli–Jordan propagator essentially coincides with one of the matrix elements of the evolution operator. One can then write down the forward and backward propagators by inserting the Heaviside

function in the appropriate places. Thus if one uses the method of evolution equations, the Pauli–Jordan propagator becomes the central object, whereas in typical approaches found in the literature, e.g., [Bär et al. 2007], the forward and backward propagators are obtained first and then used to define the Pauli–Jordan propagator. We find this (trivial) observation curious.

The assumptions of our paper, in particular their global character and the positive-mass assumptions, are adapted to the needs of nonclassical propagators, which are our main interest. However, if one is interested only in classical propagators, some of these assumptions can be relaxed.

When the Hamiltonian is merely bounded from below, we can reduce the problem to the positive-mass case by a perturbation argument. Then one can construct the evolution, and hence also the classical propagators. We remark about this fact at the end of Section 5.

Another point that can be relaxed are the global assumptions. We know that the propagation of solutions to the Klein–Gordon equation has finite speed — this can be proven independently under a weak assumption on the regularity; see, e.g., Appendix E. Therefore, to construct the evolution, it is sufficient to have local information about our system. We do not discuss this point further in our paper.

As already stated above, our main interest is the nonclassical propagators. Unfortunately, in the nonstationary case it is not obvious how to define them. The most popular view on this subject says that instead of a single positive-frequency bisolution one should consider a whole class of bisolutions locally similar to the Minkowski two-point function, known as *Hadamard states*. There exists considerable literature about them; in particular we would like to mention [Radzikowski 1996; Kay and Wald 1991]. Properties of Hadamard states play a central role in most formulations of perturbation theory and renormalization on curved spacetimes; see, e.g., [Hollands and Wald 2001; 2002]. Moreover, the expectation value of time-ordered fields in every Hadamard state is the integral kernel of an inverse of K and can be viewed as a possible generalization of the usual Feynman propagator to the generic case.

One of possibilities is to use spectral projections of the generator of the evolution at a fixed instance of time, as we describe in Section 8. This allows us to define *instantaneous positive- and negative-frequency bisolutions*, which yield the so-called *instantaneous vacua*. One also has the corresponding *instantaneous Feynman inverses*.

One can criticize these propagators on physical grounds. Not only do they depend on an arbitrary and unphysical choice of a preferred time, but it is folklore knowledge that they are generally not Hadamard states. In a forthcoming article we will show, using methods from our formalism, that an instantaneous positive-frequency bisolution yields a Hadamard state if the Klein–Gordon operator K is infinitesimally stationary at the Cauchy surface where the positive/negative-frequency splitting was performed.

Spacetimes that become asymptotically stationary in the past and the future form a class that in our opinion is especially natural from the point of view of quantum field theory and scattering theory. For such spacetimes one can define positive/negative-frequency bisolutions corresponding to the asymptotic past and future; see Section 9. We can call them *in/out-positive/negative-frequency bisolutions*. One can argue that the corresponding *in-vacuum* yields the representation of incoming states (prepared in the experiment) and the corresponding *out-vacuum* gives the representation of final observables (measured in the experiment). Therefore, the in- and out-states are not only distinguished, they also have a clear and important physical meaning. If the spacetime becomes stationary sufficiently fast, it can be shown that the states thus defined are Hadamard [Gérard and Wrochna 2017].

As we described above, and is well known, spacetimes with asymptotically stationary past and future possess two pairs of distinguished and physically well-motivated propagators: the in/out-positive/negative-frequency bisolution. It is perhaps less known that a large class of such spacetimes possesses another pair of natural and physically motivated propagators: the so-called *canonical Feynman* and *anti-Feynman propagators* (*inverses*). The Feynman propagator appears naturally when we evaluate Feynman diagrams. A study of these propagators will be presented in a forthcoming article, where the formalism and results of the present paper will play an important role.

Let us mention that the canonical Feynman and anti-Feynman propagators are related to the intriguing and poorly understood question about the self-adjointness of the Klein–Gordon operator. It is easy to see that the Klein–Gordon operator is Hermitian; however, the existence of a distinguished self-adjoint extension seems to be difficult to prove and is known only in special cases: in the static case [Dereziński and Siemssen 2018] and (since very recently) for a class of asymptotically Minkowskian spaces [Vasy 2017]. Note that heuristically the canonical Feynman or anti-Feynman propagator is the boundary value at zero from above or below, respectively, of the resolvent of the Klein–Gordon operator. One could also argue that the adjective *canonical* is not needed for both propagators, that they should simply be called *the* Feynman and anti-Feynman propagators.

Let us compare our work with the literature. The construction of classical propagators is described in numerous sources. Typically, one shows first the well-posedness of the Cauchy problem. Then the existence of the classical propagators and their properties easily follow; see, e.g., [Kay 1978; Dimock and Kay 1982], and also the more recent works [Drago and Gérard 2017; Gérard and Wrochna 2014; Gérard et al. 2017]. Standard methods include the Hadamard parametrix method [Bär et al. 2007; Friedlander 1975] and energy estimates obtained via the divergence theorem. Another popular method relies on the factorization of the Klein–Gordon operator into the product of first-order scalar operators (see, e.g., the treatment of [Hörmander 1985], which also covers n-th order hyperbolic equations). A brief history of the Cauchy problem for hyperbolic equations with references to various approaches can be found in [Hörmander 1985, Notes to Chapter XXIII].

In our opinion, the method of evolution equations used in this paper provides a natural and powerful approach to analyze the Klein–Gordon equation on curved spacetimes, especially concerning questions relevant to quantum field theory. Therefore, we were greatly surprised that it is difficult to find a treatment of this problem similar to ours in the existing literature. We are only aware of one more publication where the methods of evolution equations have been applied to the problem at hand in the nonstationary case: in [Furlani 1997] the evolution is constructed under quite restrictive assumptions, namely, assuming that Cauchy surfaces are compact and have a decreasing volume along a finite time-interval. The treatment of some papers, such as [Dimock and Kay 1982; Kay 1978; Gérard et al. 2017; Gérard and Wrochna 2014], may also resemble our method. However, in almost all papers that we know, the existence of the evolution is taken for granted, is given by the local theory, and is not constructed within the formalism of evolution equations on some Banach spaces.

The literature devoted to classical propagators on curved spacetimes usually does not use a global functional-analytic setting. As we discussed above, from the point of view of classical propagators, the method of our paper seems to impose unnecessary limitations, because of the global assumptions on the spacetime. However, to define and study nonclassical propagators, some kind of global assumptions are usually indispensable.

Most authors do not consider low-regularity situations; for an exception we refer to [Sanchez and Vickers 2018]. For example, the propagators are typically understood from $C_{\mathrm{c}}^\infty(M)$ to $C^\infty(M)$. As far as we know, the constructions found in the literature require more stringent regularity assumptions than ours.

Throughout our paper we impose rather weak assumptions on the regularity of various objects (the metric, electromagnetic potential and the scalar potential). Nevertheless, we did not write this work with any particular nonregular examples in mind, even though low regularity is present in some interesting physical applications (e.g., boundaries of astrophysical objects, shock waves) and singularities appear generically in solutions of the Einstein equation. Instead, the main reason for the chosen approach is our conviction that weak assumptions play an important theoretical role, because they impose a certain discipline on a mathematical theory, forcing us to find better arguments and a more natural setting for the problem.

We think that our approach is rather natural and direct if one wants to treat the simplest examples of spacetimes (from the point of view of quantum field theory) such as local perturbations of Minkowski spacetime and cosmological spacetimes. However, it is also flexible enough to treat some less obvious examples, such as certain nonglobally hyperbolic spacetimes, including spacetimes with boundaries, provided we impose appropriate boundary conditions. This includes for example compactifications of anti-de Sitter spacetime with appropriate conditions on its timelike boundary (see [Dappiaggi et al. 2018a; 2018b] for a recent discussion of boundary conditions on anti-de Sitter spacetime and spacetimes with a timelike boundary).

Finally, let us remark that Kato's theory of nonautonomous evolution equations has also been successfully applied in the context of quantum field theory for the Dirac equation on curved spacetimes; see, e.g., [Häfner 2009; Nicolas 2002]. The Dirac equation is simpler in this respect than the Klein–Gordon equation. For the Dirac equation there exists a natural Hilbert space. For the (nonstationary) Klein–Gordon equation no such choice exists: one is forced to work with a family of Hilbertizable spaces. Studying the evolution for the Klein–Gordon equation in time-dependent families of Hilbert spaces has also been fruitful in the context of spherical gravitational collapse (i.e., in static Schwarzschild spacetime with time-dependent boundary conditions); see [Bachelot 1999].

1.1. ***Notation and conventions.*** Throughout this paper we adopt essentially the same notation and conventions as in [Dereziński and Siemssen 2018] but for the convenience of the reader we repeat the relevant conventions. We also introduce some new notation.

Suppose that T is an operator on a Banach space $\mathcal{X}$. We denote by $\operatorname{Dom} T$ its domain and by $\operatorname{Ran} T$ its range. For its spectrum we write $\operatorname{sp} T$ and for the resolvent set $\operatorname{rs} T$.

Suppose that T is an operator on a Hilbert space $\mathcal{H}$ with inner product $(\cdot \mid \cdot)$. If T is positive, i.e., $(u \mid Tu) \geq 0$, we write $T \geq 0$. If also $\operatorname{Ker} T = \{0\}$, then we write $T > 0$.

A useful function is the so-called "Japanese bracket", defined as $\langle T \rangle := (1 + |T|^2)^{1/2}$.

A topological vector space $\mathcal{X}$ is called *Hilbertizable* if there exists a scalar product on $\mathcal{X}$ that determines its topology and makes it into a Hilbert space. Clearly, two scalar products determine the topology of $\mathcal{X}$ if and only if they are equivalent.

The p-times continuously differentiable $\mathcal{X}$-valued functions on a manifold M are denoted by $C^p(M;\mathcal{X})$; if $\mathcal{X}=\mathbb{C}$, we simply write $C^p(M)$. Sets of compactly supported or bounded functions are indicated by a subscript "c" or "b".

$\mathrm{AC}(\mathbb{R})$ denotes the set of absolutely continuous functions, i.e., functions whose distributional derivative belongs to $L^1_{\mathrm{loc}}(\mathbb{R})$. $\mathrm{AC}^1(\mathbb{R})$ denotes the set of functions whose distributional derivative belongs to $\mathrm{AC}(\mathbb{R})$.

When calculating integrals, we denote by $\int'$ the "Cauchy principal value" at infinity, e.g.,

$$\int'_{\mathrm{i}\mathbb{R}} f(t)\,\mathrm{d}t = \lim_{R\to\infty}\int_{-\mathrm{i}R}^{\mathrm{i}R} f(t)\,\mathrm{d}t.$$

Observe that we pass to infinity symmetrically in the lower and upper integration limits.

Suppose we fix a positive density γ on M. The space $L^2(M,\gamma)$ of square-integrable functions on M is then defined as the completion of $C_{\mathrm{c}}^\infty(M)$ with respect to the scalar product

$$(u\,|\,v)_\gamma := \int_M \bar{u}\,v\,\gamma, \qquad u, v \in C_{\mathrm{c}}^\infty(M).$$

If g is the metric tensor g on M (of any signature), then we set $|g| := |\det[g_{\mu\nu}]|$. M is then equipped with a canonical density $|g|^{1/2}$. Sometimes it is however convenient to fix a density γ independent of the metric tensor.

Often it is convenient to use the formalism of (complexified) half-densities on M. If γ is a positive density on M, then $\gamma^{1/2}$ is a half-density. The canonical example for a half-density on a pseudo-Riemannian manifold is $|g|^{1/4}$. Since the integral over a density on a manifold is well-defined, half-densities come equipped with a natural L^2-structure

$$(\tilde{u}\,|\,\tilde{v}) = \int_M \bar{\tilde{u}}\,\tilde{v}, \qquad \tilde{u}, \tilde{v} \in C_{\mathrm{c}}^\infty(\Omega^{1/2}M).$$

We denote by $L^2(\Omega^{1/2}M)$ the completion of $C_{\mathrm{c}}^\infty(\Omega^{1/2}M)$ with respect to the corresponding norm. Note that if we fix an everywhere-positive density γ, then

$$L^2(M,\gamma) \ni u \mapsto \tilde{u} := u\gamma^{1/2} \in L^2(\Omega^{1/2}M)$$

is the natural unitary identification of the L^2-space in the scalar formalism and in the half-density formalism.

The operator $D=-\mathrm{i}\partial$ acts naturally on scalars, and $D^\gamma = \gamma^{1/2}D\gamma^{-1/2}$ acts naturally on half-densities.

In our paper we generally prefer to use the half-density formalism rather than the scalar formalism. The Klein–Gordon operator K is presented in (1-1) in the scalar formalism. Transformed to the half-density formalism it is

$$K_{\frac{1}{2}} := |g|^{1/4}K|g|^{-1/4} = |g|^{-1/4}(D_\mu - A_\mu)|g|^{1/2}g^{\mu\nu}(D_\nu - A_\nu)|g|^{-1/4} + Y. \tag{1-2}$$

In what follows we drop the subscript $\frac{1}{2}$ from $K_{1/2}$ and by K we will mean (1-2).

2. Assumptions and setting

2.1. $1+3$ *splitting.* We consider smooth manifolds M and Σ such that there exists a (fixed) diffeomorphism $\mathbb{R}\times\Sigma\to M$. This means that we have a distinguished time function t on M, and the leaves $\Sigma_t=\{t\}\times\Sigma$ provide a foliation of M with a family of diffeomorphisms $\epsilon_t:\Sigma\to\Sigma_t\subset M$. We define the time vector field

$$\partial_t := \frac{\mathrm{d}}{\mathrm{d}t}\epsilon_t.$$

Note that $\mathrm{d}t\cdot\partial_t=1$.

We assume that M is equipped with a continuous Lorentzian metric g; i.e., (M,g) is a *spacetime*. The restriction of g to the tangent space of Σ_t defines a time-dependent family of metrics on Σ, denoted by $g_\Sigma(t):=\epsilon_t^* g$. We make the assumption that all $g_\Sigma(t)$ are Riemannian, or, equivalently, that the covector $\mathrm{d}t$ is everywhere timelike. This assumption allows us to define the *lapse function* α:

$$\frac{1}{\alpha^2} := -g^{-1}(\mathrm{d}t,\mathrm{d}t) > 0.$$

Note that at this moment we do not assume that the vector ∂_t is everywhere timelike, which is equivalent to

$$g_\Sigma(\beta,\beta) < \alpha^2. \tag{2-1}$$

This assumption will be forced on us later on by Assumption (1.b). The part of ∂_t orthogonal to the leaves of the foliation is the *shift vector*

$$\beta := \partial_t + \alpha^2 g^{-1}(\mathrm{d}t,\cdot).$$

The inverse metric can now be written as

$$g^{-1} = -\frac{1}{\alpha^2}(\partial_t-\beta)\otimes(\partial_t-\beta) + g_\Sigma^{-1}. \tag{2-2}$$

In coordinates, we have

$$\begin{aligned} g_{\mu\nu}\,\mathrm{d}x^\mu\,\mathrm{d}x^\nu &= -\alpha^2\,\mathrm{d}t^2 + g_{\Sigma,ij}(\mathrm{d}x^i+\beta^i\,\mathrm{d}t)(\mathrm{d}x^j+\beta^j\,\mathrm{d}t),\\ g^{\mu\nu}\partial_\mu\partial_\nu &= -\frac{1}{\alpha^2}(\partial_t-\beta^i\partial_i)^2 + g_\Sigma^{ij}\partial_i\partial_j. \end{aligned}$$

The generic notation for a point of M will be $(t,\vec{x})$. We often suppress the spatial dependence of objects defined on M; e.g., we identify $f(t)=f(t,\cdot)$ for some function f on M. Sometimes we also suppress the time-dependence, but it should be kept in mind that the central quantities considered here, the metric g, the electromagnetic potential A and the scalar potential Y, generically are time-dependent. Sometimes we denote derivatives with respect to t (i.e., the action of the vector field ∂_t) by a dot.

2.2. *Klein–Gordon operator.* The main object of our paper is the Klein–Gordon operator (1-2). Instead of the operator K on $L^2(M)$, it is more convenient to work with the operator

$$\widetilde{K} := \alpha K \alpha.$$

With the inverse metric expressed as (2-2), it can be written as

$$\begin{aligned}\widetilde{K} &= -\gamma^{-1/2}(D_t - D_i\beta^i + V)\gamma(D_t - \beta^j D_j + V)\gamma^{-1/2} + \gamma^{-1/2}(D_i - A_i)\alpha^2\gamma g_\Sigma^{ij}(D_j - A_j)\gamma^{-1/2} + \alpha^2 Y \\ &= -(D_t + W^*)(D_t + W) + L,\end{aligned}$$

where we introduce

$$\begin{aligned}\gamma &:= \alpha^{-2}|g|^{1/2} = \alpha^{-1}|g_\Sigma|^{1/2},\\ V &:= -A_0 + A_i\beta^i,\\ W &:= \beta^i D_i + V - \tfrac{1}{2}\gamma^{-1}(D_t\gamma - \beta^i D_i\gamma),\\ L &:= D_i^{A,\gamma\,*}\tilde{g}_\Sigma^{ij} D_j^{A,\gamma} + \widetilde{Y},\end{aligned}$$

and we use the shorthands

$$\begin{aligned}\tilde{g}_\Sigma^{ij}(t) &:= \alpha(t)^2 g_\Sigma^{ij}(t),\\ \widetilde{Y}(t) &:= \alpha(t)^2 Y(t),\\ D^{A,\gamma}(t) &:= \gamma(t)^{1/2}(D - A(t))\gamma(t)^{-1/2}.\end{aligned}$$

Clearly, propagators for $\widetilde{K}$ induce corresponding propagators for K.

2.3. *First-order formalism.* For each $t \in \mathbb{R}$, we (formally) define

$$B(t) := \begin{pmatrix} W(t) & \mathbb{1} \\ L(t) & W(t)^* \end{pmatrix}.$$

Setting $u_1(t) = u(t)$ and $u_2(t) = -(D_t + W(t))u(t)$, we find that

$$(\partial_t + \mathrm{i}B(t))\begin{pmatrix} u_1(t) \\ u_2(t) \end{pmatrix} = 0$$

if and only if u is a (weak) solution of the Klein–Gordon equation $\widetilde{K}u = 0$. Therefore we occasionally call $\partial_t + \mathrm{i}B(t)$ the *first-order Klein–Gordon operator*. The half-densities $u_1(t)$ and $u_2(t)$ may be called the *Cauchy data* for u at time t.

2.4. *Assumptions local in time.*

Assumption 1. We suppose that the following assumptions hold:

(1.a) For all $t \in \mathbb{R}$, $L(t)$ extends to a positive invertible self-adjoint operator on $L^2(\Omega^{1/2}\Sigma)$ (denoted by the same symbol).

(1.b) There exists $a \in C(\mathbb{R})$ such that $a(t) < 1$ and $\|W(t)L(t)^{-1/2}\| \le a(t)$.

(1.c) There exists a positive $C \in L^1_{\mathrm{loc}}(\mathbb{R})$ such that for all $|t-s| \le 1$

$$\|L(t)^{-1/2}(L(t) - L(s))L(t)^{-1/2}\| + 2\|(W(t) - W(s))L(t)^{-1/2}\| \le \left|\int_s^t C(r)\,\mathrm{d}r\right|, \tag{2-3}$$

where we place the absolute value on the right-hand side to account for the arbitrary order of t and s.

(1.d) $t \mapsto \alpha(t)^{\pm 1}$ are norm-continuous on $L(s)^{-1/2}L^2(\Omega^{1/2}\Sigma)$ for any $s \in \mathbb{R}$, and $t \mapsto \dot{\alpha}(t)$ is norm-continuous on $L^2(\Omega^{1/2}\Sigma)$.

A few remarks about these assumptions are in order:

First, Assumption (1.a) can always be realized if $\gamma(t)^{-1}\partial_i \gamma(t),\ A_i(t) \in L^2_{\mathrm{loc}}(\Sigma),\ \tilde{g}_{ij}(t) \in L^\infty_{\mathrm{loc}}(\Sigma)$ and $\widetilde{Y}(t) \in L^1_{\mathrm{loc}}(\Sigma)$ such that $\widetilde{Y}(t)$ is bounded from below by a positive constant. In that case $L(t)$ can be understood as the form

$$(u \mid L(t)\, v) = \int_\Sigma \big((\overline{D_i^{A,\gamma}(t)\, u})\, \tilde{g}^{ij}_\Sigma(t)\, (D_j^{A,\gamma}(t)\, v) + \bar{u}\, \widetilde{Y}(t)\, v \big),$$

on its (natural) maximal form domain $\operatorname{Dom} L(t)^{1/2} \supset C_c^\infty(\Omega^{1/2}\Sigma)$ (but it is not generally clear if $C_c^\infty(\Omega^{1/2}\Sigma)$ is a form core). This form then defines a self-adjoint operator in the usual way. The details of this construction are given in Appendix A; its main aspects can be found in [Kato 1966, Theorem VI.2.6].

Next, Assumption (1.b) means that $\|W(t)L(t)^{-1/2}\| < 1$. Thus the electrostatic potential $V(t)$ together with the variation of the metric expressed by $\gamma(t)^{-1}\dot{\gamma}(t)$ and the shift vector β cannot be too big compared to $L(t)$. This has to be true already on the level of the principal symbols of W and L. Therefore, for each $x = (t, \vec{x}) \in M$ and $p \in T^*_{\vec{x}}\Sigma_t$, we need to have

$$|\beta^k(x) p_k (\tilde{g}^{ij}_\Sigma(x) p_i p_j)^{-1/2}| < 1.$$

This is equivalent to

$$\tilde{g}_{\Sigma,ij}\beta^i\beta^j < 1, \tag{2-4}$$

where $\tilde{g}_{\Sigma,ij} = \alpha^{-2} g_{\Sigma,ij}$ is the inverse of $\tilde{g}^{ij}_\Sigma$, and consequently (2-4) is equivalent to (2-1). Thus Assumption (1.b) implies that ∂_t is timelike. This excludes, e.g., the ergosphere region of Kerr spacetime in stationary coordinates — in such a case one needs to switch to the nonstationary corotating coordinates.

Together, Assumptions (1.a) and (1.b) guarantee that the Hamiltonian is positive and has a positive lower bound (the "positive-mass assumption"). The positivity of the Hamiltonian and its positive lower bound have two aspects. First, they are essentially necessary if we want to construct nonclassical propagators. Second, this assumption helps us to introduce a natural family of Hilbertizable spaces, which are used in the analysis of the evolution. (A similar analysis would be possible with a positive Hamiltonian, but without a positive lower bound; however there would be some additional technical problems).

Nevertheless, as far as the derivation of the evolution and the classical propagators is concerned, Assumption (1.a) can be relaxed. In fact, for the existence of the evolution it is sufficient that there exists a constant $b > 0$ such that these assumptions are satisfied by $L(t) + b$; see also Corollary 5.5. In this case in general we do not have a positive Hamiltonian and our analysis of nonclassical propagators does not apply.

Among other things, Assumption (1.c) guarantees that for any t, s there exists $c(t, s) > 0$ such that

$$L(t) \le c(t, s) L(s). \tag{2-5}$$

Therefore, for $\delta \in [-1, 1]$ we can define the Hilbertizable spaces

$$\mathcal{K}^\delta := L(t)^{-\delta/2} L^2(\Omega^{1/2}\Sigma),$$

where the Hilbertian structures on the right-hand side are equivalent for different t because of (2-5).

Finally, Assumption (1.d) implies the norm-continuity of $t \mapsto \alpha(t)^{\pm 1}$ on $\mathcal{K}^\delta$ for $\delta \in [-1, 1]$. Indeed, by this assumption, $t \mapsto \alpha(t)^{\pm 1}$ are norm-continuous on $\mathcal{K}^{1/2}$, hence by duality also on $\mathcal{K}^{-1/2}$, and then we can interpolate using, e.g., the Heinz–Kato inequality (Theorem D.1).

While it should be obvious how Assumptions (1.a), (1.b) and (1.d) can be realized in an example, Assumption (1.c) is slightly less obvious. Therefore in Appendix B we briefly explain how Assumption (1.c) can follow from more concrete assumptions on the metric, the vector potential and the scalar potential.

2.5. ***Assumptions global in time.*** While we always require that Assumption 1 holds, the following additional assumptions are only imposed when we derive asymptotic properties of propagators.

Assumption 2. (2.a) $L(t)$ is uniformly bounded away from zero.

(2.b) There exists $a < 1$ such that $\|W(t)L(t)^{-1/2}\| \le a$ for all t.

(2.c) There exists a positive $C \in L^1(\mathbb{R})$ such that for all $t, s \in \mathbb{R}$

$$\|L(t)^{-1/2}(L(t) - L(s))L(t)^{-1/2}\| + 2\|(W(t) - W(s))L(t)^{-1/2}\| \le \left| \int_s^t C(r)\,\mathrm{d}r \right|,$$

where we place the absolute value on the right-hand side to account for the arbitrary order of t and s.

(2.d) $t \mapsto \alpha(t)^{\pm 1}$ are uniformly bounded on $\mathcal{K}^1$ and $t \mapsto \dot{\alpha}$ is uniformly bounded on $\mathcal{K}^0$.

Note that, by the same argument as for Assumption (1.d), one can show that Assumption (2.d) implies the uniform boundedness of $t \mapsto \alpha(t)^{\pm 1}$ on $\mathcal{K}^\delta$ for $\delta \in [-1, 1]$.

3. The energy space and the dynamical space

We will occasionally use the Hilbert space

$$\mathcal{H} := L^2(\Omega^{1/2}\Sigma) \oplus L^2(\Omega^{1/2}\Sigma) = \mathcal{K}^0 \oplus \mathcal{K}^0,$$

with the canonical inner product also denoted by $(\cdot \mid \cdot)$ and the corresponding norm $\|\cdot\|$.

The Hilbert space $\mathcal{H}$ plays only an auxiliary role in our work. More important are the Hilbertizable spaces $\mathcal{H}_\lambda$, $\lambda \in [-1, 1]$, defined as

$$\mathcal{H}_\lambda := \mathcal{K}^{(\lambda+1)/2} \oplus \mathcal{K}^{(\lambda-1)/2}. \tag{3-1}$$

Note that for any t

$$\mathcal{H}_\lambda = (L(t) \oplus L(t))^{-\lambda/4}\mathcal{H}_0, \quad \lambda \in [-1, 1]. \tag{3-2}$$

We will treat the space $\mathcal{H}_0$ as the central element of the family (3-2), identifying $\mathcal{H}_0$ with $\mathcal{H}_0^*$, the *antidual* of $\mathcal{H}_0$ (the space of bounded antilinear functionals on $\mathcal{H}_0$). Then we have a natural identification of $\mathcal{H}_{-\lambda}$ with $\mathcal{H}_\lambda^*$.

The central role in this work is played by the *energy space*, the *dynamical space* and the antidual of the energy space:

$$\mathcal{H}_{\mathrm{en}} := \mathcal{H}_1 = (L(t)^{-1/2} \oplus \mathbb{1})\mathcal{H} = H_0(t)^{-1/2}\mathcal{H}, \tag{3-3a}$$

$$\mathcal{H}_{\mathrm{dyn}} := \mathcal{H}_0 = (L(t)^{-1/4} \oplus L(t)^{1/4})\mathcal{H}, \tag{3-3b}$$

$$\mathcal{H}_{\mathrm{en}}^* := \mathcal{H}_{-1} = (\mathbb{1} \oplus L(t)^{1/2})\mathcal{H} = (QH_0(t)Q)^{1/2}\mathcal{H}, \tag{3-3c}$$

where we set

$$H_0(t) := L(t) \oplus \mathbb{1} = \begin{pmatrix} L(t) & 0 \\ 0 & \mathbb{1} \end{pmatrix},$$

and we also used the *charge form*

$$(u \mid Qv) := (u_1 \mid v_2) + (u_2 \mid v_1), \quad Q := \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}.$$

It is evident that the charge form is bounded on $\mathcal{H}$. More importantly, it is also bounded on $\mathcal{H}_{\mathrm{dyn}}$ (but, e.g., not on $\mathcal{H}_{\mathrm{en}}$).

Note that

$$\mathrm{Im}\,(u \mid Qv) = \frac{1}{2\mathrm{i}}((u \mid Qv) - (v \mid Qu))$$

is a symplectic form on $\mathcal{H}_{\mathrm{dyn}}$. Therefore, the formalism based on the charge form is equivalent to the symplectic formalism, commonly used in the literature.

4. Instantaneous energy spaces and instantaneous dynamical spaces

An important role in our paper is played by the instantaneous Hamiltonian, defined formally for each t as

$$H(t) = QB(t) = B(t)^* Q.$$

One can rigorously define $H(t)$ as a form-bounded perturbation of $H_0(t)$:

Proposition 4.1. *The operator*

$$H(t) := \begin{pmatrix} L(t) & W(t)^* \\ W(t) & \mathbb{1} \end{pmatrix}$$

is self-adjoint on $\mathcal{H}$ *with the form domain* $\mathcal{H}_{\mathrm{en}}$. *We have*

$$(1 - a(t)) H_0(t) \le H(t) \le (1 + a(t)) H_0(t), \tag{4-1}$$

where $0 \le a(t) < 1$ *was introduced in Assumption* (1.*b*).

Proof. We show only the right-hand side of the inequality (4-1). Set $u = \binom{u_1}{u_2}$. Using the Cauchy–Schwarz inequality and Assumption (1.b), we find

$$\begin{aligned} (u \mid H(t)\, u) &\le \|L(t)^{1/2} u_1\|^2 + \|u_2\|^2 + 2\|W(t)\, u_1\|\,\|u_2\| \\ &\le \|L(t)^{1/2} u_1\|^2 + \|u_2\|^2 + 2a(t)\|L(t)^{1/2} u_1\|\,\|u_2\| \\ &\le (1 + a(t))(\|L(t)^{1/2} u_1\|^2 + \|u_2\|^2) \\ &= (1 + a(t))(u \mid H_0(t)\, u). \end{aligned}$$ □

We define for each time $t \in \mathbb{R}$ the *(instantaneous) energy scalar products* given by

$$(u \mid v)_{\mathrm{en},t} := (u \mid H(t) v)$$

on $\mathcal{H}_{\mathrm{en}}$. By (4-1) the scalar product $(\cdot \mid \cdot)_{\mathrm{en},t}$ is compatible with the topology of $\mathcal{H}_{\mathrm{en}}$. We call the resulting Hilbert space the *instantaneous energy space at t* and denote it by $\mathcal{H}_{\mathrm{en},t}$.

Similarly, we can also define the operator $QH(t)^{-1}Q$. We find that its form domain is $\mathcal{H}_{\mathrm{en}}^*$. Indeed,

$$(1+a(t))^{-1}QH_0(t)^{-1}Q \le QH(t)^{-1}Q \le (1-a(t))^{-1}QH_0(t)^{-1}Q. \tag{4-2}$$

Then we define for each t the scalar product

$$(u \mid v)_{\mathrm{en}^*,t} := (u \mid QH(t)^{-1}Qv)$$

and note that it is compatible with the topology of $\mathcal{H}_{\mathrm{en}}^*$; we denote the resulting Hilbert space by $\mathcal{H}_{\mathrm{en},t}^*$.

The central operator in this work is $B(t)$. In the next section we construct the evolution generated by $B(t)$, solving the first-order Klein–Gordon equation.

Proposition 4.2. *Considered as an operator on* $\mathcal{H}_{\mathrm{en},t}^*$ *with domain* $\mathcal{H}_{\mathrm{en}}$,

$$B(t) := \begin{pmatrix} W(t) & \mathbb{1} \\ L(t) & W(t)^* \end{pmatrix}$$

is self-adjoint and 0 *is in its resolvent set.*

Proof. For notational simplicity, we drop the time-dependence of $B(t)$ and the other objects.

First note that, by definition, $H_0(t)^{-1/2} = (L(t)^{-1/2} \oplus \mathbb{1})$ maps $\mathcal{H}$ to $\mathcal{H}_{\mathrm{en}}$, and $(QH_0(t)Q)^{-1/2} = (\mathbb{1} \oplus L(t)^{-1/2})$ maps $\mathcal{H}_{\mathrm{en}}^*$ to $\mathcal{H}$. Now, to check that $B(t)$ is well-defined, we calculate

$$\begin{pmatrix} \mathbb{1} & 0 \\ 0 & L^{-1/2} \end{pmatrix} \begin{pmatrix} W & \mathbb{1} \\ L & W^* \end{pmatrix} \begin{pmatrix} L^{-1/2} & 0 \\ 0 & \mathbb{1} \end{pmatrix} = \begin{pmatrix} WL^{-1/2} & \mathbb{1} \\ \mathbb{1} & L^{-1/2}W^* \end{pmatrix},$$

which is bounded by Assumption (1.b).

Next, we show that $0 \in \operatorname{rs} B$, and consequently also that B is closed. We rewrite B as

$$B = \begin{pmatrix} \mathbb{1} & 0 \\ W^* & \mathbb{1} \end{pmatrix} \begin{pmatrix} 0 & \mathbb{1} \\ L - W^*W & 0 \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ W & \mathbb{1} \end{pmatrix}$$

and check that B^{-1} is bounded from $\mathcal{H}_{\mathrm{en}}^*$ to $\mathcal{H}_{\mathrm{en}}$:

$$\begin{pmatrix} L^{1/2} & 0 \\ 0 & \mathbb{1} \end{pmatrix} B^{-1} \begin{pmatrix} \mathbb{1} & 0 \\ 0 & L^{1/2} \end{pmatrix} = \begin{pmatrix} \mathbb{1} & 0 \\ -L^{-1/2}W^* & \mathbb{1} \end{pmatrix} \begin{pmatrix} 0 & (\mathbb{1} - L^{-1/2}W^*WL^{-1/2})^{-1} \\ \mathbb{1} & 0 \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ -WL^{-1/2} & \mathbb{1} \end{pmatrix},$$

where the first and last factors on the right-hand side are bounded by Assumption (1.b), and

$$\mathbb{1} - L^{-1/2}W^*WL^{-1/2}$$

is invertible because $\|L^{-1/2}W^*WL^{-1/2}\| < 1$, also by Assumption (1.b).

Finally, we check that B is Hermitian on $\mathcal{H}_{\mathrm{en}}^*$. We calculate

$$(QHQ)^{-1}B^{-1} = (BQHQ)^{-1} = (QHQHQ)^{-1} = (QHQB^*)^{-1} = B^{*-1}(QHQ)^{-1}. \qquad \square$$

We can now define for each time $t \in \mathbb{R}$ a whole scale of Hilbert spaces

$$\mathcal{H}_{\lambda,t} := |B(t)|^{-(1+\lambda)/2}\mathcal{H}_{\mathrm{en},t}^*, \quad \lambda \in \mathbb{R},$$

with scalar products

$$(u \mid v)_{\lambda,t} := (u \mid |B(t)|^{1+\lambda} v)_{\mathrm{en}^*,t}, \quad u, v \in \mathcal{H}_{\lambda,t}.$$

Above we performed the polar decomposition with respect to the Hilbert space $\mathcal{H}^*_{\mathrm{en},t}$, where we have

$$|B(t)| = \sqrt{B(t)^2} = \sqrt{QH(t)QH(t)}.$$

It follows from its definition, that $B(t)$ extends/restricts to a self-adjoint operator on each of the spaces $\mathcal{H}_{\lambda,t}$. When $B(t)$ is interpreted as an operator on $\mathcal{H}_{\lambda,t}$, its domain is $\mathcal{H}_{\lambda+2,t}$.

Clearly the scales $\mathcal{H}_{\lambda,t}$ contain $\mathcal{H}^*_{\mathrm{en},t} = \mathcal{H}_{-1,t}$. They also contain the (instantaneous) energy spaces $\mathcal{H}_{\mathrm{en},t} = \mathcal{H}_{1,t}$, because a short calculation shows $H(t) = QH(t)^{-1}Q|B(t)|^2$. Furthermore, we define the (*instantaneous*) *dynamical spaces*

$$\mathcal{H}_{\mathrm{dyn},t} := \mathcal{H}_{0,t},$$

which are treated as the central spaces in these scales. Note that $\mathcal{H}_{\mathrm{dyn},t}$ is the form domain of $B(t)$. We identify $\mathcal{H}^*_{0,t}$ with $\mathcal{H}_{0,t}$, and hence $\mathcal{H}^*_{\lambda,t}$ is identified with $\mathcal{H}_{-\lambda,t}$. Thus we obtain the rigged Hilbert space setting

$$\mathcal{H}_{\mathrm{en},t} \subset \mathcal{H}_{\mathrm{dyn},t} \subset \mathcal{H}^*_{\mathrm{en},t}.$$

Proposition 4.3. *In the sense of Hilbertizable spaces, we have*

$$\mathcal{H}_{\lambda,t} = \mathcal{H}_\lambda, \quad \lambda \in [-1, 1], \tag{4-3}$$

thus justifying our notation. In particular,

$$\mathcal{H}_{\mathrm{en},t} = \mathcal{H}_{\mathrm{en}}, \quad \mathcal{H}_{\mathrm{dyn},t} = \mathcal{H}_{\mathrm{dyn}}, \quad \mathcal{H}^*_{\mathrm{en},t} = \mathcal{H}^*_{\mathrm{en}}.$$

Proof. It follows from (4-1) and (4-2) that $\mathcal{H}_{\mathrm{en},t} = \mathcal{H}_{\mathrm{en}}$ and $\mathcal{H}^*_{\mathrm{en},t} = \mathcal{H}^*_{\mathrm{en}}$. Since both $L(t)^{1/2} \oplus L(t)^{1/2}$ and $|B|$ can be understood as invertible bounded operators from $\mathcal{H}_{\mathrm{en}}$ to $\mathcal{H}^*_{\mathrm{en}}$, there exists $c > 1$ such that

$$c^{-1}\|(L(t) \oplus L(t))^{1/2}u\|_{\mathrm{en}^*} \le \||B(t)|u\|_{\mathrm{en}^*} \le c\|(L(t) \oplus L(t))^{1/2}u\|_{\mathrm{en}^*}.$$

By interpolation (e.g., using the Heinz–Kato inequality, Theorem D.1),

$$c^{-\delta}\|(L(t) \oplus L(t))^{\delta/2}u\|_{\mathrm{en}^*} \le \||B(t)|^\delta u\|_{\mathrm{en}^*} \le c^\delta\|(L(t) \oplus L(t))^{\delta/2}u\|_{\mathrm{en}^*}$$

for $\delta \in [0, 1]$. It follows that the norms for $\mathcal{H}_\lambda$ and $\mathcal{H}_{\lambda,t}$ with $\lambda \in [-1, 1]$ are equivalent and thus (4-3) follows. □

Note that for $|\lambda| > 1$ the spaces $\mathcal{H}_{\lambda,t}$ may depend on t and do not have to coincide with $\mathcal{H}_\lambda$.

5. Evolution

In the last section we laid the foundations for an application of the theory of nonautonomous evolution equations to the situation at hand, i.e., the first-order Klein–Gordon equation

$$\partial_t u(t) + \mathrm{i}B(t)u(t) = 0.$$

Autonomous evolution equations (viz., with a time-independent generator) possess a well-understood theory in terms of the theory of strongly continuous semigroups and groups. The theory for nonautonomous evolution equations is significantly more complicated and subtle. In Appendix C we discuss the relevant results based on [Kato 1970].

Here we apply Theorem C.10 to the operator $B(t)$ on the spaces

$$\mathcal{X}_t = \mathcal{H}^*_{\mathrm{en},t} \quad \text{and} \quad \mathcal{Y}_t = \mathcal{H}_{\mathrm{en},t}. \tag{5-1}$$

For this purpose, we need to check whether the conditions (a)–(c) of Theorem C.10 hold. The self-adjointness condition (c) is clearly true; see Section 3. The next proposition implies that condition (b), a continuity condition on the norms of the Hilbert spaces $\mathcal{H}_{\mathrm{en},t}$ and $\mathcal{H}^*_{\mathrm{en},t}$, holds:

Proposition 5.1. *Let $C \in L^1_{\mathrm{loc}}(\mathbb{R})$ as in Assumption (1.c), $a(t) \in C(\mathbb{R})$ as in Assumption (1.b) and $|t-s| \le 1$ with $t \ge s$. Set*

$$c_{s,t} := \sup_{\tau\in[s,t]} (1-a(\tau))^{-1}.$$

Then, for $\lambda \in [-1, 1]$,

$$\|u\|_{\lambda,t} \exp\biggl(-c_{s,t}\int_s^t C(\tau)\,\mathrm{d}\tau\biggr) \le \|u\|_{\lambda,s} \le \|u\|_{\lambda,t} \exp\biggl(c_{s,t}\int_s^t C(\tau)\,\mathrm{d}\tau\biggr). \tag{5-2}$$

Proof. First we show (5-2) for $\lambda = 1$, i.e., for the energy space.

By Assumption (1.c), we have

$$\begin{aligned}\|(L(t)^{-1/2} \oplus \mathbb{1})&(H(s)-H(t))(L(t)^{-1/2} \oplus \mathbb{1})\| \\ &\le \|L(t)^{-1/2}(L(s)-L(t))L(t)^{-1/2}\| + 2\|(W(s)-W(t))L(t)^{-1/2}\| \\ &\le \int_s^t C(\tau)\,\mathrm{d}\tau. \end{aligned}\tag{5-3}$$

Equation (4-1) then implies

$$\|H(t)^{-1/2}(L(t)\oplus\mathbb{1})H(t)^{-1/2}\| \le c_{s,t}. \tag{5-4}$$

Putting together (5-3) and (5-4), we obtain

$$\|H(t)^{-1/2}(H(s)-H(t))H(t)^{-1/2}\| \le c_{s,t}\int_s^t C(\tau)\,\mathrm{d}\tau.$$

Consequently we have

$$\bigl|\|u\|^2_{\mathrm{en},s} - \|u\|^2_{\mathrm{en},t}\bigr| \le \|u\|^2_{\mathrm{en},t}\biggl(c_{s,t}\int_s^t C(\tau)\,\mathrm{d}\tau\biggr).$$

Therefore

$$\|u\|^2_{\mathrm{en},s} \le \|u\|^2_{\mathrm{en},t}\biggl(1 + c_{s,t}\int_s^t C(\tau)\,\mathrm{d}\tau\biggr) \le \|u\|^2_{\mathrm{en},t} \exp\biggl(c_{s,t}\int_s^t C(\tau)\,\mathrm{d}\tau\biggr)$$

and, exchanging the roles of t and s, we can similarly derive

$$\|u\|^2_{\mathrm{en},s} \ge \|u\|^2_{\mathrm{en},t} \exp\biggl(-c_{s,t}\int_s^t C(\tau)\,\mathrm{d}\tau\biggr),$$

so that the inequality (5-2) for $\lambda = 1$ follows.

For $\lambda = -1$ the inequality follows by duality. Using interpolation, we can then extend the inequality to the remaining values of λ. □

To show that condition (a) of Theorem C.10 holds, we only need to show the norm-continuity of $t \mapsto B(t)$; the remaining statements are obvious.

Proposition 5.2. *With $C \in L^1_{\mathrm{loc}}(\mathbb{R})$ as in Assumption (1.c), $c_{s,t}$ as in (4-1) and $|t-s| \le 1$,*

$$\|(B(s) - B(t))u\|_{\mathrm{en}^*,t} \le \|u\|_{\mathrm{en},t} \left| c_{s,t} \int_s^t C(\tau)\,\mathrm{d}\tau \right|,$$

where we place the absolute value on the right-hand side because $t \ge s$ or $t \le s$. In particular, $t \mapsto B(t)$ is norm-continuous as an operator from $\mathcal{H}_{\mathrm{en},t}$ to $\mathcal{H}^*_{\mathrm{en},t}$.

Proof. We reduce the problem to the inequalities

$$\begin{aligned}\|(\mathbb{1} \oplus L(t)^{-1/2})(B(s) - B(t))(L(t)^{-1/2} \oplus \mathbb{1})\| &= \|Q(L(t)^{-1/2} \oplus \mathbb{1})Q(B(s) - B(t))(L(t)^{-1/2} \oplus \mathbb{1})\| \\ &\le \|(L(t)^{-1/2} \oplus \mathbb{1})(H(s) - H(t))(L(t)^{-1/2} \oplus \mathbb{1})\| \\ &\le \left| \int_s^t C(\tau)\,\mathrm{d}\tau \right|\end{aligned}$$

and proceed much as in the proof of Proposition 5.1. Since the integral is continuous, the required norm-continuity follows. □

It follows that we can globally define an evolution for $B(t)$:

Theorem 5.3. *There exists a unique, strongly continuous family of bounded operators $\{U(t,s)\}_{s,t\in\mathbb{R}}$ on $\mathcal{H}^*_{\mathrm{en}}$, the* evolution generated by $B(t)$, *with the following properties:*

(i) *For all $r, s, t \in \mathbb{R}$, we have the identities*

$$U(t,t) = \mathbb{1}, \quad U(t,r)U(r,s) = U(t,s). \tag{5-5}$$

(ii) *For $\lambda \in [-1, 1]$, $U(t,s)\mathcal{H}_\lambda \subset \mathcal{H}_\lambda$, $(t,s) \mapsto U(t,s)$ is strongly $\mathcal{H}_\lambda$-continuous and satisfies the bounds*

$$\|U(t,r)\|_{\lambda,s} \le \exp\left(2c_{r,t} \int_r^t C(\tau)\,\mathrm{d}\tau\right), \tag{5-6a}$$

$$\|U(r,t)\|_{\lambda,s} \le \exp\left(2c_{r,t} \int_r^t C(\tau)\,\mathrm{d}\tau\right), \tag{5-6b}$$

with C, c as in Proposition 5.1 and $r \le s \le t$, where $|t-r| \le 1$.

(iii) *For all $u \in \mathcal{H}_{\mathrm{en}}$, $U(t,s)u$ is continuously differentiable in $s, t \in \mathbb{R}$ with respect to the strong topology of $\mathcal{H}^*_{\mathrm{en}}$ and it satisfies*

$$\mathrm{i}\partial_t U(t,s)u = B(t)U(t,s)u, \tag{5-7a}$$

$$-\mathrm{i}\partial_s U(t,s)u = U(t,s)B(s)u. \tag{5-7b}$$

Proof. Propositions 5.1 and 5.2 as well as the results of Section 3 show that Theorem C.10 can be applied to our operator $B(t)$, understood as an operator from $\mathcal{H}_{\mathrm{en}}$ to $\mathcal{H}_{\mathrm{en}}^*$ (or, equivalently, as a form on $\mathcal{H}_{\mathrm{dyn}}$ with form domain $\mathcal{H}_{\mathrm{en}}$). We thus obtain for every sufficiently small compact interval $I \subset \mathbb{R}$ an evolution $U(t,s)$ with the properties (i)–(iv) of Theorem C.10. In particular, we have for $r, t \in I$ and $r \le s \le t$

$$\|U(t,r)\|_{\mathrm{en},s} \le \exp\biggl(2c_{r,t}\int_r^t C(\tau)\,\mathrm{d}\tau\biggr),$$

$$\|U(t,r)\|_{\mathrm{en}^*,s} \le \exp\biggl(2c_{r,t}\int_r^t C(\tau)\,\mathrm{d}\tau\biggr).$$

The same bounds also hold for $\|U(r,t)\|_{\mathrm{en},s}$ and $\|U(r,t)\|_{\mathrm{en}^*,s}$. By interpolation we find (5-6).

We cover $\mathbb{R}$ by compact intervals. Using the identity (5-5), we thereby define the evolution $U(t,s)$ on the whole real axis by gluing. For finite s, t, it has the properties (i)–(iv) of Theorem C.10. □

Equation (5-6) states that $U(t,s)$ is bounded for finite t, s. To obtain stronger results later, we can choose more stringent assumptions:

Corollary 5.4. *If Assumption* (2.c) *holds, and we set* $C_1(t) := 2(1-a)^{-1}C(t)$, *then*

$$\|U(t,s)\|_{\lambda,r} \le \exp\biggl(\int_{\mathbb{R}} C_1(\tau)\,\mathrm{d}\tau\biggr)$$

for all $r, s, t \in \mathbb{R}$ *and any* $\lambda \in [-1, 1]$.

In Assumption (1.a) we supposed that $L(t)$ is positive and invertible. Actually, the main results of this section remain true if $L(t)$ is only bounded from below:

Corollary 5.5. *Instead of Assumption 1, suppose that there exists a constant* $b > 0$ *such that Assumption 1 holds for* $L(t)+b$. *Then Theorem 5.3 holds with respect to the scale of Hilbert spaces and constants obtained from* $L(t)+b$, *and with the bounds* (5-6) *replaced by*

$$\|U(t,r)\|_{\lambda,s} \le \exp\biggl(2c_{r,t}\int_r^t C(\tau)\,\mathrm{d}\tau + (t-r)b\|(L(s)+b)^{-1/2}\|\biggr),$$

$$\|U(r,t)\|_{\lambda,s} \le \exp\biggl(2c_{r,t}\int_r^t C(\tau)\,\mathrm{d}\tau + (t-r)b\|(L(s)+b)^{-1/2}\|\biggr).$$

Proof. Replacing $L(t)$ in $B(t)$ by $L(t)+b$, we obtain a new operator

$$B_b(t) = B(t) + \begin{pmatrix} 0 & 0 \\ b & 0 \end{pmatrix}.$$

We also replace $L(t)$ by $L(t)+b$ in all definitions concerning the Hilbert and Hilbertizable spaces that we need. According to Theorem 5.3, $B_b(t)$ has an evolution $U_b(t,s)$ with the properties stated in the theorem. Note that $\left(\begin{smallmatrix} 0 & 0 \\ b & 0 \end{smallmatrix}\right)$ is a bounded operator on $\mathcal{H}_{\mathrm{en}}^*$. Indeed, this follows from the boundedness of

$$\begin{pmatrix} \mathbb{1} & 0 \\ 0 & L^{-1/2} \end{pmatrix}\begin{pmatrix} 0 & 0 \\ b & 0 \end{pmatrix}\begin{pmatrix} \mathbb{1} & 0 \\ 0 & L^{1/2} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ L^{-1/2}b & 0 \end{pmatrix}$$

on $\mathcal{H}$. Since $B(t)$ is a bounded perturbation of $B_b(t)$, we can apply Theorem C.11 to find the evolution for $B(t)$. □

Remark 5.6. Our choice of spaces (5-1) to prove Theorem 5.3 is natural, especially given our low-regularity setup. Under more restrictive assumptions on the smoothness and boundedness of coefficients of the Klein–Gordon operator K, other spaces in the scale $\mathcal{H}_{\lambda,t}$, $\lambda \in \mathbb{R}$, could be used. This would lead to improved regularity results of the type $U(t,s)\mathcal{H}_\lambda \subset \mathcal{H}_\lambda$ and continuous differentiability of $U(t,s)\mathcal{H}_\lambda$ in $\mathcal{H}_{\lambda-2}$.

Remark 5.7. In the stationary case, i.e., if B does not depend on time, there exist distinguished Hilbert spaces $\mathcal{H}_\lambda$ and the evolution family $U(t,s)$ simplifies to a unitary group $U(t-s) = U(t,s)$ on $\mathcal{H}_\lambda$.

6. Solutions of the Klein–Gordon equation

Solutions of the Klein–Gordon equation are closely related to solutions of the first-order Klein–Gordon equation.

Let us introduce the projection onto the second component:

$$\pi_2 \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} := u_2.$$

We also define embeddings

$$\iota_2 u := \begin{pmatrix} 0 \\ u \end{pmatrix}, \quad \rho u := \begin{pmatrix} u \\ -(D_t + W)u \end{pmatrix}.$$

A formal calculation then shows that[2]

$$\widetilde{K} = -\mathrm{i}\pi_2(\partial_t + \mathrm{i}B)\rho \quad \text{and} \quad K = -\mathrm{i}\alpha^{-1}\pi_2(\partial_t + \mathrm{i}B)\rho\alpha^{-1}. \tag{6-1}$$

Therefore, if $Ku = f$ or, equivalently, $\widetilde{K}\tilde{u} = \tilde{f}$ with $\tilde{u} = \alpha^{-1}u$, $\tilde{f} = \alpha f$, then

$$-\mathrm{i}(\partial_t + \mathrm{i}B)\rho\tilde{u} = \iota_2\tilde{f}.$$

The projection π_2 and the embeddings ρ, ι_2, which relate solutions of the Klein–Gordon equation and the first-order Klein–Gordon equation, can be understood between various spaces. It follows from the definition of $\mathcal{H}_\lambda$ in (3-1) that, for $\lambda \in [-1, 1]$,

$$\pi_2 : \mathcal{H}_\lambda \to \mathcal{K}^{(\lambda-1)/2}, \tag{6-2a}$$

$$\pi_2 Q : \mathcal{H}_\lambda \to \mathcal{K}^{(\lambda+1)/2}, \tag{6-2b}$$

$$\iota_2 : \mathcal{K}^{(\lambda-1)/2} \to \mathcal{H}_\lambda. \tag{6-2c}$$

These projections and embeddings already allow us to easily prove an existence and uniqueness result regarding solutions of the Klein–Gordon equation with Cauchy data in the energy space:

Theorem 6.1. *Let* $s \in \mathbb{R}$, $\binom{u_1(s)}{u_2(s)} \in \mathcal{H}_{\mathrm{en}}$ *and* $f \in L^1_{\mathrm{loc}}(\mathbb{R}; \mathcal{K}^0)$. *Set*

$$\begin{pmatrix} \tilde{u}_1(s) \\ \tilde{u}_2(s) \end{pmatrix} = \alpha(s)^{-1} \begin{pmatrix} u_1(s) \\ u_2(s) \end{pmatrix} \quad \textit{and} \quad \tilde{f} = \alpha f.$$

[2]Note that there is a sign error in the corresponding equation in [Dereziński and Siemssen 2018] which also affects the definition of the associated propagators.

Then $u = \alpha\tilde{u}$, *with*

$$\tilde{u}(t) = \pi_2 Q U(t,s)\begin{pmatrix}\tilde{u}_1(s)\\ \tilde{u}_2(s)\end{pmatrix} + \mathrm{i}\int_s^t \pi_2 Q U(t,r)\iota_2 \tilde{f}(r)\,\mathrm{d}r,$$

is the unique solution of $Ku = f$ *such that*

$$u \in C(\mathbb{R};\mathcal{K}^1)\cap C^1(\mathbb{R};\mathcal{K}^0) \quad \textit{and} \quad \rho\tilde{u}(s) = \begin{pmatrix}\tilde{u}_1(s)\\ \tilde{u}_2(s)\end{pmatrix}. \tag{6-3}$$

Proof. We have the following special cases of (6-2):

$$\iota_2 : \mathcal{K}^0 \to \mathcal{H}_{\mathrm{en}}, \tag{6-4a}$$

$$\pi_2 Q : \mathcal{H}_{\mathrm{en}} \to \mathcal{K}^1, \tag{6-4b}$$

$$\pi_2 Q : \mathcal{H}_{\mathrm{en}}^* \to \mathcal{K}^0. \tag{6-4c}$$

By (6-4a), (6-4b) and Assumption (1.d), u belongs to $C(\mathbb{R};\mathcal{K}^1)$. By (6-4a), (6-4c) and Assumption (1.d), $\partial_t u$ belongs to $C(\mathbb{R};\mathcal{K}^0)$. Hence the first part of (6-3) is true. The second part of (6-3) is obvious.

Set

$$\begin{pmatrix}\tilde{u}_1(t)\\ \tilde{u}_2(t)\end{pmatrix} = U(t,s)\begin{pmatrix}\tilde{u}_1(s)\\ \tilde{u}_2(s)\end{pmatrix} + \mathrm{i}\int_s^t U(t,r)\iota_2\tilde{f}(r)\,\mathrm{d}r. \tag{6-5}$$

Differentiating (6-5) we obtain

$$\mathrm{i}\partial_t\begin{pmatrix}\tilde{u}_1(t)\\ \tilde{u}_2(t)\end{pmatrix} = B(t)\begin{pmatrix}\tilde{u}_1(t)\\ \tilde{u}_2(t)\end{pmatrix} - \iota_2\tilde{f}(t). \tag{6-6}$$

Clearly, $\tilde{u}(t) = \tilde{u}_1(t)$. The first component of (6-6) yields $\tilde{u}_2(t) = -(D_t + W(t))\tilde{u}_1(t)$. Hence

$$\rho\tilde{u}(t) = \begin{pmatrix}\tilde{u}_1(t)\\ \tilde{u}_2(t)\end{pmatrix}. \tag{6-7}$$

The second component of (6-6) and then insertion of (6-7) yield

$$\tilde{f}(t) = -\mathrm{i}\pi_2(\partial_t + \mathrm{i}B)\begin{pmatrix}\tilde{u}_1(t)\\ \tilde{u}_2(t)\end{pmatrix} = -\mathrm{i}\pi_2(\partial_t + \mathrm{i}B)\rho\tilde{u}(t) = \widetilde{K}\tilde{u}(t),$$

whence we have shown that $\tilde{u}$ solves $\widetilde{K}\tilde{u} = \tilde{f}$ and thus $Ku = f$.

Uniqueness of the solution follows from the uniqueness of the evolution $U(t,s)$, and the linearity of K, ρ by the standard argument: if u, u' satisfy

$$Ku = Ku' = f \quad \text{and} \quad \rho\tilde{u}(s) = \rho\tilde{u}'(s) = \begin{pmatrix}\tilde{u}_1(s)\\ \tilde{u}_2(s)\end{pmatrix},$$

where $\tilde{u}' = \alpha^{-1}u'$, then $K(u-u') = 0$, $\rho(\tilde{u}-\tilde{u}')(s) = 0$ and thus $u = u'$. □

It is well known that solutions of the Klein–Gordon equation propagate slower than the speed of light. The method of evolution equations together with the freedom of the choice of the time-variable provide a rather obvious heuristic argument for the propagation at a finite speed. However, when one tries to convert this argument into a rigorous proof, technical problems appear which make such a proof difficult to formulate.

In the literature the finiteness of the speed of propagation is usually shown for the Klein–Gordon equation with smooth coefficients. In Appendix E, in particular in Theorem E.1, we show that solutions of the Klein–Gordon propagate at a finite speed also in a low-regularity setup typical for our paper.

7. Classical propagators

Having constructed the evolution for $B(t)$ in Section 5, it is not difficult to find the classical propagators for the first-order Klein–Gordon operator $\partial_t + \mathrm{i}B$. To wit, the *Pauli–Jordan propagator* E^{PJ} and the *forward/backward propagator* $E^{\vee/\wedge}$ are given by the integral kernels

$$E^{\mathrm{PJ}}(t,s) := U(t,s), \tag{7-1a}$$

$$E^{\vee}(t,s) := \theta(t-s)\,U(t,s), \tag{7-1b}$$

$$E^{\wedge}(t,s) := -\theta(s-t)\,U(t,s), \tag{7-1c}$$

where θ denotes the Heaviside step function, via

$$(E^{\bullet} f)(t) = \int_{\mathbb{R}} E^{\bullet}(t,s) f(s)\,\mathrm{d}s. \tag{7-2}$$

Theorem 7.1. *Let* $\lambda \in [-1, 1]$:

(i) *The classical propagators* E^{PJ} *and* $E^{\vee/\wedge}$ *are well-defined between the spaces*

$$E^{\bullet} : L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{H}_\lambda) \to C(\mathbb{R}; \mathcal{H}_\lambda),$$
$$E^{\bullet} : L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{H}_{\mathrm{en}}) \to C^1(\mathbb{R}; \mathcal{H}^*_{\mathrm{en}}).$$

(ii) *The forward and backward propagators* $E^{\vee/\wedge}$ *are well-defined between the spaces*

$$E^{\vee/\wedge} : L^1_{\mathrm{loc}}(I; \mathcal{H}_\lambda) \to C(I; \mathcal{H}_\lambda),$$
$$E^{\vee/\wedge} : L^1_{\mathrm{loc}}(I; \mathcal{H}_{\mathrm{en}}) \to C^1(I; \mathcal{H}^*_{\mathrm{en}}),$$

where $I = [a, +\infty[$ *or* $]-\infty, a]$, *respectively*, *for some* $a \in \mathbb{R}$.

(iii) *If Assumption 2 is satisfied*, *the classical propagators* E^{PJ} *and* $E^{\vee/\wedge}$ *are bounded between the spaces*

$$E^{\bullet} : L^1(\mathbb{R}; \mathcal{H}_\lambda) \to C_{\mathrm{b}}(\mathbb{R}; \mathcal{H}_\lambda),$$
$$E^{\bullet} : L^1(\mathbb{R}; \mathcal{H}_{\mathrm{en}}) \to C^1_{\mathrm{b}}(\mathbb{R}; \mathcal{H}^*_{\mathrm{en}}).$$

(iv) E^{PJ} *is a bisolution of* $\partial_t + \mathrm{i}B$:

$$(\partial_t + \mathrm{i}B) E^{\mathrm{PJ}} f = 0, \qquad f \in L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{H}_{\mathrm{en}}), \tag{7-3}$$

$$E^{\mathrm{PJ}}(\partial_t + \mathrm{i}B) f = 0, \qquad f \in L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{H}_{\mathrm{en}}) \cap \mathrm{AC}_{\mathrm{c}}(\mathbb{R}; \mathcal{H}^*_{\mathrm{en}}). \tag{7-4}$$

(v) *$E^{\vee/\wedge}$ are the unique inverses of $\partial_t + \mathrm{i}B$ such that*

$$(\partial_t + \mathrm{i}B)E^{\vee/\wedge} f = f, \quad f \in L^1_{\mathrm{loc}}(I, \mathcal{H}_{\mathrm{en}}), \tag{7-5}$$

$$E^{\vee/\wedge}(\partial_t + \mathrm{i}B) f = f, \quad f \in L^1_{\mathrm{loc}}(I; \mathcal{H}_{\mathrm{en}}) \cap \mathrm{AC}(I, \mathcal{H}^*_{\mathrm{en}}), \tag{7-6}$$

with $I = [a, +\infty[$ or $]-\infty, a]$, respectively, for some $a \in \mathbb{R}$.

(vi) *The relation $E^{\mathrm{PJ}} = E^{\vee} - E^{\wedge}$ holds.*

Proof. Parts (i)–(iii) follow from the properties of the evolution $U(t, s)$ (see Theorem 5.3 and Corollary 5.4) and the definition of the kernels (7-1).

Consider next (iv) and (v). We first need to check that the products contained in these properties are well-defined. Indeed, by (i), the maps

$$E^{\bullet} : L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{H}_{\mathrm{en}}) \to C(\mathbb{R}; \mathcal{H}_{\mathrm{en}}) \cap C^1(\mathbb{R}; \mathcal{H}^*_{\mathrm{en}}), \tag{7-7a}$$

$$(\partial_t + \mathrm{i}B) : C(\mathbb{R}; \mathcal{H}_{\mathrm{en}}) \cap C^1(\mathbb{R}; \mathcal{H}^*_{\mathrm{en}}) \to C(\mathbb{R}; \mathcal{H}^*_{\mathrm{en}}), \tag{7-7b}$$

are well-defined, which shows that (7-3) and (7-5) make sense. Similarly, by (i), we have

$$(\partial_t + \mathrm{i}B) : L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{H}_{\mathrm{en}}) \cap \mathrm{AC}_{\mathrm{c}}(\mathbb{R}; \mathcal{H}^*_{\mathrm{en}}) \to L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{H}^*_{\mathrm{en}}), \tag{7-8a}$$

$$E^{\bullet} : L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{H}^*_{\mathrm{en}}) \to C(\mathbb{R}; \mathcal{H}^*_{\mathrm{en}}), \tag{7-8b}$$

and hence the products in (7-4) and (7-6) make sense. Then we show (7-3)–(7-6) using (7-2) and (5-7). For (7-4) and (7-6) we also need to apply an integration by parts. □

We can also state an L^2 version of Theorem 7.1(iii):

Theorem 7.2. *Let $s > \frac{1}{2}$ and $\lambda \in [-1, 1]$. If Assumption 2 is satisfied, the classical propagators E^{PJ} and $E^{\vee/\wedge}$ are bounded between the spaces*

$$E^{\bullet} : \langle t\rangle^{-s} L^2(\mathbb{R}; \mathcal{H}_{\lambda}) \to \langle t\rangle^{s} L^2(\mathbb{R}; \mathcal{H}_{\lambda}),$$
$$E^{\bullet} : \langle t\rangle^{-s} L^2(\mathbb{R}; \mathcal{H}_{\mathrm{en}}) \to \langle t\rangle^{s} \langle \partial_t\rangle^{-1} L^2(\mathbb{R}; \mathcal{H}^*_{\mathrm{en}}).$$

Proof. We use the embeddings

$$\langle t\rangle^{-s} L^2(\mathbb{R}; \mathcal{X}) \subset L^1(\mathbb{R}; \mathcal{X}) \quad \text{and} \quad \langle t\rangle^{s} L^2(\mathbb{R}; \mathcal{X}) \supset C_{\mathrm{b}}(\mathbb{R}; \mathcal{X})$$

for any Banach space $\mathcal{X}$ and $s > \frac{1}{2}$. □

The classical propagators for the first-order Klein–Gordon operator can also be understood between various spaces other than those considered in Theorems 7.1 and 7.2, but our choices are quite natural. At the same time, this setup leads to an almost straightforward derivation of the propagators for the Klein–Gordon operator K.

Since $\partial_t + \mathrm{i}B$ and K are related via (6-1), also the propagators of these operators are closely related. At least formally, it can be shown that if $E^{\bullet}$ is a propagator for $\partial_t + \mathrm{i}B$, then $\mathrm{i}\pi_2 Q E^{\bullet}\iota_2$ is a propagator for $\widetilde{K}$, and hence

$$G^{\bullet} = \mathrm{i}\alpha\pi_2 Q E^{\bullet}\iota_2\alpha \tag{7-9}$$

is a propagator for the Klein–Gordon operator K. As we shall see now, this is indeed true if the domain of $G^\bullet$ is carefully chosen:

Theorem 7.3. *Let* $\delta \in [0, 1]$:

(i) *The classical propagators* G^{PJ} *and* $G^{\vee/\wedge}$ *are well-defined between the spaces*

$$G^\bullet : L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^{-\delta}) \to C(\mathbb{R}; \mathcal{K}^{1-\delta}), \tag{7-10}$$

$$G^\bullet : L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^{0}) \to C^1(\mathbb{R}; \mathcal{K}^{0}). \tag{7-11}$$

(ii) *The forward and backward propagators* $G^{\vee/\wedge}$ *are well-defined between the spaces*

$$G^{\vee/\wedge} : L^1_{\mathrm{loc}}(I; \mathcal{K}^{-\delta}) \to C(I; \mathcal{K}^{1-\delta}),$$
$$G^{\vee/\wedge} : L^1_{\mathrm{loc}}(I; \mathcal{K}^{0}) \to C^1(I; \mathcal{K}^{0}),$$

where $I = [a, +\infty[$ *or* $]-\infty, a]$, *respectively*, *for some* $a \in \mathbb{R}$.

(iii) *If Assumption 2 is satisfied*, *the classical propagators* G^{PJ} *and* $G^{\vee/\wedge}$ *are bounded between the spaces*

$$G^\bullet : L^1(\mathbb{R}; \mathcal{K}^{-\delta}) \to C_{\mathrm{b}}(\mathbb{R}; \mathcal{K}^{1-\delta}),$$
$$G^\bullet : L^1(\mathbb{R}; \mathcal{K}^{0}) \to C^1_{\mathrm{b}}(\mathbb{R}; \mathcal{K}^{0}).$$

(iv) G^{PJ} *is a bisolution of* K:

$$K G^{\mathrm{PJ}} f = 0, \quad f \in L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^0), \tag{7-12}$$

$$G^{\mathrm{PJ}} K f = 0, \quad f \in L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^1) \cap \mathrm{AC}_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^0) \cap \mathrm{AC}^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^{-1}). \tag{7-13}$$

(v) $G^{\vee/\wedge}$ *are the unique inverses of* K *such that*

$$K G^{\vee/\wedge} f = f, \quad f \in L^1_{\mathrm{loc}}(I; \mathcal{K}^0), \tag{7-14}$$

$$G^{\vee/\wedge} K f = f, \quad f \in L^1_{\mathrm{loc}}(I; \mathcal{K}^1) \cap \mathrm{AC}(\mathbb{R}; \mathcal{K}^0) \cap \mathrm{AC}^1(I; \mathcal{K}^{-1}), \tag{7-15}$$

with $I = [a, +\infty[$ *or* $]-\infty, a]$, *respectively*, *for some* $a \in \mathbb{R}$.

(vi) *The relation* $G^{\mathrm{PJ}} = G^\vee - G^\wedge$ *holds.*

Proof. These results are a direct consequence of Theorem 7.1. In (i)–(iii) we used (6-2) and Assumption (1.d).

Let us check that the products in (iv) and (v) are well-defined. From the definition of ρ we can read off that

$$\rho : C(\mathbb{R}; \mathcal{K}^1) \cap C^1(\mathbb{R}; \mathcal{K}^0) \to C(\mathbb{R}; \mathcal{H}_{\mathrm{en}}),$$
$$\rho : L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^1) \cap \mathrm{AC}_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^0) \to L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{H}_{\mathrm{en}}),$$
$$\rho : \mathrm{AC}_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^0) \cap \mathrm{AC}^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^{-1}) \to \mathrm{AC}_{\mathrm{c}}(\mathbb{R}; \mathcal{H}^*_{\mathrm{en}}).$$

Then, by (i) and also using (7-7), we have

$$G^\bullet : L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^0) \to C(\mathbb{R}; \mathcal{K}^1) \cap C^1(\mathbb{R}; \mathcal{K}^0),$$
$$K : C(\mathbb{R}; \mathcal{K}^1) \cap C^1(\mathbb{R}; \mathcal{K}^0) \to C^{-1}(\mathbb{R}; \mathcal{K}^0) \cap C(\mathbb{R}; \mathcal{K}^{-1}),$$

where $C^{-1}(\mathbb{R})$ denotes the space of distributional derivatives of continuous functions. This shows that (7-12) and (7-14) make sense. Similarly, by (i) and (7-8), we have

$$K : L^1_c(\mathbb{R}; \mathcal{K}^1) \cap \mathrm{AC}_c(\mathbb{R}; \mathcal{K}^0) \cap \mathrm{AC}^1_c(\mathbb{R}; \mathcal{K}^{-1}) \to L^1_c(\mathbb{R}; \mathcal{K}^{-1}),$$
$$G^\bullet : L^1_c(\mathbb{R}; \mathcal{K}^{-1}) \to C(\mathbb{R}; \mathcal{K}^0),$$

and hence the products in (7-13) and (7-15) make sense. □

Here is an L^2 version of Theorem 7.3(iii):

Theorem 7.4. *Let $s > \frac{1}{2}$. If Assumption 2 is satisfied, the classical propagators G^{PJ} and $G^{\vee/\wedge}$ are bounded between the spaces*

$$G^\bullet : \langle t\rangle^{-s} L^2(\Omega^{1/2}M) \to \langle t\rangle^{s} L(t)^{-1/2} L^2(\Omega^{1/2}M), \tag{7-16a}$$
$$G^\bullet : \langle t\rangle^{-s} L^2(\Omega^{1/2}M) \to \langle t\rangle^{s} \langle \partial_t\rangle^{-1} L^2(\Omega^{1/2}M). \tag{7-16b}$$

Proof. By (7-10), for $\delta \in [0, 1]$ we have

$$G^\bullet : \langle t\rangle^{-s} L^2(\mathbb{R}; \mathcal{K}^{-\delta}) \to \langle t\rangle^{s} L^2(\mathbb{R}; \mathcal{K}^{1-\delta}). \tag{7-17}$$

Setting $\delta = 0$ we obtain

$$G^\bullet : \langle t\rangle^{-s} L^2(\mathbb{R}; \mathcal{K}^0) \to \langle t\rangle^{s} L(t)^{-1/2} L^2(\mathbb{R}; \mathcal{K}^0). \tag{7-18}$$

But $L^2(\mathbb{R}; \mathcal{K}^0) = L^2(\mathbb{R}; L^2(\Omega^{1/2}\Sigma))$ and $L^2(\Omega^{1/2}M)$ can naturally be identified, which proves (7-16a).

It follows from (7-11) that

$$G^\bullet : \langle t\rangle^{-s} L^2(\mathbb{R}; \mathcal{K}^0) \to \langle t\rangle^{s} \langle \partial_t\rangle^{-1} L^2(\mathbb{R}; \mathcal{K}^0).$$

This yields (7-16b). □

Observe that in other approaches, e.g., [Bär et al. 2007], the retarded and advanced propagators are the central objects and the Pauli–Jordan propagator is defined as their difference. Here, instead, the Pauli–Jordan propagator follows immediately from the evolution $U(t, s)$ and should be seen as the central object, while the retarded and advanced propagators are derived objects.

Using the Pauli–Jordan propagator G^{PJ}, we can associate to every sufficiently regular compactly supported function a solution of the homogeneous Klein–Gordon equation. In fact, as the following proposition shows, also the converse is true.

Proposition 7.5. *Suppose that $u \in L^1_{\mathrm{loc}}(\mathbb{R}; \mathcal{K}^1) \cap \mathrm{AC}(\mathbb{R}; \mathcal{K}) \cap \mathrm{AC}^1(\mathbb{R}; \mathcal{K}^{-1})$ satisfies $Ku = 0$. Then there exists a (nonunique) $f \in L^1_c(\mathbb{R}; \mathcal{K}^{-1})$ such that $u = G^{\mathrm{PJ}} f$.*

Proof. Choose any $r, s \in \mathbb{R}$, $r < s$, and $\chi \in C^\infty(M)$ such that $\chi(t) = 0$ for $t < r$, $0 \le \chi(t) \le 1$ for $r \le t \le s$ and $\chi(t) = 1$ for $t > s$. Clearly,

$$0 = Ku = K\chi u - K(\chi - 1)u$$

and thus $\mathrm{supp}(K\chi u) \subset [r, s] \times \Sigma$. Besides, $K\chi u \in L^1_c(\mathbb{R}; \mathcal{K}^{-1})$. Therefore, we can act with G^{PJ} on $K\chi u$, obtaining

$$G^{\mathrm{PJ}} K\chi u = G^\vee K\chi u - G^\wedge K(\chi - 1)u = u.$$

That is, $f = K\chi u$ is the desired function. □

Our construction of the classical propagators starts from the propagators for the first-order Klein–Gordon operator; i.e., given $E^\bullet$, we derive $G^\bullet$ using (7-9). If, instead, $G^\bullet$ is provided, then $E^\bullet$ can be derived:

(i) If $G^\bullet$ is an inverse of K then
$$E^\bullet = -\mathrm{i}\begin{pmatrix} -\alpha^{-1}G^\bullet\alpha^{-1}(D_t+W^*) & \alpha^{-1}G^\bullet\alpha^{-1} \\ \mathbb{1}+(D_t+W)\alpha^{-1}G^\bullet\alpha^{-1}(D_t+W^*) & -(D_t+W)\alpha^{-1}G^\bullet\alpha^{-1}\end{pmatrix}$$
is (formally) an inverse of $(\partial_t + \mathrm{i}B)$.

(ii) If $G^\bullet$ is a bisolution of K then
$$E^\bullet = -\mathrm{i}\begin{pmatrix} -\alpha^{-1}G^\bullet\alpha^{-1}(D_t+W^*) & \alpha^{-1}G^\bullet\alpha^{-1} \\ (D_t+W)\alpha^{-1}G^\bullet\alpha^{-1}(D_t+W^*) & -(D_t+W)\alpha^{-1}G^\bullet\alpha^{-1}\end{pmatrix}$$
is (formally) a bisolution of $(\partial_t + \mathrm{i}B)$.

Note the subtle difference in the formulas for inverses and bisolutions. No such difference appears in (7-9), which yields $G^\bullet$ given $E^\bullet$.

8. Instantaneous nonclassical propagators

Consider an arbitrary reference time τ. According to Proposition 4.2, $B(\tau)$ is a self-adjoint operator on $\mathcal{H}^*_{\mathrm{en},\tau}$. Therefore we can use the functional calculus to define the projections onto the positive and negative parts of the spectrum of $B(\tau)$:
$$\Pi^{(\pm)}_\tau := \mathbb{1}_{[0,\infty[}(\pm B(\tau)). \tag{8-1}$$

Zero is in the resolvent set of $B(\tau)$, and therefore the projections in (8-1) are complementary.

Proposition 8.1. $\Pi^{(\pm)}_\tau$ *restrict to complementary projections on* $\mathcal{H}_\lambda$ *for* $\lambda \in [-1, 1]$, *and have the following properties*:

(i) $\Pi^{(\pm)}_\tau B(\tau) = B(\tau)\Pi^{(\pm)}_\tau$.

(ii) $\Pi^{(+)}_\tau - \Pi^{(-)}_\tau = \operatorname{sgn} B(\tau)$.

(iii) $\operatorname{sp}(\pm\Pi^{(\pm)}_\tau B(\tau)) \subset\,]0, \infty[$.

(iv) $\Pi^{(\pm)}_\tau$ *are self-adjoint with respect to* $\mathcal{H}_{\lambda,\tau}$.

Moreover, the projections $\Pi^{(\pm)}_\tau$ split $\mathcal{H}_{\lambda,\tau}$ into subspaces of positive and negative charge (with respect to the charge form Q):

Proposition 8.2.
$$\pm(u \mid Q\Pi^{(\pm)}_\tau u) = \pm(\Pi^{(\pm)}_\tau u \mid Qu) = \pm(\Pi^{(\pm)}_\tau u \mid Q\Pi^{(\pm)}_\tau u) \geq 0 \tag{8-2}$$
for all $u \in \mathcal{H}_\lambda$ *with* $\lambda \in [-1, 1]$.

Proof. The proof is the same as that of [Dereziński and Siemssen 2018, Proposition 6.3]. □

The projections $\Pi_\tau^{(\pm)}$ can be used to define *instantaneous positive/negative-frequency bisolutions* $E_\tau^{(\pm)}$, given by their integral kernels as

$$E_\tau^{(\pm)}(t,s) := \pm U(t,\tau)\Pi_\tau^{(\pm)}U(\tau,s). \tag{8-3}$$

Using step functions, we then define the kernels of the *instantaneous Feynman and anti-Feynman inverses of* $\partial_t + \mathrm{i}B$:

$$\begin{aligned} E_\tau^{\mathrm{F}}(t,s) &:= \theta(t-s)E_\tau^{(+)}(t,s) + \theta(s-t)E_\tau^{(-)}(t,s), \\ E_\tau^{\bar{\mathrm{F}}}(t,s) &:= -\theta(t-s)E_\tau^{(-)}(t,s) - \theta(s-t)E_\tau^{(+)}(t,s). \end{aligned}$$

It is easy to see that these kernels can also be expressed using the retarded and advanced propagators:

$$E_\tau^{\mathrm{F}}(t,s) = E^{\wedge}(t,s) + E_\tau^{(+)}(t,s) = E^{\vee}(t,s) + E_\tau^{(-)}(t,s), \tag{8-4a}$$

$$E_\tau^{\bar{\mathrm{F}}}(t,s) = E^{\vee}(t,s) - E_\tau^{(+)}(t,s) = E^{\wedge}(t,s) - E_\tau^{(-)}(t,s). \tag{8-4b}$$

As before, these kernels define the corresponding propagators via (7-2):

Theorem 8.3. *Let* $\lambda \in [-1, 1]$:

(i) *The instantaneous nonclassical propagators* $E_\tau^{(\pm)}$ *and* $E_\tau^{\mathrm{F}/\bar{\mathrm{F}}}$ *are well-defined between the spaces*

$$\begin{aligned} E_\tau^\bullet &: L_\mathrm{c}^1(\mathbb{R};\mathcal{H}_\lambda) \to C(\mathbb{R};\mathcal{H}_\lambda), \\ E_\tau^\bullet &: L_\mathrm{c}^1(\mathbb{R};\mathcal{H}_\mathrm{en}) \to C^1(\mathbb{R};\mathcal{H}_\mathrm{en}^*). \end{aligned}$$

(ii) *If Assumption 2 is satisfied,* $E_\tau^{(\pm)}$ *and* $E_\tau^{\mathrm{F}/\bar{\mathrm{F}}}$ *are bounded between the spaces*

$$\begin{aligned} E_\tau^\bullet &: L^1(\mathbb{R};\mathcal{H}_\lambda) \to C_\mathrm{b}(\mathbb{R};\mathcal{H}_\lambda), \\ E_\tau^\bullet &: L^1(\mathbb{R};\mathcal{H}_\mathrm{en}) \to C_\mathrm{b}^1(\mathbb{R};\mathcal{H}_\mathrm{en}^*). \end{aligned}$$

(iii) $E_\tau^{(\pm)}$ *are bisolutions of* $\partial_t + \mathrm{i}B$:

$$\begin{aligned} (\partial_t + \mathrm{i}B)E_\tau^{(\pm)}f &= 0, \quad f \in L_\mathrm{c}^1(\mathbb{R};\mathcal{H}_\mathrm{en}), \\ E_\tau^{(\pm)}(\partial_t + \mathrm{i}B)f &= 0, \quad f \in L_\mathrm{c}^1(\mathbb{R};\mathcal{H}_\mathrm{en}) \cap \mathrm{AC}_\mathrm{c}(\mathbb{R};\mathcal{H}_\mathrm{en}^*). \end{aligned}$$

(iv) $E_\tau^{\mathrm{F}/\bar{\mathrm{F}}}$ *are inverses of* $\partial_t + \mathrm{i}B$:

$$\begin{aligned} (\partial_t + \mathrm{i}B)E_\tau^{\mathrm{F}/\bar{\mathrm{F}}}f &= f, \quad f \in L_\mathrm{c}^1(\mathbb{R};\mathcal{H}_\mathrm{en}), \\ E_\tau^{\mathrm{F}/\bar{\mathrm{F}}}(\partial_t + \mathrm{i}B)f &= f, \quad f \in L_\mathrm{c}^1(\mathbb{R};\mathcal{H}_\mathrm{en}) \cap \mathrm{AC}_\mathrm{c}(\mathbb{R};\mathcal{H}_\mathrm{en}^*). \end{aligned}$$

(v) *The instantaneous nonclassical propagators satisfy the relations*

$$\begin{aligned} &E_\tau^{\mathrm{F}} = E^{\wedge} + E_\tau^{(+)} = E^{\vee} + E_\tau^{(-)}, \qquad E_\tau^{\mathrm{F}} + E_\tau^{\bar{\mathrm{F}}} = E^{\vee} + E^{\wedge}, \qquad E_\tau^{(+)} - E_\tau^{(-)} = E^{\mathrm{PJ}}, \\ &E_\tau^{\bar{\mathrm{F}}} = E^{\vee} - E_\tau^{(+)} = E^{\wedge} - E_\tau^{(-)}, \qquad E_\tau^{\mathrm{F}} - E_\tau^{\bar{\mathrm{F}}} = E_\tau^{(+)} + E_\tau^{(-)}. \end{aligned}$$

Proof. The various properties of the nonclassical propagators can be shown along the same lines as in Theorem 7.1 so we will omit the proofs. Property (v) in particular follows from (8-4) and its linear combinations. □

As for the classical propagators, we can also find an L^2 version of Theorem 8.3(ii):

Theorem 8.4. *Let $s>\frac{1}{2}$ and $\lambda \in [-1,1]$. If Assumption 2 is satisfied, the instantaneous nonclassical propagators $E_\tau^{(\pm)}$ and $E_\tau^{\mathrm{F}/\bar{\mathrm{F}}}$ are bounded between the spaces*

$$E_\tau^\bullet : \langle t\rangle^{-s} L^2(\mathbb{R}; \mathcal{H}_\lambda) \to \langle t\rangle^{s} L^2(\mathbb{R}; \mathcal{H}_\lambda),$$
$$E_\tau^\bullet : \langle t\rangle^{-s} L^2(\mathbb{R}; \mathcal{H}_{\mathrm{en}}) \to \langle t\rangle^{s} \langle \partial_t\rangle^{-1} L^2(\mathbb{R}; \mathcal{H}_{\mathrm{en}}^*).$$

Similarly to (7-9), we define the instantaneous nonclassical propagators $G_\tau^{(\pm)}$ and $G_\tau^{\mathrm{F}/\bar{\mathrm{F}}}$ for the Klein–Gordon operator K by

$$G_\tau^{(\pm)} := \alpha\pi_2 Q E_\tau^{(\pm)} \iota_2\alpha, \qquad G_\tau^{\mathrm{F}/\bar{\mathrm{F}}} := \mathrm{i}\alpha\pi_2 Q E_\tau^{\mathrm{F}/\bar{\mathrm{F}}} \iota_2\alpha.$$

Note the absence of the complex unit in the definition of $G_\tau^{(\pm)}$ so that $G_\tau^{(\pm)}$ define positive forms; see property (vi) below.

Analogously to Theorem 7.3, we find:

Theorem 8.5. *Let $\delta \in [-1,1]$:*

(i) *The instantaneous nonclassical propagators $G_\tau^{(\pm)}$ and $G_\tau^{\mathrm{F}/\bar{\mathrm{F}}}$ are well-defined between the spaces*

$$G_\tau^\bullet : L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^{-\delta}) \to C(\mathbb{R}; \mathcal{K}^{1-\delta}),$$
$$G_\tau^\bullet : L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^{0}) \to C^1(\mathbb{R}; \mathcal{K}^{0}).$$

(ii) *If Assumption 2 is satisfied, $G_\tau^{(\pm)}$ and $G_\tau^{\mathrm{F}/\bar{\mathrm{F}}}$ are bounded between the spaces*

$$G_\tau^\bullet : L^1(\mathbb{R}; \mathcal{K}^{-\delta}) \to C_{\mathrm{b}}(\mathbb{R}; \mathcal{K}^{1-\delta}),$$
$$G_\tau^\bullet : L^1(\mathbb{R}; \mathcal{K}^{0}) \to C^1_{\mathrm{b}}(\mathbb{R}; \mathcal{K}^{0}).$$

(iii) *$G_\tau^{(\pm)}$ are bisolutions of K:*

$$K G_\tau^{(\pm)} f = 0, \qquad f \in L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^0),$$
$$G_\tau^{(\pm)} K f = 0, \qquad f \in L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^1) \cap \mathrm{AC}_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^0) \cap \mathrm{AC}^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^{-1}).$$

(iv) *$G_\tau^{\mathrm{F}/\bar{\mathrm{F}}}$ are inverses of K:*

$$K G_\tau^{\mathrm{F}/\bar{\mathrm{F}}} f = f, \qquad f \in L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^0),$$
$$G_\tau^{\mathrm{F}/\bar{\mathrm{F}}} K f = f, \qquad f \in L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^1) \cap \mathrm{AC}_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^0) \cap \mathrm{AC}^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^{-1}).$$

(v) *The instantaneous nonclassical propagators satisfy the relations:*

$$G_\tau^{\mathrm{F}} = G^\wedge + \mathrm{i}G_\tau^{(+)} = G^\vee + \mathrm{i}G_\tau^{(-)}, \qquad G_\tau^{\mathrm{F}} + G_\tau^{\bar{\mathrm{F}}} = G^\vee + G^\wedge, \qquad G_\tau^{(+)} - G_\tau^{(-)} = -\mathrm{i}G^{\mathrm{PJ}},$$
$$G_\tau^{\bar{\mathrm{F}}} = G^\vee - \mathrm{i}G_\tau^{(+)} = G^\wedge - \mathrm{i}G_\tau^{(-)}, \qquad G_\tau^{\mathrm{F}} - G_\tau^{\bar{\mathrm{F}}} = \mathrm{i}G_\tau^{(+)} + \mathrm{i}G_\tau^{(-)}.$$

(vi) *The instantaneous positive/negative-frequency bisolutions are positive:*

$$(f \mid G_\tau^{(\pm)} f) = \int_M \bar{f}\, G_\tau^{(\pm)} f \geq 0$$

for $f \in L^1_{\mathrm{c}}(\mathbb{R}; \mathcal{K}^0)$.

Proof. We only show (vi); the remaining properties follow from corresponding properties of $E_\tau^\bullet$ in Theorem 8.3 and can be shown as in Theorem 7.3. For (vi), we note that

$$\begin{aligned}(f \mid G_\tau^{(\pm)} f) &= \iint (\iota_2 \tilde{f}(t) \mid Q E_\tau^{(\pm)}(t,s)\iota_2 \tilde{f}(s))\, \mathrm{d}s\, \mathrm{d}t \\ &= (\tilde{u}(\tau) \mid Q\Pi_\tau^{(\pm)} \tilde{u}(\tau)) \geq 0\end{aligned}$$

by Proposition 8.2, where we set

$$\tilde{f} = \alpha f \quad \text{and} \quad \tilde{u}(\tau) = \int U(\tau,t)\tilde{f}(t)\, \mathrm{d}t \in \mathcal{H}_{\mathrm{en}}. \qquad \square$$

The L^2 version of Theorem 8.5(ii) is:

Theorem 8.6. *Let $s > \frac{1}{2}$. If Assumption 2 is satisfied, the instantaneous nonclassical propagators $G_\tau^{(\pm)}$ and $G_\tau^{\mathrm{F}/\bar{\mathrm{F}}}$ are bounded between the spaces*

$$\begin{aligned}G_\tau^\bullet &: \langle t\rangle^{-s} L^2(\Omega^{1/2}M) \to \langle t\rangle^{s} L(t)^{-1/2} L^2(\Omega^{1/2}M), \\ G_\tau^\bullet &: \langle t\rangle^{-s} L^2(\Omega^{1/2}M) \to \langle t\rangle^{s} \langle \partial_t\rangle^{-1} L^2(\Omega^{1/2}M).\end{aligned}$$

In the static case, the nonclassical propagators defined above do not depend on τ. They are the natural propagators to consider in that situation; see also our earlier work [Dereziński and Siemssen 2018].

In the nonstatic case, however, the instantaneous nonclassical propagators just defined have deficiencies from the physical point of view; see, e.g., [Fulling 1979]. First of all, their definition hinges on the arbitrary choice of a fixed instance of time and, even more seriously, on the choice of a time function. Secondly, instantaneous positive-frequency bisolutions usually do not satisfy the microlocal spectrum condition of [Radzikowski 1996] (in other words, they do not define Hadamard states).

Nevertheless, the situation improves if the Klein–Gordon operator is infinitesimally static at the time when the positive/negative-frequency splitting is performed. In a forthcoming article we will show (using methods of evolution equations) that the corresponding instantaneous positive-frequency bisolutions, which we define in the following section, satisfy then the microlocal spectrum condition of [Radzikowski 1996].

9. Asymptotic nonclassical propagators

Throughout this section we assume that Assumption 2 is satisfied. It follows, in particular, that $B(t)$ converges to $B(\pm\infty)$ as $t \to \pm\infty$ in norm as an operator from $\mathcal{H}_{\mathrm{en}}$ to $\mathcal{H}_{\mathrm{en}}^*$. We define the *out/in-positive/negative-frequency projections*

$$\begin{aligned}\Pi_+^{(\pm)} &:= \mathbb{1}_{[0,\infty[}(\pm B(+\infty)), \\ \Pi_-^{(\pm)} &:= \mathbb{1}_{[0,\infty[}(\pm B(-\infty)).\end{aligned}$$

Theorem 9.1. *The strong limits*

$$\Pi_+^{(\pm)}(t) := \operatorname*{s-lim}_{\tau\to+\infty} U(t,\tau)\Pi_+^{(\pm)} U(\tau,t), \tag{9-1a}$$

$$\Pi_-^{(\pm)}(t) := \operatorname*{s-lim}_{\tau\to-\infty} U(t,\tau)\Pi_-^{(\pm)} U(\tau,t) \tag{9-1b}$$

exist as bounded operators on $\mathcal{H}_\lambda$ with $\lambda \in [-1, 1]$. They satisfy the obvious analogs of Propositions 8.1 and 8.2. Additionally,

$$U(s,t)\Pi_+^{(\pm)}(t)U(t,s) = \Pi_+^{(\pm)}(s), \tag{9-2}$$

$$U(s,t)\Pi_-^{(\pm)}(t)U(t,s) = \Pi_-^{(\pm)}(s). \tag{9-3}$$

Proof. We only prove the theorem for (9-1a) because the proof for (9-1b) is the same. We have

$$U(t,r)\Pi_+^{(\pm)}U(r,t) = U(t,r)\mathrm{e}^{\mathrm{i}(t-r)B(+\infty)}\Pi_+^{(\pm)}\mathrm{e}^{\mathrm{i}(r-t)B(+\infty)}U(r,t).$$

We analyze separately the limit $r \to +\infty$ of the operators left and right of the projection. Since both operators are bounded on $\mathcal{H}_{\lambda,\tau}$, $\lambda \in [-1, 1]$, uniformly in t, r for arbitrary $\tau \in \mathbb{R}$, it is sufficient to show the convergence on $\mathcal{H}_{\mathrm{en}}$ with respect to the norm on $\mathcal{H}^*_{\mathrm{en},\tau}$.

We may assume that $r > t$. For $u \in \mathcal{H}_{\mathrm{en}}$ we have

$$\begin{aligned} U(t,r)\mathrm{e}^{\mathrm{i}(t-r)B(+\infty)}u &= u + \int_t^r \partial_s(U(t,s)\mathrm{e}^{\mathrm{i}(t-s)B(+\infty)})u\,\mathrm{d}s \\ &= u - \mathrm{i}\int_t^r U(t,s)(B(s)-B(+\infty))\mathrm{e}^{\mathrm{i}(t-s)B(+\infty)}u\,\mathrm{d}s, \end{aligned}$$

by the fundamental theorem of calculus and Theorem 5.3(iii). Taking the norm of this expression in $\mathcal{H}^*_{\mathrm{en},\tau}$, we find

$$\|U(t,r)\mathrm{e}^{\mathrm{i}(t-r)B(+\infty)}u - u\|_{\mathrm{en}^*,\tau} \le C\|u\|_{\mathrm{en},\tau}\int_t^r \big\|(\mathbb{1}\oplus L(\tau)^{-1/2})(B(s)-B(+\infty))(L(\tau)^{-1/2}\oplus\mathbb{1})\big\|\,\mathrm{d}s,$$

since $U(t,s)$ is uniformly bounded on $\mathcal{H}^*_{\mathrm{en},\tau}$.

It follows from the proof of Proposition 5.2 that

$$\|(\mathbb{1}\oplus L(\tau)^{-1/2})(B(s)-B(+\infty))(L(\tau)^{-1/2}\oplus\mathbb{1})\|$$

is uniformly bounded. Therefore,

$$\|U(t,r)\mathrm{e}^{\mathrm{i}(t-r)B(+\infty)}u - u\|_{\mathrm{en}^*,\tau} \to 0$$

as $t, r \to +\infty$ and the desired convergence follows.

The proof for $U(t,r)\mathrm{e}^{\mathrm{i}(t-r)B(+\infty)}$ is essentially the same. The main difference is that we use the uniform boundedness of $U(t,s)$ on $\mathcal{H}_{\mathrm{en},\tau}$. □

We also define

$$E_+^{(\pm)}(t,s) := \pm U(t,\tau)\Pi_+^{(\pm)}(\tau)U(\tau,s), \tag{9-4}$$

$$E_-^{(\pm)}(t,s) := \pm U(t,\tau)\Pi_-^{(\pm)}(\tau)U(\tau,s). \tag{9-5}$$

Clearly, the definitions above do not depend on τ.

The kernels $E_\pm^{(\pm)}(t,s)$ yield the *positive/negative-frequency bisolutions at future* and *past infinity*. They are often called *out* and *in*, or jointly *asymptotic*. Moreover, we may use them together with the advanced and retarded propagators to define corresponding *asymptotic Feynman* and *anti-Feynman propagators*:

$$E_{\pm}^{\mathrm{F}} = E^{\wedge} + E_{\pm}^{(+)} = E^{\vee} + E_{\pm}^{(-)},$$
$$E_{\pm}^{\bar{\mathrm{F}}} = E^{\vee} - E_{\pm}^{(+)} = E^{\wedge} - E_{\pm}^{(-)}.$$

As before, the propagators $E_{\pm}^{\bullet}$ for $\partial_t + \mathrm{i}B$ induce the corresponding propagators $G_{\pm}^{\bullet}$ for K. Obviously, the asymptotic nonclassical propagators defined here have analogs to Theorems 8.3 and 8.5; we only have to replace occurrences of τ with $\pm$.

The asymptotic propagators defined above have various advantages over the instantaneous ones of the previous section. For one, they do not depend on an arbitrarily chosen instant of time. Under rather broad assumptions one can show that they even do not depend on the choice of the time function, but only on the spacetime itself. Finally, as recently discussed in [Gérard and Wrochna 2017], if the spacetime becomes asymptotically static sufficiently fast, they satisfy the microlocal spectrum condition of [Radzikowski 1996].

Appendix A: Second-order differential operators

Consider a manifold Σ. Every second-order Hermitian differential operator on $L^2(\Omega^{1/2}\Sigma)$ can locally be written as

$$L = D_i g^{ij}(x) D_j - A^i(x) D_i - D_i A^i(x) + Y_0(x), \tag{A-1}$$

where $g^{ij} = g^{ji}$, Y_0 and A^i are real-valued.

L can be often rewritten in the form

$$L = (D_i - A_i) g^{ij} (D_j - A_j) + Y_1. \tag{A-2}$$

This is possible in particular if g^{ij} is everywhere nondegenerate, viz., g determines a (pseudo-)Riemannian structure on M. Then (A-2) holds with

$$A_i := g_{ij} A^j, \quad Y_1 := Y_0 - A^i g_{ij} A^j,$$

where g_{ij} denotes the inverse of g^{ij}.

Let γ be an everywhere nonzero function. Then the operator L can be rewritten as

$$L = \gamma^{-1/2} (D_i - A_i) \gamma g^{ij} (D_j - A_j) \gamma^{-1/2} + Y_\gamma, \tag{A-3}$$

where

$$Y_\gamma := Y - \tfrac{1}{2}(D_i g^{ij} \gamma^{-1} (D_j \gamma)) - \tfrac{1}{4} g^{ij} \gamma^{-2} (D_i \gamma)(D_j \gamma).$$

In particular, if we set $\gamma := |g|^{1/2}$, where $|g| := |\det[g_{ij}]|$ is the canonical density induced by the metric, and $Y := Y_{|g|^{1/2}}$, then (A-3) yields the geometric form of the operator L:

$$L = |g|^{-1/4} (D_i - A_i) |g|^{1/2} g^{ij} (D_j - A_j) |g|^{-1/4} + Y. \tag{A-4}$$

If g is a metric tensor, A a 1-form, and Y a scalar, then the right-hand side of (A-4) transforms covariantly and L is well-defined as a differential operator acting on half-densities. We can rewrite (A-4) using the

Levi-Civita derivative ∇ for g as

$$L = g^{ij}(\mathrm{i}\nabla_i + A_i)(\mathrm{i}\nabla_j + A_j) + Y. \tag{A-5}$$

Note that in (A-5) the right ∇ acts on half-densities and the left ∇ acts on half-densitized covectors.

If the metric is Riemannian, the differential part of the operator (A-4) can be called a (*magnetic*) *Laplace–Beltrami operator*, and the full operator can be called a (*magnetic*) *Schrödinger operator*. If the metric is Lorentzian, the differential part of the operator (A-4) can be called an (*electromagnetic*) *d'Alembertian*, and the full operator can be called an (*electromagnetic*) *Klein–Gordon operator*.

It is however sometimes convenient to consider a density γ independent of the metric tensor g, i.e., to work with (A-3) instead of (A-4). Using the derivative

$$D^{A,\gamma} := \gamma^{1/2}(D - A)\gamma^{-1/2}, \tag{A-6}$$

L can be written as a quadratic form on half-densities:

$$(u \mid Lv) = \int_\Sigma ((\overline{D_i^{A,\gamma} u}) g^{ij} (D_j^{A,\gamma} v) + \bar{u}\, Y_\gamma\, v). \tag{A-7}$$

Assumption 3. In the remaining part of this appendix we assume that g is a Riemannian metric. We also assume that $\gamma^{-1}\partial_i\gamma,\ A_i \in L^2_{\mathrm{loc}}(\Sigma),\ g^{ij} \in L^\infty_{\mathrm{loc}}(\Sigma)$ and $Y_\gamma \in L^1_{\mathrm{loc}}(\Sigma)$ such that $Y_\gamma \geq C$ for some $C \in \mathbb{R}$.

We will see that under the above assumption L can be understood as a self-adjoint operator on $L^2(\Omega^{1/2}\Sigma)$ in at least two natural ways. First we reinterpret (A-7) by introducing the form

$$l_{\mathrm{mx}}[u, v] = \int_\Sigma ((\overline{D_i^{A,\gamma} u}) g^{ij} (D_j^{A,\gamma} v) + \bar{u}\, Y_\gamma\, v) \tag{A-8}$$

on its maximal form domain

$$\operatorname{dom} l_{\mathrm{mx}} = \{u \in L^2(\Omega^{1/2}\Sigma) \mid D^{A,\gamma}u \in L^2(\Omega^{1/2}T^*\Sigma, g),\ Y_\gamma^{1/2}u \in L^2(\Omega^{1/2}\Sigma)\}.$$

Here we denote by $L^2(\Omega^{1/2}T^*\Sigma, g)$ the completion of $C_{\mathrm{c}}^\infty(\Omega^{1/2}T^*\Sigma)$ with respect to the norm given by

$$u \mapsto \left(\int_\Sigma \bar{u}_i\, g^{ij} u_j\right)^{1/2}.$$

We remark that $C_{\mathrm{c}}^\infty(\Omega^{1/2}\Sigma) \subset \operatorname{dom} l_{\mathrm{mx}}$.

The following is a standard proof and has been adapted from [Leinfelder and Simader 1981, Lemma 1].

Lemma A.1. *The form l_{mx} is closed and Hermitian. It defines a unique self-adjoint operator L_{mx} on*

$$\operatorname{Dom} L_{\mathrm{mx}} = \{v \in \operatorname{dom} l_{\mathrm{mx}} \mid |l_{\mathrm{mx}}[u, v]| \leq C_v\|u\| \text{ for all } u \in L^2(\Omega^{1/2}\Sigma)\}$$

satisfying

$$(u \mid L_{\mathrm{mx}}v) = l_{\mathrm{mx}}[u, v]$$

for $u \in \operatorname{dom} l_{\mathrm{mx}}$ and $v \in \operatorname{Dom} L_{\mathrm{mx}}$. Moreover, $\operatorname{dom} l_{\mathrm{mx}} = \operatorname{Dom} L_{\mathrm{mx}}^{1/2}$.

Proof. Suppose that $\{u_n\} \subset \operatorname{dom} l_{\mathrm{mx}}$ is a Cauchy sequence with respect to the norm

$$\operatorname{dom} l_{\mathrm{mx}} \ni u \mapsto (l_{\mathrm{mx}}[u, u] + (1 - C)\|u\|^2)^{1/2}.$$

Then there exist $u, v \in L^2(\Omega^{1/2}\Sigma)$ and $w \in L^2(\Omega^{1/2}T^*\Sigma, g)$ such that

$$u_n \to u, \quad Y_\gamma^{1/2} u_n \to v \quad \text{in } L^2(\Omega^{1/2}\Sigma)$$

and

$$D^{A,\gamma} u_n \to w \quad \text{in } L^2(\Omega^{1/2}T^*\Sigma, g).$$

Moreover, $Y_\gamma^{1/2} u_n \to Y_\gamma^{1/2} u$ and $D^{A,\gamma} u_n \to D^{A,\gamma} u$ weakly, and thus $v = Y_\gamma^{1/2} u$ and $w = D^{A,\gamma} u$ because v, w must coincide with the weak limits. It follows that l_{mx} is a closed form (and manifestly Hermitian). Therefore, by the first representation theorem [Kato 1966, Theorem VI.2.6], l_{mx} defines a unique self-adjoint operator with the stated properties. □

An alternative to l_{mx} is the form l_{mn} given by the completion of the form (A-8) on $C_c^\infty(\Omega^{1/2}\Sigma)$, and the corresponding operator L_{mn}. l_{mn} may have a strictly smaller domain than l_{mx} because of boundary effects. If $l_{\mathrm{mn}} = l_{\mathrm{mx}}$, then $C_c^\infty(\Omega^{1/2}\Sigma)$ is a core of l_{mx}. Note that for $\Sigma = \mathbb{R}^3$ with the Euclidean metric this is known to be true; see, e.g., [Leinfelder and Simader 1981].

Certainly the setting considered in this appendix is not the most general possible. For example, the assumption that Y is bounded from below can certainly be relaxed.

Appendix B: Concrete assumptions

The objective of this appendix is to elucidate how Assumption (1.c) may be realized in practice. Recall that $(\Sigma, \tilde{g}_\Sigma(t))$ is a family of Riemannian manifolds, $\gamma(t) > 0$ are densities on Σ, $A(t)$ are real-valued 1-forms and $\widetilde{Y}(t)$ are real-valued scalar potentials. For simplicity, we write $\tilde{g}$ for $\tilde{g}_\Sigma$. As in Assumption 3 in Appendix A, we assume that $\gamma^{-1}(t)\partial_i\gamma(t),\ A_i(t) \in L^2_{\mathrm{loc}}(\Sigma),\ \tilde{g}^{ij} \in L^\infty_{\mathrm{loc}}(\Sigma)$, and $\widetilde{Y} \in L^1_{\mathrm{loc}}(\Sigma)$ is bounded from below.

Let us recall the definition of the operators $W(t)$ and $L(t)$ on $L^2(\Omega^{1/2}\Sigma)$:

$$W(t) := \beta(t)^i D_i + V(t) - \tfrac{1}{2}\gamma(t)^{-1}(D_t\gamma(t) - \beta(t)^i D_i\gamma(t)),$$

$$(u \mid L(t)\, v) := \int_\Sigma \big(\overline{(D_i^{A,\gamma}(t)\, u)}\, \tilde{g}^{ij}(t)\, (D_j^{A,\gamma}(t)\, v) + \bar{u}\, \widetilde{Y}(t)\, v\big), \tag{B-1}$$

where $L(t)$ is interpreted, say, as the maximal operator given by (B-1), as in Appendix A. Assumption (1.c) now says that there exists a positive $C \in L^1_{\mathrm{loc}}(\mathbb{R})$ such that for all $|t - s| \le 1$

$$\|L(t)^{-1/2}(L(t) - L(s))L(t)^{-1/2}\| + 2\|(W(t) - W(s))L(t)^{-1/2}\| \le \left|\int_s^t C(r)\, \mathrm{d}r\right| \tag{B-2}$$

for some $C \in L^1_{\mathrm{loc}}(\mathbb{R})$.

We also introduce the family of norms

$$\|X\|_t = \left(\int_\Sigma \tilde{g}^{ij}(t)\, \overline{X}_i X_j\right)^{1/2}$$

for half-densitized 1-forms X on Σ.

Proposition B.1. *Suppose that there are positive $C_Y, C_g, C_W \in L^1_{\mathrm{loc}}(\mathbb{R})$, $C_A, C_\gamma \in L^2_{\mathrm{loc}}(\mathbb{R})$ such that for all $|t-s| \le 1$*

$$\begin{aligned} \|L(t)^{-1/2}\partial_s \widetilde{Y}(s) L(t)^{-1/2}\| &\le C_Y(s), \\ \|\partial_s W(s) L(t)^{-1/2}\| &\le C_W(s), \\ \|\partial_s A(s) L(t)^{-1/2}\|_t &\le C_A(s), \\ \|\partial_s \gamma(s)^{-1}\,\mathrm{d}\gamma(s) L(t)^{-1/2}\|_t &\le C_\gamma(s), \\ |\partial_s \tilde{g}^{ij}(s) X_i X_j| &\le C_g(s)\tilde{g}^{ij}(t) X_i X_j, \qquad X \in C(T^*\Sigma). \end{aligned}$$

Then (B-2) *holds and thus Assumption* (1.*c*) *is true.*

Proof. To avoid notational clutter within this proof, we simply write D_i for $D_i^{A,\gamma}$. Clearly, the assumptions of the proposition imply

$$\|L(t)^{-1/2}(\widetilde{Y}(t) - \widetilde{Y}(s))L(t)^{-1/2}\| \le \left|\int_s^t C_Y(r)\,\mathrm{d}r\right|, \tag{B-3a}$$

$$\|(W(t) - W(s))L(t)^{-1/2}\| \le \left|\int_s^t C_W(r)\,\mathrm{d}r\right|, \tag{B-3b}$$

$$\|(A(t) - A(s))L(t)^{-1/2}\|_t \le \left|\int_s^t C_A(r)\,\mathrm{d}r\right|, \tag{B-3c}$$

$$\|(\gamma(t)^{-1}\,\mathrm{d}\gamma(t) - \gamma(s)^{-1}\,\mathrm{d}\gamma(s))L(t)^{-1/2}\|_t \le \left|\int_s^t C_\gamma(r)\,\mathrm{d}r\right|, \tag{B-3d}$$

$$|\tilde{g}^{ij}(t) X_i X_j - \tilde{g}^{ij}(s) X_i X_j| \le \left|\int_s^t C_g(r)\,\mathrm{d}r\right| \tilde{g}^{ij}(t) X_i X_j. \tag{B-3e}$$

We compute

$$\begin{aligned} &(u \mid (L(t) - L(s))u) \\ &\quad = \int_\Sigma \tilde{g}^{ij}(t)\big((\overline{D_i(t)u})(D_j(t)u - D_j(s)u) + (\overline{D_i(t)u - D_i(s)u})(D_j(t)u) \\ &\qquad\qquad - (\overline{D_i(t)u - D_i(s)u})(D_j(t)u - D_j(s)u)\big) \\ &\qquad + \int_\Sigma (\tilde{g}^{ij}(t) - \tilde{g}^{ij}(s))\big((\overline{D_i(t)u})(D_j(t)u) - (\overline{D_i(t)u})(D_j(t)u - D_j(s)u) \\ &\qquad\qquad - (\overline{D_i(t)u - D_i(s)u})(D_j(t)u) + (\overline{D_i(t)u - D_i(s)u})(D_j(t)u - D_j(s)u)\big) \\ &\qquad + \int_\Sigma (\widetilde{Y}(t) - \widetilde{Y}(s))|u|^2, \end{aligned}$$

where

$$D_i(t) - D_i(s) = -A_i(t) + A_i(s) + \frac{\mathrm{i}}{2}\gamma(t)^{-1}\partial_i\gamma(t) - \frac{\mathrm{i}}{2}\gamma(s)^{-1}\partial_i\gamma(s).$$

Estimating each term separately using (B-3), we find

$$|(u \mid (L(t) - L(s))u)| \le \widetilde{C}(t,s)(u \mid L(t)u),$$

where

$$\widetilde{C}(t,s) = 2\left|\int_s^t C_D(r)\,\mathrm{d}r\right| + \left|\int_s^t C_D(r)\,\mathrm{d}r\right|^2 + \left|\int_s^t C_g(r)\,\mathrm{d}r\right|\left(1 + \left|\int_s^t C_D(r)\,\mathrm{d}r\right|\right)^2 + \left|\int_s^t C_Y(r)\,\mathrm{d}r\right|,$$

with $C_D = C_A + C_\gamma/2$. After two applications of

$$\left|\int_s^t C_D(r)\,\mathrm{d}r\right|^2 \le |t-s|\left|\int_s^t C_D(r)^2\,\mathrm{d}r\right| \le \left|\int_s^t C_D(r)^2\,\mathrm{d}r\right|,$$

which is a simple consequence of the Cauchy–Schwarz inequality, we obtain

$$\widetilde{C}(t,s) \le \left|\int_s^t (c(t)(2C_D + C_D^2) + C_\gamma + C_g)\,\mathrm{d}r\right|,$$

where $c(t) := 1 + \int_{t-1}^{t+1} C_g(r)\,\mathrm{d}r$. Thus Assumption (1.c) is true with $C(t) = \widetilde{C}(t) + C_W(t)$. □

The inequalities (B-3) in the last proposition were stated with respect to $L(t)$. For a more convenient criterion, fix a (time-independent) Riemannian metric g_0 on Σ and set $\gamma_0 := |g_0|^{1/2}$. Consider the operator L_0 defined by the form

$$(u \mid L_0 v) := \int_\Sigma \big((\overline{D_i^{\gamma_0} u}) g_0^{ij}(t)(D_j^{\gamma_0} v) + \bar{u}\, v\big).$$

Proposition B.2. *Assume that there exists a positive $C_g \in C(\mathbb{R})$ such that*

$$\tilde{g}^{ij}(t) X_i X_j \ge C_g(t) g_0^{ij} X_i X_j. \tag{B-4}$$

Further, suppose that there exist $\varepsilon_0 \in C(\mathbb{R})$, $\varepsilon_0(t) \in \,]0,1[$, and a positive $C_0 \in C(\mathbb{R})$ such that

$$\varepsilon_0(t)\gamma_0^2\gamma(t)^{-2}(\partial_i \gamma_0^{-1}\gamma(t))\,\tilde{g}^{ij}(t)\,(\partial_j \gamma_0^{-1}\gamma(t)) + \widetilde{Y}(t) \ge C_0(t). \tag{B-5}$$

Then there exists a positive $C \in C(\mathbb{R})$ such that L_0 satisfies the inequality

$$\|L(t)^{1/2}u\| \ge C(t)\|L_0^{1/2}|u|\|, \quad u \in \operatorname{Dom} L(t)^{1/2}. \tag{B-6}$$

Proof. Let $\varepsilon(t) := (1 - 4\varepsilon_0(t))^{-1}$, so that $\varepsilon_0(t) = \frac{1}{4}(1 - \varepsilon(t)^{-1})$. Then

$$\begin{aligned}
&(u \mid L(t)u)\\
&\ge \int_\Sigma \big(-(D_i^\gamma(t)|u|)\tilde{g}^{ij}(t)(D_j^\gamma(t)|u|) + \widetilde{Y}(t)\,|u|^2\big)\\
&\ge \int_\Sigma (\varepsilon(t)-1)(D_i^{\gamma_0}|u|)\tilde{g}^{ij}(t)(D_j^{\gamma_0}|u|) + \int_\Sigma \big(\varepsilon_0(t)\gamma_0^2\gamma(t)^{-2}(\partial_i\gamma_0^{-1}\gamma(t))\tilde{g}^{ij}(t)(\partial_j\gamma_0^{-1}\gamma(t)) + \widetilde{Y}(t)\big)|u|^2\\
&\ge \min\big(C_g(t)(1-\varepsilon(t)), C_0(t)\big)\,(|u| \mid L_0|u|).
\end{aligned}$$

In the first step we used the diamagnetic inequality

$$|(\partial_x - \mathrm{i}V(x))f(x)| \ge |\partial_x|f(x)||$$

almost everywhere for real V and f such that $(\partial_x - \mathrm{i}V)f$ exists almost everywhere. In the second step we used the Cauchy–Schwarz inequality. □

We can apply the preceding proposition to restate Proposition B.1 using L_0 instead of $L(t)$. For this purpose we introduce another norm on half-densitized 1-forms:

$$\|X\| = \left(\int_\Sigma g_0^{ij}\,\overline{X}_i X_j\right)^{1/2}.$$

Proposition B.3. *In addition to* (B-4) *and* (B-5) *we suppose that for some* $C_g \in C(\mathbb{R})$

$$\tilde{g}^{ij}(t)X_iX_j \leq C_g(t)g_0^{ij}X_iX_j, \quad X \in C(T^*\Sigma).$$

Moreover, we assume that there are positive $C_{Y,0}, C_{g,0}, C_{W,0} \in L^1_{\mathrm{loc}}(\mathbb{R})$, $C_{A,0}, C_{\gamma,0} \in L^2_{\mathrm{loc}}(\mathbb{R})$ *such that for all* $t \in \mathbb{R}$

$$\begin{aligned} \|L_0^{-1/2}|\partial_t \widetilde{Y}(t)|L_0^{-1/2}\| &\leq C_{Y,0}(t), \\ \|\partial_t W(t)L_0^{-1/2}\| &\leq C_{W,0}(t), \\ \|\partial_t A(t)L_0^{-1/2}\| &\leq C_{A,0}(t), \\ \|\partial_t \gamma(t)^{-1}\,\mathrm{d}\gamma(t)L_0^{-1/2}\| &\leq C_{\gamma,0}(t), \\ |\partial_t \tilde{g}^{ij}(t)X_iX_j| &\leq C_{g,0}(t)g_0^{ij}X_iX_j, \quad X \in C(T^*\Sigma). \end{aligned}$$

Then Assumption (1.*c*) *is true.*

Appendix C: Nonautonomous evolution equations

To make this paper more self-contained, we explain in this appendix relevant aspects of the theory of linear evolution equations. We are more general than strictly necessary for the purposes of this paper, but in anticipation of our upcoming work this generality could be useful. The results stated in this appendix can be found in similar form in [Kato 1970] and in the monographs [Pazy 1983; Tanabe 1997]. We also wish to refer to the appendix of [Bach and Bru 2016], which uses slightly different assumptions that essentially coincide with ours for the Hilbertian case. Finally, we would like to mention [Schmid and Griesemer 2017] which also discusses the theory of nonautonomous evolution equations on uniformly convex Banach spaces.

Let $\mathcal{X}$ be a Banach space. We recall that a linear operator A on $\mathcal{X}$ is the generator of a strongly continuous (one-parameter) semigroup $[0,\infty[\, \ni t \mapsto \mathrm{e}^{tA}$ if and only if A is densely defined, closed and there exist constants $M \geq 1$, $\beta \in \mathbb{R}$ such that its resolvent satisfies

$$\|(A-\lambda)^{-n}\| \leq M(\lambda-\beta)^{-n}, \quad \lambda > \beta, \quad n = 1, 2, \dots. \tag{C-1}$$

Then we have $\|\mathrm{e}^{tA}\| \leq M\mathrm{e}^{\beta t}$ and say that e^{tA} is a semigroup of type (M,β). If both A and $-A$ generate strongly continuous semigroups, they generate a strongly continuous (one-parameter) group $\mathbb{R} \ni t \mapsto \mathrm{e}^{tA}$.

If

$$\|(A-\lambda)^{-1}\| \leq (\lambda-\beta)^{-1}, \quad \lambda > \beta, \tag{C-2}$$

then (C-1) is true with $M = 1$. Thus $\|\mathrm{e}^{tA}\| \leq M\mathrm{e}^{\beta t}$, so that $\mathrm{e}^{t(A-\beta)}$ is a semigroup of contractions.

Let $\mathcal{Y}$ be another Banach space which is densely and continuously embedded in $\mathcal{X}$.

Definition C.1. By the *part of* A *on* $\mathcal{Y}$ we mean the operator $\tilde{A}$, which is the restriction of A to the domain

$$\mathrm{Dom}(\tilde{A}) := \{y \in \mathrm{Dom}(A) \cap \mathcal{Y} \mid Ay \in \mathcal{Y}\}.$$

Definition C.2. $\mathcal{Y}$ is called A-*admissible* if the semigroup e^{tA}, $t \in [0,\infty[$, leaves $\mathcal{Y}$ invariant and its restriction to $\mathcal{Y}$ is a strongly continuous semigroup on $\mathcal{Y}$.

In the following we consider a family $\{A(t)\}_{t\in[0,T]}$ of generators of a strongly continuous semigroup. We chose the interval $[0, T]$ for convenience and definiteness; the generalization to other intervals is straightforward.

Definition C.3. The family $\{A(t)\}_{t\in[0,T]}$ is called *stable* with stability constants $M \geq 1,\ \beta \in \mathbb{R}$, if

$$\left\| \prod_{j=1}^{k} (A(t_j) - \lambda)^{-1} \right\| \leq M(\lambda - \beta)^{-k}, \quad \lambda > \beta,$$

for all finite sequences $0 \leq t_1 \leq t_2 \leq \cdots \leq t_k \leq T,\ k = 1, 2, \ldots.$ Here and below such products are time-ordered (viz., factors with a larger t_j are to the left of factors with a smaller t_j).

Proposition C.4. *If $\{A(t)\}_{t\in[0,T]}$ is stable with stability constants M, β, then*

$$\left\| \prod_{j=1}^{k} \mathrm{e}^{\mu_j A(t_j)} \right\| \leq M \mathrm{e}^{\beta(\mu_1+\cdots+\mu_k)}, \quad \mu_j \geq 0.$$

Proof. The proof is straightforward; see, e.g., [Tanabe 1997, Proposition 7.3]. □

The following simple generalization of [Kato 1970, Proposition 3.4] gives a criterion for the stability using an assumption of the form (C-2) for a time-dependent norm:

Proposition C.5. *For each $t \in [0, T]$, let $\|\cdot\|_t$ be an equivalent norm on $\mathcal{X}$ and $C \in L^1[0, T]$ positive such that*

$$\|u\|_s \leq \|u\|_t \exp\left| \int_s^t C(r)\,\mathrm{d}r \right|, \quad u \in \mathcal{X},\ s, t \in [0, T]. \tag{C-3}$$

If $\{A(t)\}$ satisfies

$$\|(A(t) - \lambda)^{-1}\|_t \leq (\lambda - \beta)^{-1}, \quad \lambda > \beta, \tag{C-4}$$

for all $t \in [0, T]$, then for any $s \in [0, T]$

$$\left\| \prod_{j=1}^{k} (A(t_j) - \lambda)^{-1} \right\|_s \leq (\lambda - \beta)^{-k} \exp\left(\int_0^T 2C(r)\,\mathrm{d}r \right), \quad t_1 \leq s \leq t_k,$$

for every finite sequence $0 \leq t_1 \leq t_2 \leq \cdots \leq t_k \leq T$.

Proof. Repeated application of (C-3) and (C-4) yields

$$\begin{aligned} \left\| \prod_{j=1}^{k} (A(t_j) - \lambda)^{-1} u \right\|_{t_k} &\leq (\lambda - \beta)^{-1} \left\| \prod_{j=1}^{k-1} (A(t_j) - \lambda)^{-1} u \right\|_{t_k} \\ &\leq (\lambda - \beta)^{-1} \exp\left(\int_{t_{k-1}}^{t_k} C(r)\,\mathrm{d}r \right) \left\| \prod_{j=1}^{k-1} (A(t_j) - \lambda)^{-1} u \right\|_{t_{k-1}} \\ &\vdots \\ &\leq (\lambda - \beta)^{-k} \exp\left(\int_{t_1}^{t_k} C(r)\,\mathrm{d}r \right) \|u\|_{t_1}. \end{aligned}$$

Applying (C-3) twice more (for s and t_k, as well as s and t_1), we obtain the desired result. □

Let us start with a rather general theorem on the construction of evolution operators; see also [Kato 1970, Theorem 4.1; Tanabe 1997, Theorem 7.1]. Note that the properties of the evolution operator described in this theorem are rather modest.

Theorem C.6. *Assume that*:

(a) $\{A(t)\}_{t\in[0,T]}$ *is stable with constants* M, β.

(b) $\mathcal{Y}$ *is* $A(t)$*-admissible for each* t, *and the part* $\tilde{A}(t)$ *of* $A(t)$ *in* $\mathcal{Y}$ *is stable with constants* $\widetilde{M}$, $\tilde{\beta}$.

(c) $\mathcal{Y} \subset \operatorname{Dom} A(t)$ *so that* $A(t) \in B(\mathcal{Y}, \mathcal{X})$ *for each* t, *and* $t \mapsto A(t)$ *is norm-continuous in the norm of* $B(\mathcal{Y}, \mathcal{X})$.

Then there exists a unique family of bounded operators $\{U(t, s)\}_{0\le s\le t\le T}$, *on* $\mathcal{X}$, *called the* evolution (operator) *generated by* $A(t)$, *with the following properties*:

(i) *For all* $0 \le r \le s \le t \le T$, *we have the identities*

$$U(t, t) = \mathbb{1}, \quad U(t, s)U(s, r) = U(t, r).$$

(ii) $(t, s) \mapsto U(t, s)$ *is strongly* $\mathcal{X}$*-continuous and* $\|U(t, s)\|_{\mathcal{X}} \le M e^{\beta(t-s)}$.

(iii) *For all* $y \in \mathcal{Y}$ *and* $0 \le s \le t \le T$,

$$\partial_t^+ U(t, s)y|_{t=s} = A(s)y, \tag{C-5a}$$

$$-\partial_s U(t, s)y = U(t, s)A(s)y, \tag{C-5b}$$

where the right derivative ∂_t^+ *and the derivative* ∂_s (*right derivative if* $s = 0$ *and left derivative if* $s = t$) *are in the strong topology of* $\mathcal{X}$.

Proof. We approximate $A(t)$ by step functions: Set

$$A_n(t) = A(T\lfloor tn/T\rfloor/n),$$

where $\lfloor\cdot\rfloor$ denotes the floor function, viz., rounding to the integral part. Since $t \mapsto A(t)$ is norm-continuous in the norm of $B(\mathcal{Y}, \mathcal{X})$, we have

$$\|A_n(t) - A(t)\|_{B(\mathcal{Y},\mathcal{X})} \to 0 \quad \text{as } n \to \infty \tag{C-6}$$

uniformly in t. It follows immediately that also $A_n(t)$ and $\tilde{A}_n(t)$ are stable with constants M, β and $\widetilde{M}$, $\tilde{\beta}$, respectively.

Corresponding to $A_n(t)$ we construct approximating evolution operators $U_n(t, s)$ by setting

$$U_n(t, s) = e^{(t-s)A_n(s)}$$

if s, t belong to the closure of an interval where A_n is constant, and by imposing the relation

$$U_n(t, s) = U_n(t, r)U_n(r, s)$$

to determine $U_n(t, s)$ for other values of s, t. Clearly, $U_n(t, t) = \mathbb{1}$ and $(t, s) \mapsto U_n(t, s)$ is strongly $\mathcal{X}$-continuous. We also have

$$\|U_n(t, s)\|_{\mathcal{X}} \le M e^{\beta(t-s)}, \quad \|U_n(t, s)\|_{\mathcal{Y}} \le \widetilde{M} e^{\tilde{\beta}(t-s)} \tag{C-7}$$

by Proposition C.4, and $U_n(t,s)\mathcal{Y}\subset\mathcal{Y}$ because $\mathcal{Y}$ is $A(t)$-admissible. Furthermore, because $\mathcal{Y}\subset\operatorname{Dom}A(t)$ we have for $y\in\mathcal{Y}$

$$\partial_t U_n(t,s)y = A_n(t)U_n(t,s)y,$$
$$\partial_s U_n(t,s)y = -U_n(t,s)A_n(s)y,$$

for any t or s, respectively, that is not on the boundary of an interval where A_n is constant.

Next we show that $U_n(t,s)$ converges to $U(t,s)$ strongly in $\mathcal{X}$ uniformly in s,t: By the fundamental theorem of calculus, we have

$$U_n(t,r)y - U_m(t,r)y = \int_r^t U_n(t,s)(A_n(s)-A_m(s))U_m(s,r)y\,\mathrm{d}s.$$

Applying (C-7), we thus obtain

$$\|U_n(t,r)y - U_m(t,r)y\|_{\mathcal{X}} \le M\widetilde{M}\mathrm{e}^{\gamma(t-r)}\|y\|_{\mathcal{Y}}\int_r^t \|A_n(s)-A_m(s)\|_{B(\mathcal{Y},\mathcal{X})}\,\mathrm{d}s,$$

where $\gamma=\max(\beta,\tilde{\beta})$. Therefore it follows from (C-6) that $U_n(t,s)y$ converges in the strong topology of $\mathcal{X}$ uniformly in s,t. Since $\mathcal{Y}$ is dense in $\mathcal{X}$ and $U_n(t,s)$ is uniformly bounded in n, $U_n(t,s)$ converges strongly in $\mathcal{X}$ and we set

$$U(t,s) = \operatorname*{s-lim}_{n\to\infty} U_n(t,s).$$

It is immediate that the properties (i) and (ii) follow from the corresponding properties for $U_n(t,s)$.

Finally, we show uniqueness and (iii): If $\{V(t,s)\}_{0\le s\le t\le T}$ satisfies (i)–(iii) for a stable family of operators $\{A'(t)\}_{t\in[0,T]}$ with the same stability constants, then we apply the fundamental theorem of calculus to find

$$U_n(t,s)y - V(t,s)y = \int_s^t U_n(t,r)(A_n(r)-A'(r))V(r,s)y\,\mathrm{d}r,$$

and therefore

$$\|U_n(t,s)y - V(t,s)y\|_{\mathcal{X}} \le M\widetilde{M}\mathrm{e}^{\gamma(t-s)}\|y\|_{\mathcal{Y}}\int_s^t \|A_n(r)-A'(r)\|_{B(\mathcal{Y},\mathcal{X})}\,\mathrm{d}r. \tag{C-8}$$

If we set $A'(t)=A(t)$ and let $n\to\infty$, we thus find that $U(t,s)y=V(t,s)y$ and by density $U(t,s)=V(t,s)$ on the whole of $\mathcal{X}$. We conclude that $U(t,s)$ is unique.

Now, in (C-8), we set $A'(t)=A(\tau)=\text{const}$ for $\tau\in[0,T]$, divide by $t-s$ and let $n\to\infty$ to obtain

$$(t-s)^{-1}\|U(t,s)y-\mathrm{e}^{(t-s)A(\tau)}y\|_{\mathcal{X}} \le (t-s)^{-1}M\widetilde{M}\mathrm{e}^{\gamma(t-s)}\|y\|_{\mathcal{Y}}\int_s^t \|A_n(r)-A(\tau)\|_{B(\mathcal{Y},\mathcal{X})}\,\mathrm{d}r.$$

On the one hand, for $\tau=s$, we find (C-5a) in the limit $t\to s$. On the other hand, setting $\tau=t$ and letting $t\to s$, we find

$$\partial_s^- U(t,s)y|_{s=t} = -A(t)y. \tag{C-9}$$

To find (C-5b), we check the right and left derivative separately. Applying (C-5a) and (C-9), we obtain

$$\begin{aligned}\partial_s^+ U(t,s)y &= \operatorname*{s-lim}_{h\searrow 0} h^{-1}(U(t,s+h)y - U(t,s)y)\\ &= U(t,s+h)\operatorname*{s-lim}_{h\searrow 0} h^{-1}(y-U(s+h,s)y) = -U(t,s)A(s)y,\end{aligned} \tag{C-10a}$$

$$\partial_s^- U(t,s)y = \operatorname*{s-lim}_{h\searrow 0} h^{-1}(U(t,s)y - U(t,s-h)y)$$
$$= U(t,s) \operatorname*{s-lim}_{h\searrow 0} h^{-1}(y - U(s,s-h)y) = -U(t,s)A(s)y. \tag{C-10b}$$

Therefore we have completed the proof also for (iii). □

We say that a Banach space $\mathcal{Y}$ possesses a predual if there exists a Banach space $\mathcal{Y}_*$ such that $\mathcal{Y}$ is the dual of $\mathcal{Y}_*$. Having fixed a predual $\mathcal{Y}_*$, we can equip $\mathcal{Y}$ with the so-called weak* topology, which is generated by the seminorms $y \mapsto |\xi(y)|$, where $\xi \in \mathcal{Y}_*$. Note in particular that every reflexive Banach space possesses a unique predual (namely, its dual). For reflexive Banach spaces the weak* convergence clearly coincides with the weak convergence.

For Banach spaces possessing a predual one can slightly improve the previous theorem; see also [Kato 1970, Theorem 5.1].

Theorem C.7. *In addition to the assumptions of Theorem C.6, assume that*:

(d) *$\mathcal{Y}$ possesses a predual.*

Then, *in addition to* (i)–(iii), *the evolution* $\{U(t,s)\}_{0\le s\le t\le T}$ *has the following properties*:

(iv) $U(t,s)\mathcal{Y} \subset \mathcal{Y}$, $(t,s) \mapsto U(t,s)$ *is weakly* continuous and*

$$\|U(t,r)\|_{\mathcal{Y}} \le \widetilde{M}e^{\tilde{\beta}(t-s)}, \quad 0 \le r \le s \le t \le T. \tag{C-11}$$

Proof. Note that for fixed $s,t \in [0,T]$ and $y \in \mathcal{Y}$, $U_n(t,s)y$ is a uniformly bounded sequence in $\mathcal{Y}$, and thus, by the Banach–Alaoglu theorem, it contains a weakly* convergent subsequence. Moreover, by our previous results, $U_n(t,s)y \to U(t,s)y$ in $\mathcal{X}$. But $U(t,s)y$ must be equal to the weak* limit, and thus lie in $\mathcal{Y}$; i.e., $U(t,s)\mathcal{Y} \subset \mathcal{Y}$. The inequality then follows from (C-7).

Now, let $(t_j)_j$, $(s_j)_j$ be sequences with $t_j \to t$, $s_j \to s$ and $y \in \mathcal{Y}$. Recall that $U(t_j,s_j)y \to U(t,s)y$ in $\mathcal{X}$ because $(t,s) \mapsto U(t,s)$ is $\mathcal{X}$-strongly continuous. By the Banach–Alaoglu theorem, since $U(t_j,s_j)$ is uniformly bounded, $U(t_j,s_j)y$ contains a weakly* convergent subsequence. The weak* limit of $U(t_j,s_j)y$ is thus $U(t,s)y$ and must lie in $\mathcal{Y}$. In other words, $U(t,s)$ is weakly* continuous on $\mathcal{Y}$. □

We recall that a normed space is called *uniformly convex* if for every $\varepsilon > 0$ and unit vectors $\|x\| = \|y\| = 1$ there exists $\delta > 0$ such that

$$\|x-y\| \ge \varepsilon \quad \Longrightarrow \quad \left\|\frac{x+y}{2}\right\| \le 1-\delta.$$

We note that all uniformly convex Banach spaces are reflexive. Additionally, on uniformly convex Banach spaces, $\|x_n\| \to \|x\|$ and the weak convergence $x_n \rightharpoonup x$ implies the strong convergence. All Hilbert spaces are uniformly convex.

If we assume that the Banach space $\mathcal{Y}$ is uniformly convex, stronger results about the evolution can be derived. They are described in the following theorem, which is a part of [Kato 1970, Theorem 5.2]:

Theorem C.8. *In addition to the assumptions of Theorem C.6, assume that*:

(d′) *$\mathcal{Y}$ is uniformly convex.*

(e) *For every t there exist on $\mathcal{Y}$ an equivalent norm $\|\cdot\|_{\mathcal{Y},t}$ as well as a positive $C \in L^1[0,T]$ such that*

$$\|y\|_{\mathcal{Y},s} \leq \|y\|_{\mathcal{Y},t} \exp\left|\int_s^t C(r)\,\mathrm{d}r\right|, \quad s,t \in [0,T]. \tag{C-12}$$

Additionally, there exists $\tilde{\beta} \in \mathbb{R}$ such that

$$\|(\tilde{A}(t)-\lambda)^{-1}\|_{\mathcal{Y},t} \leq (\lambda-\tilde{\beta})^{-1}, \quad \lambda > \tilde{\beta},$$

for all $t \in [0,T]$.

Then, in addition to (i)–(iii), *the evolution $\{U(t,s)\}_{0\leq s\leq t\leq T}$ has the following property, which is an improved version of* (iv):

(iv′) *$U(t,s)$ preserves $\mathcal{Y}$, is $\mathcal{Y}$-strongly continuous in s for fixed t and $\mathcal{Y}$-strongly right-continuous in t for fixed s, and*

$$\|U(t,r)\|_{\mathcal{Y},s} \leq \exp\left(\int_r^t (\tilde{\beta}+2C(\tau))\,\mathrm{d}\tau\right), \quad 0\leq r\leq s\leq t\leq T. \tag{C-13}$$

Proof. Since $\mathcal{Y}$ is uniformly convex, it is also reflexive, and thus Theorem C.7(iv) holds. Then we use Propositions C.4 and C.5 to find (C-13).

Let us prove the strong continuity. By (iv), for any $y \in \mathcal{Y}$ we have $\text{w-lim}_{t,r\to s} U(t,r)y \to y$. Using this, and then the bound (C-13), we obtain

$$\begin{aligned}\|y\| &\leq \liminf_{r,t\to s} \|U(t,r)y\|_{\mathcal{Y},s} \leq \limsup_{r,t\to s} \|U(t,r)y\|_{\mathcal{Y},s} \\ &\leq \limsup_{r,t\to s} \exp\left(\int_r^t (\tilde{\beta}+2C(\tau))\,\mathrm{d}\tau\right)\|y\| = \|y\|.\end{aligned}$$

Hence, $\lim_{r,t\to s} \|U(t,r)y\|_{\mathcal{Y},s} = \|y\|$. But $\mathcal{Y}$ is uniformly convex, so this implies

$$\lim_{r,t\to s} U(t,r)y = y.$$

Let $0\leq s\leq s'\leq t\leq T$ and $y \in \mathcal{Y}$. Then

$$\|U(t,s')y - U(t,s)y\|_{\mathcal{Y}} \leq \|U(t,s')\|_{\mathcal{Y}}\|y - U(s',s)y\|_{\mathcal{Y}} \to 0$$

as $s' \to s$ or $s \to s'$. Similarly, for $0\leq s\leq t\leq t'\leq T$ we find

$$\|U(t',s)y - U(t,s)y\|_{\mathcal{Y}} \leq \|(U(t',t)-\mathbb{1})U(t,s)y\|_{\mathcal{Y}} \to 0$$

as $t' \to t$. □

In the previous theorem we still had to distinguish between the t- and s-properties of $U(t,s)$. If the reversed operator $-A(T-t)$ also satisfies the assumptions of the theorems above, this distinction can be dropped; see also [Kato 1970, Remark 5.3]:

Theorem C.9. *Suppose that both $\{A(t)\}_{t\in[0,T]}$ and the reversed family $\{-A(T-t)\}_{t\in[0,T]}$ satisfy the assumptions of Theorems C.6 and C.8. Then the unique family of bounded operators $\{U(t,s)\}_{s,t\in\mathbb{R}}$ described in the previous theorems satisfies the following improved versions of* (i), (iii), *and* (iv′):

(i′) *For all* $r, s, t \in [0, T]$, *we have the identities*

$$U(t,t) = \mathbb{1}, \quad U(t,s)U(s,r) = U(t,r).$$

(iii′) *For all* $y \in \mathcal{Y}$ *and* $s, t \in [0, T]$,

$$\partial_t U(t,s)y = A(t)U(t,s)y, \tag{C-14a}$$

$$-\partial_s U(t,s)y = U(t,s)A(s)y, \tag{C-14b}$$

where the derivatives (*right/left derivatives at the boundaries of* $[0, T]$) *are in the strong topology of* $\mathcal{X}$.

(iv″) $(t,s) \mapsto U(t,s)$ *preserves* $\mathcal{Y}$, *is* $\mathcal{Y}$*-strongly continuous and satisfies* (C-13).

Proof. Denote the evolution for $\{A(t)\}_{t\in[0,T]}$ by $U(t,s)$ and the evolution for $\{-A(T-t)\}_{t\in[0,T]}$ by $V(t,s)$. For $0 \le s \le t \le T$, we define

$$U(s,t) = V(T-s, T-t).$$

From the approximations $U_n(t,s)$ and $V_n(t,s)$, it is easy to see that

$$U(t,s)U(s,t) = \mathbb{1}$$

for $s, t \in \mathbb{R}$. This proves (i′).

It is clear that

$$\partial_t U(t,s)y|_{t=s} = A(s)y,$$

$$-\partial_s U(t,s)y = U(t,s)A(s)y$$

for $s, t \in [0, T]$. Then we can proceed as in (C-10) to find also

$$\partial_t U(t,s)y = A(t)U(t,s)y.$$

Finally, the strong continuity of $U(t,s)$ follows from (iv′) applied to both $U(t,s)$ and $V(t,s)$, which implies, in particular, that $U(t,s)$ is strongly right- and left-continuous in t for fixed s. □

Theorem C.9 implies the following; see also [Yajima 2011, Theorem 3.2]:

Theorem C.10. *Let* $\mathcal{X}$ *and* $\mathcal{Y}$ *be Hilbert spaces such that* $\mathcal{Y}$ *is densely and continuously embedded in* $\mathcal{X}$. *Let* $I \subset \mathbb{R}$ *be a compact interval, and* $\{A(t)\}_{t\in I}$ *a family of densely defined, closed operators on* $\mathcal{X}$. *Suppose that the following is satisfied*:

(a) $\mathcal{Y} \subset \operatorname{Dom} A(t)$ *so that* $A(t) \in B(\mathcal{Y}, \mathcal{X})$ *and* $t \mapsto A(t)$ *is norm-continuous in the norm of* $B(\mathcal{Y}, \mathcal{X})$.

(b) *For every* $t \in I$, *there exist on* $\mathcal{X}$ *and* $\mathcal{Y}$ *Hilbert structures* $(\cdot|\cdot)_{\mathcal{X},t}$ *and* $(\cdot|\cdot)_{\mathcal{Y},t}$, *which are equivalent to the original ones and for a positive* $C \in L^1(I)$ *and all* $s, t \in I$

$$\|x\|_{\mathcal{X},s} \le \|x\|_{\mathcal{X},t} \exp\left|\int_s^t C(r)\,\mathrm{d}r\right|,$$

$$\|y\|_{\mathcal{Y},s} \le \|y\|_{\mathcal{Y},t} \exp\left|\int_s^t C(r)\,\mathrm{d}r\right|.$$

Denote the corresponding Hilbert spaces by $\mathcal{X}_t$ *and* $\mathcal{Y}_t$.

(c) *$A(t)$ is self-adjoint with respect to $\mathcal{X}_t$ and the part $\tilde{A}(t)$ of $A(t)$ in $\mathcal{Y}_t$ is self-adjoint in $\mathcal{Y}_t$.*

*Then there exists a unique family of bounded operators $\{U(t,s)\}_{s,t\in I}$, in $\mathcal{X}$, called the **evolution** (**operator**) generated by $A(t)$, with the following properties*:

(i) *For all $r, s, t \in I$, we have the identities*

$$U(t,t) = \mathbb{1}, \quad U(t,s)U(s,r) = U(t,r).$$

(ii) *$U(t,s)$ is $\mathcal{X}$-strongly continuous and*

$$\|U(t,s)\|_{\mathcal{X},s} \le \exp\left|\int_s^t 2C(r)\,\mathrm{d}r\right|, \quad s,t \in I.$$

(iii) *For all $y \in \mathcal{Y}$ and $s, t \in I$,*

$$\mathrm{i}\partial_t U(t,s)y = A(t)U(t,s)y,$$
$$-\mathrm{i}\partial_s U(t,s)y = U(t,s)A(s)y,$$

where the derivatives (*right/left derivatives at the boundaries of I*) *are in the strong topology of $\mathcal{X}$.*

(iv) *$U(t,s)\mathcal{Y} \subset \mathcal{Y}$, $U(t,s)$ is $\mathcal{Y}$-strongly continuous and*

$$\|U(t,s)\|_{\mathcal{Y},s} \le \exp\left|\int_s^t 2C(r)\,\mathrm{d}r\right|, \quad s,t \in I.$$

The following perturbation theorem is essentially [Kato 1966, Theorem 4.5]. We leave the proof as an exercise to the reader.

Theorem C.11. *Suppose that $\{A(t)\}_{t\in[0,T]}$ satisfies the assumptions of Theorem C.6. Let $\{B(t)\}_{t\in[0,T]}$ be a family of bounded operators in $\mathcal{X}$ such that $t \mapsto B(t)$ is strongly continuous with respect to $\mathcal{X}$ and $K = \sup_t \|B(t)\|_{\mathcal{X}}$. Then there exists a unique evolution $V(t,s)$ for $\{A(t)+B(t)\}_{t\in[0,T]}$ satisfying the properties* (i)–(iii), *but with the estimate*

$$\|V(t,s)\| \le M\mathrm{e}^{(\beta+KM)(t-s)}.$$

Suppose that $\{A(t)\}_{t\in[0,T]}$ also satisfies the stronger assumptions of Theorem C.7, C.8 or C.9, and $\{B(t)\}_{t\in[0,T]}$ preserves $\mathcal{Y}$ and its part $\{\tilde{B}(t)\}_{t\in[0,T]}$ in $\mathcal{Y}$ is bounded in $\mathcal{Y}$ with $\widetilde{K} = \sup_t \|B(t)\|_{\mathcal{Y}}$. Then the evolution $V(t,s)$ satisfies the corresponding stronger properties, where the estimate (C-11) *needs to be multiplied by $\mathrm{e}^{\widetilde{K}\widetilde{M}(t-s)}$, and the estimate* (C-13) *by $\mathrm{e}^{\widetilde{K}(t-s)}$.*

The evolution $V(t,s)$ in the theorem above is given symbolically by

$$V = U + U * B * U + U * B * U * B * U + \cdots,$$

where $* B *$ denotes a Volterra-type convolution with "density" $B(t)$. For example,

$$(U * B * U)(t,r) = \int_r^t U(t,s)B(s)U(s,r)\,\mathrm{d}s.$$

Appendix D: Heinz–Kato inequality

We recall the Heinz–Kato inequality [Heinz 1951; Kato 1961], which is an elementary but very useful result for the interpolation of operators:

Theorem D.1. *Suppose that A, B are positive operators on Hilbert spaces $\mathcal{X}$, $\mathcal{Y}$, respectively. If T is a bounded operator from $\mathcal{X}$ to $\mathcal{Y}$ such that $T(\operatorname{Dom} A) \subset \operatorname{Dom} B$ and*

$$\|Tx\| \leq C_0\|x\|, \quad \|BTx\| \leq C_1\|Ax\|,$$

for $x \in \operatorname{Dom} A$, then

$$\|B^\lambda Tx\| \leq C_0^\lambda C_1^{1-\lambda}\|A^\lambda x\|, \quad \lambda \in [0,1]. \tag{D-1}$$

Appendix E: Finite speed of propagation

In this appendix we prove the finite speed of propagation for solutions of the Klein–Gordon equation with coefficients of low regularity.

In this section we prefer to work with the Klein–Gordon equation in the scalar formalism, given by (1-1), which can be locally written as

$$Ku := -g^{\mu\nu}(\nabla_\mu - \mathrm{i}A_\mu)(\nabla_\nu - \mathrm{i}A_\nu)u + Yu, \tag{E-1}$$

with pseudo-Riemannian metric g and the corresponding Levi-Civita derivative ∇, vector potential A, and scalar potential Y. Our standing assumptions in this appendix are as follows:

Assumption 4. $M = \mathbb{R} \times \Sigma$ is equipped with a continuous Lorentzian metric $g = -\alpha^2\,\mathrm{d}t^2 + g_\Sigma$, where $\alpha > 0$ and g_Σ are continuous, and g_Σ restricts to a family of Riemannian metrics on Σ. (Recall that every globally hyperbolic spacetime can be brought into this form [Bernal and Sánchez 2005].) We assume that $A_\mu(t) \in L^\infty_{\mathrm{loc}}(\Sigma)$ for all t, and $A_\mu, \dot{A}_\mu, Y \in L^\infty_{\mathrm{loc}}(M)$. Moreover, in every compact neighborhood $U \subset M$ there is $C_g > 0$ such that

$$|\dot{g}^{\mu\nu}X_\mu X_\nu| \leq C_g|g^{\mu\nu}X_\mu X_\nu|$$

almost everywhere in U for all covectors X.

Under these assumption we will show the following theorem on the finite speed of propagation:

Theorem E.1. *If $u \in C^1(\mathbb{R}; L^2_{\mathrm{loc}}(\Sigma))$ with $\partial_i u \in C(\mathbb{R}; L^2_{\mathrm{loc}}(\Sigma))$ and $Ku \in L^2_{\mathrm{loc}}(M)$, then*

$$\operatorname{supp} u \subset J\big(\operatorname{supp} Ku \cup \{t\}\times(\operatorname{supp} u(t) \cup \operatorname{supp} \dot{u}(t))\big)$$

for any $t \in \mathbb{R}$. That is, u is supported in the causal shadow of the union of Ku and of the support of its Cauchy data on $\{t\} \times \Sigma$.

Equation (E-1) can be obtained via the Euler–Lagrange equations from the *Lagrangian density*

$$\mathcal{L}[u] := -|g|^{1/2}\big(((\partial_\mu + \mathrm{i}A_\mu)\bar{u})g^{\mu\nu}((\partial_\nu - \mathrm{i}A_\nu)u) + Y|u|^2\big).$$

To the Lagrangian density $\mathcal{L}$ we can associate the *momentum flux density*

$$\mathcal{P}^{\mu}[u] := -\delta_0^{\mu}\mathcal{L}[u] + \frac{\partial\mathcal{L}[u]}{\partial(\partial_\mu \bar{u})}\partial_t \bar{u} + \frac{\partial\mathcal{L}[u]}{\partial(\partial_\mu u)}\partial_t u.$$

If the action for $\mathcal{L}$ is invariant under infinitesimal time-translations, Noether's theorem says that the momentum flux is conserved. If the action is not time-translation invariant, $\mathcal{P}$ is in general not conserved, but it is still a useful quantity.

The energy density $\mathcal{E} = \mathcal{P}^0$ obtained from $\mathcal{L}$ is not necessarily positive. Therefore, for technical reasons it will be convenient to replace $\mathcal{L}$ with the modified Lagrangian density

$$\widetilde{\mathcal{L}}[u] := -|g|^{1/2}\big(((\partial_\mu + \mathrm{i}A_\mu)\bar{u})g^{\mu\nu}((\partial_\nu - \mathrm{i}A_\nu)u) - (1+\alpha^{-2}A_0^2)|u|^2\big),$$

denoting the corresponding momentum flux density by $\widetilde{\mathcal{P}}$. Using the special form of the metric, we find the energy density

$$\widetilde{\mathcal{E}}[u] := \widetilde{\mathcal{P}}^0[u] = |g|^{1/2}\big(\alpha^{-2}|\dot{u}|^2 + ((\partial_i + \mathrm{i}A_i)\bar{u})g_\Sigma^{ij}((\partial_j - \mathrm{i}A_j)u) + |u|^2\big)$$

and the spatial momentum flux density

$$\widetilde{\mathcal{P}}^i[u] = \mathcal{P}^i[u] = -|g|^{1/2}\big(\dot{\bar{u}}g_\Sigma^{ij}((\partial_j - \mathrm{i}A_j)u) + \dot{u}g_\Sigma^{ij}((\partial_j + \mathrm{i}A_j)\bar{u})\big).$$

Below we will integrate $\partial_\mu\widetilde{\mathcal{P}}^\mu$ over a region which is delimited by two constant-time surfaces and the backward lightcone of a point as described in Figure 1. To rewrite this integral as an integral over the boundary of said region via Stokes' theorem, it is useful to assume that $\partial J_g^{\pm}(\Omega)$ is a Lipschitz topological hypersurface; see [Beem et al. 1996, Theorem 3.9]. Here we denote by $J_g^{\pm}(\Omega)$ the causal future (+) or causal past (−) of Ω, i.e., the set of points which can be reached from Ω by future-directed or, respectively, past-directed causal curves with respect to the metric g. Moreover, we write $J_g(\Omega) = J_g^+(\Omega) \cup J_g^-(\Omega)$.

If g is not smooth (or at least C^2), it is not guaranteed that $\partial J_g^{\pm}(\Omega)$ is a Lipschitz topological hypersurface. However, we can approximate g by smooth metrics:

If a Lorentzian metric $\hat{g}$ has strictly larger lightcones than g, i.e., each nonvanishing g-causal vector X^μ ($g_{\mu\nu}X^\mu X^\nu \le 0$) is $\hat{g}$-timelike ($\hat{g}_{\mu\nu}X^\mu X^\nu < 0$), then we write

$$\hat{g} \succ g.$$

As shown in [Chruściel and Grant 2012, Proposition 1.2], there always exists a *smooth* Lorentzian metric $\hat{g}$ with strictly larger lightcones which approximates g arbitrarily well.

Proposition E.2. *Let $\hat{g} \succ g$ be smooth and consider the situation depicted in Figure 1. Then there exists $C > 0$ such that*

$$\mathrm{e}^{C(s-t)}\int_{K_t}\widetilde{\mathcal{E}}[u](t) \le \int_{K_s}\widetilde{\mathcal{E}}[u](s) + \int_\Omega |g|^{1/2}|Ku|^2 \tag{E-2}$$

for all $u \in C^1(\mathbb{R}; L^2_{\mathrm{loc}}(\Sigma))$ with $\partial_i u \in C(\mathbb{R}; L^2_{\mathrm{loc}}(\Sigma))$ and $Ku \in L^2_{\mathrm{loc}}(M)$.

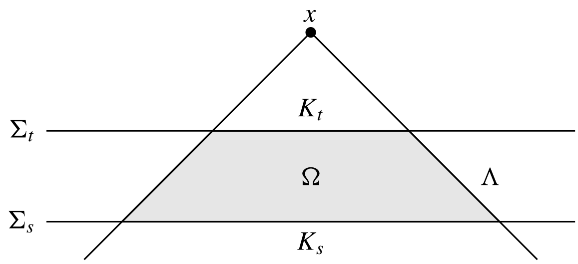

Figure 1. The truncated cone given by the backward lightcone $J^-_{\hat{g}}(x)$ of a point, and two constant-time surfaces $\Sigma_t = \{t\} \times \Sigma$ and Σ_s (with $t > s$). We write $K_t = J^-_{\hat{g}}(x) \cap (\{t\} \times \Sigma)$ and K_s for the caps, and $\Lambda = \partial J^-_{\hat{g}}(x) \cap ([s, t] \times \Sigma)$ for the mantle of the truncated cone $\Omega = J^-_{\hat{g}}(x) \cap ([s, t] \times \Sigma)$.

Proof. We derive

$$\begin{aligned}
\partial_\mu \widetilde{\mathcal{P}}^\mu[u] &= -\partial_t \widetilde{\mathcal{L}}[u] + \Big(\partial_\mu \frac{\partial \widetilde{\mathcal{L}}[u]}{\partial(\partial_\mu \bar{u})}\Big)\dot{\bar{u}} + \frac{\partial \widetilde{\mathcal{L}}}{\partial(\partial_\mu \bar{u})} \partial_\mu \partial_t \bar{u} + \Big(\partial_\mu \frac{\partial \widetilde{\mathcal{L}}}{\partial(\partial_\mu u)}\Big)\dot{u} + \frac{\partial \widetilde{\mathcal{L}}[u]}{\partial(\partial_\mu u)} \partial_\mu \partial_t u \\
&= -\partial_t \widetilde{\mathcal{L}}[u] + \Big(|g|^{1/2} \widetilde{K} u + \frac{\partial \widetilde{\mathcal{L}}[u]}{\partial \bar{u}}\Big)\dot{\bar{u}} + \frac{\partial \widetilde{\mathcal{L}}[u]}{\partial(\partial_\mu \bar{u})} \partial_t \partial_\mu \bar{u} + \Big(|g|^{1/2} \overline{\widetilde{K} u} + \frac{\partial \widetilde{\mathcal{L}}[u]}{\partial u}\Big)\dot{u} + \frac{\partial \widetilde{\mathcal{L}}[u]}{\partial(\partial_\mu u)} \partial_t \partial_\mu u \\
&= -2|g|^{1/2} \operatorname{Re}(\dot{\bar{u}} \widetilde{K} u) - \frac{\partial \widetilde{\mathcal{L}}[u]}{\partial g^{\mu\nu}} \dot{g}^{\mu\nu} - \frac{\partial \widetilde{\mathcal{L}}[u]}{\partial A_\mu} \dot{A}_\mu - \frac{\partial \widetilde{\mathcal{L}}[u]}{\partial |g|} \partial_t |g| \\
&= |g|^{1/2} \big(2 \operatorname{Re}(\dot{\bar{u}} \widetilde{K} u) + ((\partial_\mu + \mathrm{i} A_\mu)\bar{u}) \dot{g}^{\mu\nu} ((\partial_\nu - \mathrm{i} A_\nu) u) - 2\alpha^{-3} \dot{\alpha} A_0^2 |u|^2 \\
&\qquad - 2 \operatorname{Im}(\bar{u} \dot{A}_\mu g^{\mu\nu} (\partial_\nu - \mathrm{i} A_\nu) u) + 2\alpha^{-2} A_0 \dot{A}_0 |u|^2 - \tfrac{1}{2} |g|^{-1} (\partial_t |g|) \widetilde{\mathcal{L}}[u]\big).
\end{aligned}$$

where, in the second step, we used the Euler–Lagrange equations with

$$\widetilde{K} = K - Y + 1 + \alpha^{-2} A_0^2$$

being the Klein–Gordon operator associated to $\widetilde{\mathcal{L}}$. Estimating each term separately using our assumptions and the Cauchy–Schwarz inequality yields

$$\partial_\mu \widetilde{\mathcal{P}}^\mu[u] \leq |g|^{1/2} \big(|Ku|^2 + C_1 \alpha^{-2} |\dot{u}|^2 + C_2 ((\partial_i + \mathrm{i} A_i)\bar{u}) g_\Sigma^{ij} ((\partial_j + \mathrm{i} A_j) u) + C_3 |u|^2\big)$$

for $C_1, C_2, C_3 > 0$ which do not depend on u. Therefore we find

$$\int_\Omega \partial_\mu \widetilde{\mathcal{P}}^\mu[u] \leq \int_\Omega (|g|^{1/2} |Ku|^2 + C \widetilde{\mathcal{E}}[u]) \tag{E-3}$$

for some constant $C > 0$.

By Stokes' theorem,

$$\int_\Omega \partial_\mu \widetilde{\mathcal{P}}^\mu[u] = \int_{\partial\Omega} n_\mu \widetilde{\mathcal{P}}^\mu[u] = \int_{K_t} \widetilde{\mathcal{E}}[u](t) - \int_{K_s} \widetilde{\mathcal{E}}[u](s) + \int_\Lambda n_\mu \widetilde{\mathcal{P}}^\mu[u], \tag{E-4}$$

where n is the outward-directed normal field to $\partial\Omega$. For any future-directed causal covector field ξ (i.e., $g^{\mu\nu}\xi_\mu\xi_\nu \le 0$ and $\xi_0 \ge 0$) with $|\vec{\xi}| = (g_\Sigma^{ij}\xi_i\xi_j)^{1/2}$,

$$\begin{aligned}\xi_\mu \widetilde{\mathcal{P}}^\mu[u] &= \xi_0\widetilde{\mathcal{E}}[u] - 2|g|^{1/2}\operatorname{Re}(\xi_i \dot{\bar{u}} g_\Sigma^{ij}(\partial_j - \mathrm{i}A_j)u) \\ &\ge \xi_0\widetilde{\mathcal{E}}[u] - |g|^{1/2}\alpha|\vec{\xi}|\big(\alpha^{-2}|\dot{u}|^2 + ((\partial_i + \mathrm{i}A_i)\bar{u})g_\Sigma^{ij}((\partial_j - \mathrm{i}A_j)u)\big) \\ &\ge (\xi_0 - \alpha|\vec{\xi}|)\widetilde{\mathcal{E}}[u] \ge 0\end{aligned}$$

almost everywhere. Consequently, we can estimate the last term in (E-4) as $\int_\Lambda n_\mu \widetilde{\mathcal{P}}^\mu \ge 0$.

Combining (E-3) and (E-4), we obtain

$$\int_{K_t} \widetilde{\mathcal{E}}[u](t) - \int_{K_s} \widetilde{\mathcal{E}}[u](s) \le \int_s^t \left(\int_{K_r} (|g|^{1/2}|Ku(r)|^2 + C\widetilde{\mathcal{E}}[u](r)) \right) \mathrm{d}r,$$

and thus (E-2) by Grönwall's inequality. □

Now, using the proposition above, we can show the finite speed of propagation:

Theorem E.3. *If $u \in C^1(\mathbb{R}; L^2_{\mathrm{loc}}(\Sigma))$ with $\partial_i u \in C(\mathbb{R}; L^2_{\mathrm{loc}}(\Sigma))$ and $Ku \in L^2_{\mathrm{loc}}(M)$, then*

$$\begin{aligned}\operatorname{supp} u \cap M_\pm &\subset J_g^\pm\big((\operatorname{supp} Ku \cap M_\pm) \cup \{t\}\times(\operatorname{supp} u(t) \cup \operatorname{supp} \dot{u}(t))\big), \\ \operatorname{supp} u &\subset J_g\big(\operatorname{supp} Ku \cup \{t\}\times(\operatorname{supp} u(t) \cup \operatorname{supp} \dot{u}(t))\big)\end{aligned} \tag{E-5}$$

for any $t \in \mathbb{R}$, where $M_+ = [t, +\infty[\times \Sigma$ and $M_- =]-\infty, t] \times \Sigma$.

Proof. Note that, as a subset of Σ, we have $\operatorname{supp}\widetilde{\mathcal{E}}[u](t) = \operatorname{supp} u(t) \cup \operatorname{supp} \dot{u}(t)$. We show that $u(x) = 0$ for any

$$x \in M \setminus J_{\hat{g}}^+((\operatorname{supp} Ku \cap M_+) \cup \{t\}\times \operatorname{supp}\widetilde{\mathcal{E}}[u](t))$$

by an application of Proposition E.2 for all smooth $\hat{g} \succ g$. For any such x, $J_{\hat{g}}^-(x)$ does not intersect $(\operatorname{supp} Ku \cap M_+) \cup \{t\}\times \operatorname{supp}\widetilde{\mathcal{E}}[u](t)$. Proposition E.2 now shows that u vanishes in $J_{\hat{g}}^-(x) \cap M_+$ and thus also at x.

We have thus shown that

$$\operatorname{supp} u \cap M_\pm \subset J_{\hat{g}}^\pm\big((\operatorname{supp} Ku \cap M_\pm) \cup \{t\}\times(\operatorname{supp} u(t) \cup \operatorname{supp} \dot{u}(t))\big)$$

for all smooth $\hat{g} \succ g$. It follows that (E-5) holds, because a vector is g-causal if and only if it is $\hat{g}$-timelike for all smooth $\hat{g} \succ g$ by [Chruściel and Grant 2012, Proposition 1.5] and therefore

$$J_g^\pm(\Omega) = \bigcap_{\hat{g} \succ g} J_{\hat{g}}^\pm(\Omega), \quad \Omega \subset M.$$

The embedding for J^- follows by time reversal and the remaining embedding by the union of the embeddings for J^+ and J^-. □

Acknowledgements

We would like to thank Kenji Yajima for useful discussions. The work of Siemssen was supported by a grant of the Polish National Science Center (NCN) based on decision no. DEC-2015/16/S/ST1/00473. The work of Dereziński was supported by the National Science Center under the grant UMO-2014/15/B/ST1/00126.

References

[Bach and Bru 2016] V. Bach and J.-B. Bru, *Diagonalizing quadratic bosonic operators by non-autonomous flow equations*, Mem. Amer. Math. Soc. **1138**, Amer. Math. Soc., Providence, RI, 2016. MR Zbl

[Bachelot 1999] A. Bachelot, "The Hawking effect", *Ann. Inst. H. Poincaré Phys. Théor.* **70**:1 (1999), 41–99. MR Zbl

[Bär et al. 2007] C. Bär, N. Ginoux, and F. Pfäffle, *Wave equations on Lorentzian manifolds and quantization*, European Mathematical Society, Zürich, 2007. MR Zbl

[Beem et al. 1996] J. K. Beem, P. E. Ehrlich, and K. L. Easley, *Global Lorentzian geometry*, 2nd ed., Monographs and Textbooks in Pure and Applied Mathematics **202**, Marcel Dekker, New York, 1996. MR Zbl

[Bernal and Sánchez 2005] A. N. Bernal and M. Sánchez, "Smoothness of time functions and the metric splitting of globally hyperbolic spacetimes", *Comm. Math. Phys.* **257**:1 (2005), 43–50. MR Zbl

[Bogoliubov and Shirkov 1980] N. N. Bogoliubov and D. V. Shirkov, *Introduction to the theory of quantized fields*, John Wiley & Sons, New York, 1980. MR

[Chruściel and Grant 2012] P. T. Chruściel and J. D. E. Grant, "On Lorentzian causality with continuous metrics", *Classical Quantum Gravity* **29**:14 (2012), art. id. 145001. MR Zbl

[Dappiaggi et al. 2018a] C. Dappiaggi, N. Drago, and H. Ferreira, "Fundamental solutions for the wave operator on static Lorentzian manifolds with timelike boundary", preprint, 2018. arXiv

[Dappiaggi et al. 2018b] C. Dappiaggi, H. Ferreira, and A. Marta, "Ground states of a Klein–Gordon field with Robin boundary conditions in global anti-de Sitter spacetime", preprint, 2018. arXiv

[Dereziński and Gérard 2013] J. Dereziński and C. Gérard, *Mathematics of quantization and quantum fields*, Cambridge University Press, 2013. MR Zbl

[Dereziński and Siemssen 2018] J. Dereziński and D. Siemssen, "Feynman propagators on static spacetimes", *Rev. Math. Phys.* **30**:3 (2018), art. id. 1850006. MR Zbl

[Dimock and Kay 1982] J. Dimock and B. S. Kay, "Classical wave operators and asymptotic quantum field operators on curved space-times", *Ann. Inst. H. Poincaré Sect. A* (*N.S.*) **37**:2 (1982), 93–114. MR Zbl

[Drago and Gérard 2017] N. Drago and C. Gérard, "On the adiabatic limit of Hadamard states", *Lett. Math. Phys.* **107**:8 (2017), 1409–1438. MR Zbl

[Friedlander 1975] F. G. Friedlander, *The wave equation on a curved space-time*, Cambridge Monographs on Mathematical Physics **2**, Cambridge University Press, 1975. MR Zbl

[Fulling 1979] S. A. Fulling, "Remarks on positive frequency and Hamiltonians in expanding universes", *Gen. Relativity Gravitation* **10**:10 (1979), 807–824. MR Zbl

[Furlani 1997] E. P. Furlani, "Evolution operators and scattering theory for massive scalar fields on curved spacetimes", *J. Phys. A* **30**:17 (1997), 6065–6079. MR Zbl

[Gérard and Wrochna 2014] C. Gérard and M. Wrochna, "Construction of Hadamard states by pseudo-differential calculus", *Comm. Math. Phys.* **325**:2 (2014), 713–755. MR Zbl

[Gérard and Wrochna 2017] C. Gérard and M. Wrochna, "Hadamard property of the *in* and *out* states for Klein–Gordon fields on asymptotically static spacetimes", *Ann. Henri Poincaré* **18**:8 (2017), 2715–2756. MR Zbl

[Gérard et al. 2017] C. Gérard, O. Oulghazi, and M. Wrochna, "Hadamard states for the Klein–Gordon equation on Lorentzian manifolds of bounded geometry", *Comm. Math. Phys.* **352**:2 (2017), 519–583. MR Zbl

[Häfner 2009] D. Häfner, *Creation of fermions by rotating charged black holes*, Mém. Soc. Math. Fr. (N.S.) **117**, Soc. Math. France, Paris, 2009. MR Zbl

[Heinz 1951] E. Heinz, "Beiträge zur Störungstheorie der Spektralzerlegung", *Math. Ann.* **123** (1951), 415–438. MR Zbl

[Hollands and Wald 2001] S. Hollands and R. M. Wald, "Local Wick polynomials and time ordered products of quantum fields in curved spacetime", *Comm. Math. Phys.* **223**:2 (2001), 289–326. MR Zbl

[Hollands and Wald 2002] S. Hollands and R. M. Wald, "Existence of local covariant time ordered products of quantum field in curved spacetime", *Comm. Math. Phys.* **231**:2 (2002), 309–345. 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

[Kato 1961] T. Kato, "A generalization of the Heinz inequality", *Proc. Japan Acad.* **37** (1961), 305–308. MR Zbl

[Kato 1966] T. Kato, *Perturbation theory for linear operators*, Die Grundlehren der mathematischen Wissenschaften **132**, Springer, 1966. MR Zbl

[Kato 1970] T. Kato, "Linear evolution equations of "hyperbolic" type", *J. Fac. Sci. Univ. Tokyo Sect. I* **17** (1970), 241–258. MR Zbl

[Kay 1978] B. S. Kay, "Linear spin-zero quantum fields in external gravitational and scalar fields, I: A one particle structure for the stationary case", *Comm. Math. Phys.* **62**:1 (1978), 55–70. MR

[Kay and Wald 1991] B. S. Kay and R. M. Wald, "Theorems on the uniqueness and thermal properties of stationary, nonsingular, quasifree states on spacetimes with a bifurcate Killing horizon", *Phys. Rep.* **207**:2 (1991), 49–136. MR Zbl

[Leinfelder and Simader 1981] H. Leinfelder and C. G. Simader, "Schrödinger operators with singular magnetic vector potentials", *Math. Z.* **176**:1 (1981), 1–19. MR Zbl

[Nicolas 2002] J.-P. Nicolas, *Dirac fields on asymptotically flat space-times*, Dissertationes Math. **408**, Instytut Matematyczny Polskiej Akademii Nauk, Warsaw, 2002. MR Zbl

[Pazy 1983] A. Pazy, *Semigroups of linear operators and applications to partial differential equations*, Applied Mathematical Sciences **44**, Springer, 1983. MR Zbl

[Radzikowski 1996] M. J. Radzikowski, "Micro-local approach to the Hadamard condition in quantum field theory on curved space-time", *Comm. Math. Phys.* **179**:3 (1996), 529–553. MR Zbl

[Sanchez and Vickers 2018] Y. S. Sanchez and J. Vickers, "Green operators for low regularity spacetimes", *J. Phys. Conf. Ser.* **968** (2018), art. id. 012011.

[Schmid and Griesemer 2017] J. Schmid and M. Griesemer, "Well-posedness of non-autonomous linear evolution equations in uniformly convex spaces", *Math. Nachr.* **290**:2-3 (2017), 435–441. MR Zbl

[Tanabe 1997] H. Tanabe, *Functional analytic methods for partial differential equations*, Monographs and Textbooks in Pure and Applied Mathematics **204**, Marcel Dekker, New York, 1997. MR Zbl

[Vasy 2017] A. Vasy, "Essential self-adjointness of the wave operator and the limiting absorption principle on Lorentzian scattering spaces", preprint, 2017. arXiv

[Yajima 2011] K. Yajima, "Schrödinger equations with time-dependent unbounded singular potentials", *Rev. Math. Phys.* **23**:8 (2011), 823–838. MR Zbl

Received 16 Oct 2018. Revised 8 Feb 2019. Accepted 6 Mar 2019.

JAN DEREZIŃSKI: jan.derezinski@fuw.edu.pl
Department of Mathematical Methods in Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland

DANIEL SIEMSSEN: siemssen@uni-wuppertal.de
Department of Mathematics and Informatics, University of Wuppertal, Wuppertal, Germany

PURE and APPLIED
ANALYSIS

Vol. 1, No. 2, 2019
dx.doi.org/10.2140/paa.2019.1.263

THE INTERIOR OF DYNAMICAL EXTREMAL BLACK HOLES IN SPHERICAL SYMMETRY

DEJAN GAJIC AND JONATHAN LUK

We study the nonlinear stability of the Cauchy horizon in the interior of *extremal* Reissner–Nordström black holes under *spherical symmetry*. We consider the Einstein–Maxwell–Klein–Gordon system such that the charge of the scalar field is appropriately small in terms of the mass of the background extremal Reissner–Nordström black hole. Given spherically symmetric characteristic initial data which approach the event horizon of extremal Reissner–Nordström sufficiently fast, we prove that the solution extends beyond the Cauchy horizon in $C^{0,\frac{1}{2}} \cap W^{1,2}_{\mathrm{loc}}$, in contrast to the subextremal case (where generically the solution is $C^0 \setminus (C^{0,\frac{1}{2}} \cap W^{1,2}_{\mathrm{loc}})$). In particular, there exist nonunique spherically symmetric extensions which are moreover solutions to the Einstein–Maxwell–Klein–Gordon system. Finally, in the case that the scalar field is chargeless and massless, we additionally show that the extension can be chosen so that the scalar field remains Lipschitz.

1. Introduction

In this paper, we initiate the study of the interior of dynamical extremal black holes. The Penrose diagram corresponding to maximal analytic extremal Reissner–Nordström and Kerr spacetimes is depicted in Figure 1. In particular, if one restricts to a globally hyperbolic subset with an (incomplete) asymptotically flat Cauchy hypersurface (see the region $D^+(\Sigma)$ in Figure 1), then these spacetimes possess smooth *Cauchy horizons* $\mathcal{CH}^+$, whose stability property is the main object of study of this paper.

MSC2010: 35L51, 83C05, 83C57, 83C75.
Keywords: extremal black hole, black hole interior, Cauchy horizon, strong cosmic censorship conjecture.

Since the pioneering work [Poisson and Israel 1989] and the seminal works [Dafermos 2003; 2005] in the spherically symmetric setting, we now have a rather complete understanding of the interior of dynamical black holes which approach *subextremal* limits along the event horizon, at least regarding the *stability* of the Cauchy horizons. The works [Costa et al. 2015b; Dafermos 2003; 2005; 2014; Franzen 2016; Hintz 2017; Kommemi 2013; Luk 2018] culminated in the recent work [Dafermos and Luk 2017], which proves the C^0 stability of the Kerr Cauchy horizon without any symmetry assumptions; i.e., they show that whenever the exterior region of a black hole approaches a subextremal, strictly rotating Kerr exterior, then maximal Cauchy evolution can be extended across a nontrivial piece of Cauchy horizon as a Lorentzian manifold with continuous metric. Moreover, it is expected that for a generic subclass of initial data, the Cauchy horizon is an *essential weak null singularity*, so that there is no extension beyond the Cauchy horizon as a weak solution to the Einstein equations; see [Dafermos 2005; Gleeson 2016; Luk and Oh 2017a; 2017b; Luk and Sbierski 2016; Van de Moortel 2018] for recent progress and discussion.

On the other hand, much less is known about dynamical black holes which become extremal along the event horizon. Mathematically, the only partial progress was made for a related linear problem, namely the study of the linear scalar wave equation on extremal black hole backgrounds. For the linear scalar wave equation, the first author established [Gajic 2017a; 2017b] that in the extremal case, the Cauchy horizon is *more stable* than its subextremal counterpart. In particular, the solutions to linear wave equations are not only bounded, as in the subextremal case, but they in fact obey higher regularity bounds which *fail* in the subextremal case (see Section 1A for a more detailed discussion). Extrapolating from the linear result, it may be conjectured that in the interior of a black hole which approaches an extremal black hole along the event horizon, not only does the solution remain continuous up to the Cauchy horizon as in the subextremal case, but in fact there are nonunique extensions beyond the Cauchy horizon *as weak solutions*. This picture, if true, would also be consistent with the numerical study of this problem by Murata, Reall and Tanahashi [Murata et al. 2013].

In this paper, we prove that this picture holds in a simple nonlinear setting. More precisely, we study the Einstein–Maxwell–Klein–Gordon system of equations with spherically symmetric initial data (see Section 3 for further discussions on the system). We solve for a quintuple $(\mathcal{M}, g, \phi, A, F)$, where $(\mathcal{M}, g)$ is a Lorentzian metric, ϕ is a complex-valued function on $\mathcal{M}$, and A and F are real 1- and 2-forms on $\mathcal{M}$ respectively. The system of equations is

$$
\begin{cases}
\mathrm{Ric}_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = 8\pi (\mathbb{T}^{(\mathrm{sf})}_{\mu\nu} + \mathbb{T}^{(\mathrm{em})}_{\mu\nu}), \\
\mathbb{T}^{(\mathrm{sf})}_{\mu\nu} = \frac{1}{2} D_\mu\phi \overline{D_\nu\phi} + \frac{1}{2}\overline{D_\mu\phi} D_\nu\phi - \frac{1}{2} g_{\mu\nu}((g^{-1})^{\alpha\beta} D_\alpha\phi\overline{D_\beta\phi} + \mathfrak{m}^2|\phi|^2), \\
\mathbb{T}^{(\mathrm{em})}_{\mu\nu} = (g^{-1})^{\alpha\beta} F_{\mu\alpha} F_{\nu\beta} - \frac{1}{4} g_{\mu\nu} (g^{-1})^{\alpha\beta} (g^{-1})^{\gamma\sigma} F_{\alpha\gamma} F_{\beta\sigma}, \\
(g^{-1})^{\alpha\beta} D_\alpha D_\beta \phi = \mathfrak{m}^2 \phi, \\
F = dA, \\
(g^{-1})^{\alpha\mu} \nabla_\alpha F_{\mu\nu} = 2\pi i \mathfrak{e} (\phi \overline{D_\nu\phi} - \bar{\phi} D_\nu\phi).
\end{cases}
\tag{1-1}
$$

Here, ∇ denotes the Levi–Civita connection associated to the metric g, and Ric and R denote the Ricci tensor and the Ricci scalar, respectively. We also use the notation $D_\alpha = \nabla_\alpha + i\mathfrak{e}A_\alpha$, and $\mathfrak{m} \geq 0$, $\mathfrak{e} \in \mathbb{R}$ are fixed constants. The extremal Reissner–Nordström solution (see Section 3) is a special solution to (1-1) with a vanishing scalar field ϕ.

In the following we will restrict the parameters so that $|\mathfrak{e}|$ is sufficiently small in terms of M. More precisely, we assume

$$1-(10+5\sqrt{6}-3\sqrt{9+4\sqrt{6}})|\mathfrak{e}|M>0. \tag{1-2}$$

Under the assumption (1-2), our main result can be stated informally as follows (we refer the reader to Theorem 5.1 for a precise statement):

Theorem 1.1. *Consider the characteristic initial value problem to* (1-1) *with spherically symmetric smooth characteristic initial data on two null hypersurfaces transversely intersecting at a* 2*-sphere. Assume that one of the null hypersurfaces is affine complete and that the data approach the event horizon of extremal Reissner–Nordström at a sufficiently fast rate.*

Then, the solution to (1-1) *arising from such data, when restricted to a sufficiently small neighborhood of timelike infinity* (*i.e., a neighborhood of* i^+ *in Figure 1*), *satisfies the following properties*:

- *It possesses a nontrivial Cauchy horizon.*
- *The scalar field, the metric, the electromagnetic potential* (*in an appropriate gauge*) *and the charge can be extended in* (*spacetime*) $C^{0,\frac{1}{2}}\cap W^{1,2}_{\mathrm{loc}}$ *up to the Cauchy horizon. Moreover, the Hawking mass* (2-10) *can be extended continuously up to the Cauchy horizon.*
- *The metric converges to that of extremal Reissner–Nordström towards timelike infinity and the scalar field approaches* 0 *towards timelike infinity in an appropriate sense.*

Moreover, the maximal globally hyperbolic solution is future extendible (*nonuniquely*) *as a spherically symmetric solution to* (1-1).

Remark 1.2 (solutions with regularity below C^2). The extensions of the solution we construct have regularity below (spacetime) C^2 and as such do not make sense as classical solutions. As is well known, however, the Einstein equations admit a *weak formulation* which makes sense already if the metric is in (spacetime) $C^0\cap W^{1,2}_{\mathrm{loc}}$ and the stress-energy-momentum tensor is in spacetime L^1_{loc} [Geroch and Traschen 1987]. The weak formulation can be recast geometrically as follows: given a smooth (3+1)-dimensional manifold $\mathcal{M}$, a $C^0_{\mathrm{loc}}\cap W^{1,2}_{\mathrm{loc}}$ Lorentzian metric g and an L^1_{loc} symmetric 2-tensor T, we say that the Einstein equation $\mathrm{Ric}(g)-\frac{1}{2}gR(g)=8\pi T$ is satisfied weakly if for all smooth and compactly supported vector fields X, Y,

$$\int_{\mathcal{M}}((\nabla_\mu X)^\mu(\nabla_\nu Y)^\nu-(\nabla_\mu X)^\nu(\nabla_\nu Y)^\mu)=8\pi\int_{\mathcal{M}}\big(T(X,Y)-\tfrac{1}{2}g(X,Y)\,\mathrm{tr}_g\,T\big).$$

It is easy to check that any classical solution is indeed a weak solution in the sense above. Moreover, the extensions that we construct in Theorem 1.1 have more than sufficient regularity to be interpreted in the sense above.

However, in our setting we do not need to use the notion in [Geroch and Traschen 1987]. Instead, we introduce a stronger notion of solutions, defined on a quotient manifold for which we quotiented

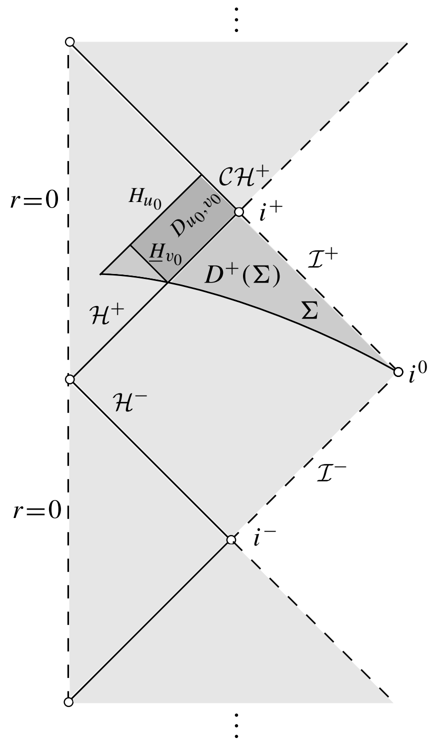

Figure 1. Maximal analytically extended extremal Reissner–Nordström.

out the spherical symmetry; see Definition 10.4. This class of solutions — even though they are not classical solutions — should be interpreted as *strong solutions* (instead of just weak solutions) since a well-posedness theory can be developed for them;[1] see Section 10.

Remark 1.3 (contrast with the subextremal case). Like in the subextremal case, the solution extends in C^0 to the Cauchy horizon. However, the $C^{0,\frac{1}{2}} \cap W^{1,2}_{\mathrm{loc}}$ extendibility and the finiteness of the Hawking mass, as well as the extendibility as a spherically symmetric solution, stand in *contrast* to the subextremal case. In particular, according to the results of [Luk and Oh 2017b; $\geq$ 2019], see also [Dafermos 2005], there are solutions which asymptote to subextremal Reissner–Nordström black holes in the exterior region such that the Hawking mass blows up at the Cauchy horizon, and the solution cannot be extended as a spherically symmetric solution to the Einstein–Maxwell-scalar field system.[2]

Remark 1.4 (regularity of the metric and extensions as solutions to (1-1)). The fact that we can extend the solutions beyond the Cauchy horizon is intimately connected to the regularity of the solutions up to

[1] In fact, in order to develop a well-posedness theory for strong solutions, one can even drop the assumption of spherical symmetry, and instead require additional regularity along the "spherical directions" with respect to an appropriately defined double null foliation gauge; see [Luk and Rodnianski 2017] for details.

[2] Though the estimates in [Luk and Oh 2017b] strongly suggest that the scalar field ceases to be in $W^{1,2}_{\mathrm{loc}}$ for any C^0 extension of the spacetime, this remains an open problem unless spherical symmetry is imposed. In particular, it is not known whether the solutions constructed in [Luk and Oh 2017b; $\geq$ 2019] can be extended as weak solutions to the Einstein–Maxwell-scalar field system if no spherical symmetry assumption is imposed.

the Cauchy horizon. In particular this relies on the fact the metric, the scalar field and the electromagnetic potential remain in (spacetime) $C^0 \cap W^{1,2}_{\text{loc}}$. In fact, the solutions are at a level of regularity for which the Einstein equations are still locally *well-posed*.[3] One can therefore construct extensions beyond the Cauchy horizon by solving appropriate characteristic initial value problems; see Section 10.

In this connection, note that we emphasized in the statement of the theorem that the solution can be extended beyond the Cauchy horizon as a spherically symmetric solution to (1-1). The emphasis on the spherical symmetry of the extension is made mostly to contrast with the situation in the subextremal case (see Remark 1.3). This should not be understood as implying that the extensions necessarily are spherically symmetric: In fact, with the bounds that we establish in this paper, one can in principle construct using the techniques in [Luk and Rodnianski 2017] extensions (still as solutions to (1-1)) without any symmetry assumptions (see footnote 1).

Remark 1.5 (assumptions on the event horizon). The assumptions we impose on the event horizon are consistent with the expected late-time behavior of the solutions in the exterior region of the black hole, at least in the $\mathfrak{e} = \mathfrak{m} = 0$ case if one extrapolates from numerical results [Murata et al. 2013]. In particular, the transversal derivative of the scalar field is not required to decay along the event horizon, and is therefore consistent with the Aretakis instability [2015]. Of course, in order to completely understand the structure of the interior, one needs to prove that the decay estimates along the event horizon indeed hold for general dynamical solutions approaching these extremal black holes. This remains an open problem.

Remark 1.6 (range of parameters of $\mathfrak{e}$ and M). Our result only covers a limited range of parameters of the model; see (1-2). This restriction comes from a Hardy-type estimate used to control the renormalized energy (see Sections 1B and 8B) and we have not made an attempt to obtain the sharp range of parameters.

Remark 1.7 (the $\mathfrak{m} = \mathfrak{e} = 0$ case and higher regularity for ϕ). In the special case $\mathfrak{m} = \mathfrak{e} = 0$, the analysis is simpler and we obtain a stronger result; namely, we show that the scalar field in fact is Lipschitz up to the Cauchy horizon (see Theorem 5.5).

Remark 1.8 (the $\mathfrak{m} \neq 0$, $\mathfrak{e} \neq 0$ case). While the result we obtain in the $\mathfrak{m} \neq 0$, $\mathfrak{e} \neq 0$ case is weaker, the general model allows for the charge of the Maxwell field to be nonconstant, and serves as a better model problem for the stability of the extremal Cauchy horizon without symmetry assumptions. Another reason that we do not restrict ourselves to the simpler $\mathfrak{m} = \mathfrak{e} = 0$ case is that in the $\mathfrak{m} = \mathfrak{e} = 0$ case, extremal black holes do not naturally arise dynamically:

- There are no one-ended black holes with nontrivial Maxwell field with regular data on $\mathbb{R}^3$ since in that setting the Maxwell field necessarily blows up at the axis of symmetry.

[3]Note that in general the Einstein equations are not locally well-posed with initial data only in $C^0 \cap W^{1,2}$. Nevertheless, when there is spherical symmetry (away from the axis of symmetry), or at least when there is additional regularity in the spherical directions (see footnote 1), one can indeed develop a local well-posedness theory with such low regularity.

- In the two-ended case, given future-admissible[4] (in the sense of [Dafermos 2014]) initial data, the solution always approaches *subextremal* black holes in each connected component of the exterior region [Kommemi 2013; Luk and Oh 2017b].

On the other hand, if $\mathfrak{e} \neq 0$, then in principle there are no such obstructions.[5]

Remark 1.9 (geometry of the black hole interior). One feature of the black hole interior of extremal Reissner–Nordström is that it is free of radial trapped surfaces — a stark contrast to the subextremal case (where every sphere of symmetry is the black hole interior is trapped!). Let us note that this feature has sometimes been taken as the defining feature of spherically symmetric extremal black holes; see for instance [Israel 1986]. We will not use this definition in this paper, and when talking about "extremal black holes", we will only be referring to black holes which converge to a stationary extremal black hole along the event horizon as in Theorem 1.1. Indeed, while our estimates imply that for the solutions in Theorem 1.1 the geometry of the black hole interior is close to that of extremal Reissner–Nordström, it remains an open problem in the general case whether the black hole interior contains any radial trapped surface.[6]

The fact that the extremal Cauchy horizons are "more stable" than their subextremal counterparts can be thought of as related to the vanishing of the surface gravity in the extremal case. Recall that in both the extremal and subextremal charged Reissner–Nordström spacetimes, there is a global infinite blue shift effect such that the frequencies of signals sent from the exterior region into the black hole are shifted infinitely to the blue [Penrose 1968]. As a result, this gives rise to an instability mechanism. Indeed, Sbierski [2015] showed[7] that for the linear scalar wave equation on *both* extremal and subextremal Reissner–Nordström spacetime, there exist *finite energy* Cauchy data which give rise to solutions that are not $W^{1,2}_{\mathrm{loc}}$ at the Cauchy horizon. On the other hand, as emphasized in [Sbierski 2015], these types of considerations do not take into account the *strength* of the blue shift effect and do not give information on the behavior of the solutions arising from more localized data. Heuristically, for localized data, one needs to quantify the amplification of the fields by a "local" blue shift effect at the Cauchy horizon, whose strength can be measured by the surface gravity. In this language, what we see in Theorem 1.1 is a manifestation of the vanishing of the local blue shift effect at the extremal limit.

This additional stability of the extremal Cauchy horizon due to the vanishing of the surface gravity may at the first sight seem to make the problem simpler than its subextremal counterpart. Ironically, from

[4]The future-admissibility condition can be thought of as an analogue of the physical "no antitrapped surface" assumption in the one-ended case.

[5]Nevertheless, it is an open problem to construct a dynamical black hole with regular data that settles down to an extremal black hole.

[6]Note however that in the $\mathfrak{e} = \mathfrak{m} = 0$ case, if we assume in addition that $\partial_U r < 0$ everywhere along the event horizon, we can in principle modify the monotonicity argument of [Kommemi 2013] in establishing the subextremality of two-ended black holes (see Remark 1.8) to show that the interior in the extremal case is free of radial trapped surfaces. Indeed, the argument of [loc. cit.] exactly proceeds by (1) showing that there are no interior trapped surfaces in the interior of extremal black holes and (2) establishing a contradiction with the future-admissibility condition. See also the appendix of [Luk and Oh 2017b].

[7]This statement is technically not explicitly proven in [Sbierski 2015], but it follows from the result there together with routine functional analytic arguments.

the point of view of the analysis, the local blue shift effect in the subextremal case in fact provides a way to prove stable estimates! This method fails at the extremal limit.

To further illustrate this, first note that in the presence of the blue shift effect, one necessarily proves *degenerate* estimates. By exploiting the geometric features of the interior of subextremal black holes, the following can be shown: when proving degenerate energy-type estimates, by choosing the weights in the estimates appropriately, one can prove that the bulk spacetime integral terms (up to a small error) have a good sign, and can be used to control the error terms; see the discussions in the introduction of [Dafermos and Luk 2017]. As a consequence, one can in fact obtain a stability result for a large class of nonlinear wave equations with a null condition, irrespective of the precise structure of the linearized system. This observation is also at the heart of [loc. cit.].

In the extremal case, however, it is not known how to obtain a sufficiently strong coercive bulk spacetime integral term when proving energy estimates. Moreover, if one naively attempts to control the spacetime integral error terms by using the boundary flux terms of the energy estimate and Grönwall's lemma, one encounters a logarithmic divergence. To handle the spacetime integral error terms, we need to use more precise structures of the equations, and we will show that there is a cancellation in the weights appearing in the bulk spacetime error terms. This improvement of the weights then allows the bulk spacetime error terms to be estimated using the boundary flux terms and a suitable adaptation[8] of Grönwall's lemma. In particular, we need to use the fact that (1) a renormalized energy can be constructed to control the scalar field and the Maxwell field *simultaneously*, and that (2) the equations for the matter fields and the equations for the geometry are "sufficiently decoupled" (see Section 1B). These structures seem to be specific to the spherically symmetric problem: to what extent this is relevant to the general problem of stability of extremal Cauchy horizons without symmetry assumptions remains to be seen.

The study of the stability properties of subextremal Cauchy horizons is often motivated by the *strong cosmic censorship conjecture*. The conjecture states that solutions arising from generic asymptotically flat initial data are *inextendible* as suitably regular Lorentzian manifolds. In particular, the conjecture, if true, would imply that *smooth* Cauchy horizons, which are present in both extremal and subextremal Reissner–Nordström spacetimes, are not generic in black hole interiors. As we have briefly discussed above, there are various results establishing this in the subextremal case; see for example [Dafermos 2005; Luk and Oh 2017b; ≥ 2019; Van de Moortel 2018]. In fact, one expects that generically, if a solution approaches a subextremal black hole at the event horizon, then the spacetime metric does not admit $W^{1,2}_{\text{loc}}$ extensions beyond the Cauchy horizon; see discussions in [Dafermos and Luk 2017]. On the other hand, our result shows that at least in our setting, this does not occur for extremal Cauchy horizons. Nevertheless, since one expects that generic dynamical black hole solutions are nonextremal, our results, which only concern black holes that become extremal in the limit, are in fact irrelevant to the strong cosmic censorship conjecture. In particular, provided that extremal black holes are indeed nongeneric as is expected, the rather strong stability that we prove in this paper does not pose a threat to cosmic censorship.

[8]In fact, using the smallness parameters in the problem, this will be implemented without explicitly resorting to Grönwall's lemma.

Finally, even though our result establishes the $C^{0,\frac{1}{2}} \cap W^{1,2}_{\mathrm{loc}}$ stability of extremal Cauchy horizons in spherical symmetry, it still leaves open the possibility of some higher derivatives of the scalar field or the metric blowing up (say, the C^k norm blows up for some $k \in \mathbb{N}$). Whether this occurs or not for generic data remains an open problem.

1A. ***Previous results on the linear wave equation.*** In this section, we review the results established in [Gajic 2017a; 2017b] concerning the behaviour of solutions to the linear wave equation $\Box_g \phi = 0$ in the interior of extremal black holes. The results concern the following cases:

- general solutions on extremal Reissner–Nordström,
- general solutions on extremal Kerr–Newman *with sufficiently small specific angular momentum*,
- *axisymmetric* solutions on extremal Kerr.

In each of these cases, the following results are proven (in a region sufficiently close to timelike infinity):

(A) ϕ is bounded and continuously extendible up to the Cauchy horizon.

(B) ϕ is $C^{0,\alpha}$ up to the Cauchy horizon for all $\alpha \in (0, 1)$.

(C) ϕ has finite energy and is $W^{1,2}_{\mathrm{loc}}$ up to the Cauchy horizon.

As we mentioned earlier, these results are in contrast with the subextremal case; (A) holds also for subextremal Reissner–Nordström and Kerr [Franzen 2016; Hintz 2017], (B) is *false*[9] on subextremal Reissner–Nordström [Dafermos 2005; Angelopoulos et al. 2018] and (C) is *false* on both subextremal Reissner–Nordström and Kerr [Luk and Oh 2017a; Luk and Sbierski 2016]. (In fact, in subextremal Reissner–Nordström, generic solutions fail to be in $W^{1,p}_{\mathrm{loc}}$ for all $p > 1$; see [Dafermos 2005; Angelopoulos et al. 2018; Gleeson 2016].)

At this point, it is not clear whether the estimates in [Gajic 2017a; 2017b] are sharp. In the special case of spherically symmetric solutions on extremal Reissner–Nordström, [Gajic 2017a] proves that the solution is in fact C^1 up to the Cauchy horizon. Moreover, if one assumes more precise asymptotics along the event horizon (motivated by numerics), then it is shown that spherically symmetric solutions are C^2.

Our results in the present paper can be viewed as an extension of those in [Gajic 2017a] to a nonlinear setting. In particular, we show that even in the nonlinear (although only spherically symmetric) setting, ϕ still obeys (A) and (C), and satisfies (B) in the subrange $\alpha \in \left(0, \frac{1}{2}\right]$. Moreover, the metric components, the electromagnetic potential, and the charge, in appropriate coordinate systems and gauges, verify similar bounds.

1B. ***Ideas of the proof.***

Model linear problems. The starting point of the analysis is to study *linear systems of wave equations* on fixed extremal Reissner–Nordström background. A simple model of such a system is the following (where $a, b, c, d \in \mathbb{R}$):

$$\Box_{g_{\mathrm{eRN}}} \phi = a\phi + b\psi, \quad \Box_{g_{\mathrm{eRN}}} \psi = c\psi + d\phi. \tag{1-3}$$

[9] This result is not explicitly stated in the literature, but can be easily inferred given the sharp asymptotics for generic solutions in [Angelopoulos et al. 2018] and the blowup result in [Dafermos 2005] appropriately adapted to the linear setting.

It turns out that in the extremal setting, we still lack an understanding of solutions to such a model system in general. (This is in contrast to the subextremal case, where the techniques of [Franzen 2016; Dafermos and Luk 2017] show that solutions to the analogue of (1-3) are globally bounded for any fixed $a, b, c, d \in \mathbb{R}$.)

Instead, we can only handle some subcases of (1-3). Namely, we need $a \geq 0,\ c \geq 0$ and $b = d = 0$. Put differently, this means that we can only treat *decoupled* Klein–Gordon equations with *nonnegative mass*. Remarkably, as we will discuss later, although the linearized equations of (1-1) around extremal Reissner–Nordström are more complicated than decoupled Klein–Gordon equations with nonnegative masses, one can find a structure in the equations so that the ideas used to handle special subcases of (1-3) can also apply to the nonlinear problem at hand.

Estimates for linear fields using ideas in [Gajic 2017a]. The most simplified case of (1-3) is the linear wave equation with zero potential $\Box_{g_{\mathrm{eRN}}}\phi = 0$. In the interior of extremal Reissner–Nordström spacetime, this has been treated by the first author in [Gajic 2017a]. That paper is based on the vector field multiplier method, which obtains L^2-based energy estimates for the derivatives of ϕ. The vector field multiplier method can be summarized as follows: Consider the stress-energy-momentum tensor

$$\mathbb{T}_{\mu\nu} = \partial_\mu\phi\, \partial_\nu\phi - \tfrac{1}{2} g_{\mu\nu}(g^{-1})^{\alpha\beta}\, \partial_\alpha\phi\, \partial_\beta\phi.$$

For a well-chosen vector field V, one can then integrate the identity for the current $\mathbb{T}_{\mu\nu} V^\nu$,

$$\nabla^\mu(\mathbb{T}_{\mu\nu} V^\nu) = \tfrac{1}{2}\mathbb{T}_{\mu\nu}(\nabla^\mu V^\nu + \nabla^\nu V^\mu),$$

to obtain an identity relating a spacetime integral and a boundary integral.

When V is casual, future-directed and Killing, the above identity yields a coercive conservation law. In the interior of extremal Reissner–Nordström $\partial_t = \frac{1}{2}(\partial_v + \partial_u)$ (see the definition of (u, v)-coordinates in Section 3) is one such vector field. This vector field, however, is too degenerate near the event horizon and the Cauchy horizon, and one expects the corresponding estimates to be of limited use in a nonlinear setting. A crucial observation in [Gajic 2017a] is that the vector field $V = |u|^2\, \partial_u + v^2\, \partial_v$ (in Eddington–Finkelstein double null coordinates, see Section 3) can give a useful, stronger, estimate. More precisely, $V = |u|^2\, \partial_u + v^2\, \partial_v$ has the following properties:

(1) V is a nondegenerate vector field at both the event horizon and the Cauchy horizon.

(2) V is causal and future-directed. Hence, together with (1), this shows that the current associated to V, when integrated over null hypersurfaces, corresponds to nondegenerate energy.

(3) Moreover, although V is not Killing, $\nabla^\mu V^\nu + \nabla^\nu V^\mu$ has a crucial cancellation[10] so that the spacetime error terms can be controlled by the boundary integrals.

These observations allow us to close the estimate and to obtain nondegenerate L^2 control for the derivatives of ϕ. Furthermore, the boundedness of such energy implies

$$|\phi|(u, v) \lesssim \mathrm{Data}(v) + |u|^{-\frac{1}{2}}, \tag{1-4}$$

[10]More precisely, $\nabla^v V^u + \nabla^u V^v = -\frac{1}{2}\Omega^{-2}(\partial_u u^2 + \partial_v v^2 + \Omega^{-2}(u^2\, \partial_u + v^2\, \partial_v)\Omega^2) \lesssim \Omega^{-2}$, whereas each single term, e.g., $\Omega^{-2}\, \partial_v v^2 \sim v\Omega^{-2}$, behaves worse as $|u|, v \to \infty$. Without this cancellation, the estimate exhibits a logarithmic divergence.

where, provided the data term decays in v, $\phi \to 0$ as $|u|, v \to \infty$. Moreover, using the embedding $W^{1,2} \hookrightarrow C^{0,\frac{1}{2}}$ in one dimension, we also conclude that $\phi \in C^{0,\frac{1}{2}}$.

In spherical symmetry, it is in fact possible to control the solution to the linear wave equation up to the Cauchy horizon using only the method of characteristics.[11] Here, however, there is an additional twist to the problem. We will need to control solutions to the *Klein–Gordon* equation with *nonzero mass*[12]

$$\Box_{g_{\mathrm{eRN}}}\phi = \mathfrak{m}^2\phi.$$

For this scalar equation, however, whenever the mass is nonvanishing, using the method of characteristics and naïve estimates leads to potential logarithmic divergences. Nonetheless, if $\mathfrak{m}^2 > 0$, the argument above which makes use of the vector field multiplier method can still be applied. In this case, one defines instead the stress-energy-momentum tensor as

$$\mathbb{T}_{\mu\nu} = \partial_\mu\phi\,\partial_\nu\phi - \tfrac{1}{2}g_{\mu\nu}((g^{-1})^{\alpha\beta}\,\partial_\alpha\phi\,\partial_\beta\phi + \mathfrak{m}^2\phi^2).$$

As it turns out, the observations (1), (2), and (3) still hold in the $\mathfrak{m}^2 > 0$ case for the vector field $V = |u|^2\,\partial_u + v^2\,\partial_v$. In particular, there is a crucial cancellation in the bulk term as above, which removes the logarithmically nonintegrable term and allows one to close the argument. Again, this consequently yields also decay estimates and $C^{0,\frac{1}{2}}$ bounds for ϕ.

Let us recap what we have achieved for the model problem (1-3). The discussions above can be used to deal fully with the case $a \geq 0$, $c \geq 0$ and $b = d = 0$. If $a < 0$ or $c < 0$, one still has a cancellation in the bulk spacetime term, but the boundary terms are not nonnegative. If, on the other hand, $b \neq 0$ or $d \neq 0$, then in general one sees a bulk term which is exactly borderline and leads to logarithmic divergence.

Renormalized energy estimates for the matter fields. In order to attack our problem at hand, the first step is to understand the propagation of the matter field even without coupling to gravity. In other words, we need to control the solution to the Maxwell-charged Klein–Gordon system in the interior of *fixed* extremal Reissner–Nordström. (A special case of this, when $\mathfrak{m} = \mathfrak{e} = 0$ is exactly what has been studied in [Gajic 2017a].)

One difficulty that arises in controlling the matter fields is that when $\mathfrak{e} \neq 0$, the energy estimates for the scalar field couple with estimates for the Maxwell field. If one naïvely estimates each field separately, while treating the coupling as error terms, one encounters logarithmically divergent terms similar to those appearing when controlling (1-3) for $b \neq 0$ or $d \neq 0$. Instead, we prove coupled estimates for the scalar field and the Maxwell field simultaneously.

In order to prove coupled energy estimates, a natural first attempt would be to use the full stress-energy-momentum tensor (i.e., the sum $\mathbb{T} = \mathbb{T}^{(\mathrm{sf})} + \mathbb{T}^{(\mathrm{em})}$) and consider the current $\mathbb{T}_{\mu\nu}V^\nu$, where

[11] In fact, as in shown in [Gajic 2017a], the method of characteristics, when combined with the energy estimates, yields more precise estimates when the initial data are assumed to be spherically symmetric. While [loc. cit.] does not give a proof of the estimates in the spherically symmetric case purely based on the method characteristics, such a proof can be inferred from the proof of Theorem 5.5 in Section 11.

[12] As we will discuss below, the need to consider the Klein–Gordon equation with nonzero mass stems not only from our desire to include mass in the matter field in (1-1), but when attempting to control the metric components, one naturally encounters a Klein–Gordon equation with positive mass.

$V = |u|^2\,\partial_u + v^2\,\partial_v$ as in [Gajic 2017a]. However, since the charge is expected to asymptote to a *nonzero* value (as it does initially along the event horizon), this energy is *infinite*!

Instead, we *renormalize* the energy to take out the infinite contribution from the background charge. We are then faced with two new issues:

- The renormalized energy is not manifestly nonnegative.
- Additional error terms are introduced.

Here, it turns out that one can use a Hardy-type inequality to show that the renormalized energy is coercive. (This is the step for which we need a restriction on the parameters of the problem.) Moreover, the additional spacetime error terms that are introduced in the energy estimates also exhibit the cancellation described in footnote 10 on page 271.

Estimates for the metric components. Having understood the uncoupled Maxwell–Klein–Gordon system, we now discuss the problem where the Maxwell–Klein–Gordon system is coupled with the Einstein equations. First, we write the metric in *double null* coordinates:

$$g = -\Omega^2(u, v)\,du\,dv + r^2(u, v)\sigma_{\mathbb{S}^2},$$

where $\sigma_{\mathbb{S}^2}$ is the standard round metric on $\mathbb{S}^2$ (with radius 1). In such a gauge, the metric components r and Ω satisfy nonlinear wave equations with ϕ and $\partial\phi$ as sources. In addition, r satisfies the Raychaudhuri equations, which can be interpreted as constraint equations.

We control r directly using the method of characteristics. As noted before, using the method of characteristics for wave equations with nontrivial zeroth-order terms[13] leads to potentially logarithmically divergent terms. To circumvent this, we use both the wave equation and the Raychaudhuri equations satisfied by r: using different equations in different regions of spacetime, one can show using the method of characteristics that

$$|r - M| \lesssim v^{-1} + |u|^{-1}, \quad |\partial_v r| \lesssim v^{-2}, \quad |\partial_u r| \lesssim |u|^{-2}.$$

For Ω, instead of controlling it directly, we bound the difference $\log\Omega - \log\Omega_0$, where Ω_0 corresponds to the metric component of the background extremal Reissner–Nordström spacetime. We will control it using the wave equation satisfied by Ω; see (2-2). Again, as is already apparent in the discussion of (1-3), to obtain wave equation estimates, we need to use the structure of the equation. Using the estimates for ϕ and r, the equation for $\log\Omega - \log\Omega_0$ can be thought of as follows (modulo terms that are easier to deal with and are represented by $\cdots$):

$$\partial_u\partial_v \log\frac{\Omega}{\Omega_0} = -\tfrac{1}{4}M^2(e^{\log\Omega^2} - e^{\log\Omega_0^2}) + \cdots . \tag{1-5}$$

Thus, when Ω is close to Ω_0, (1-5) can be viewed as a nonlinear perturbation of the Klein–Gordon equation with positive mass, which is moreover essentially decoupled from the other equations. Hence, as long as we can control the error terms and justify the approximation (1-5), we can handle this equation

[13]The wave equation for r indeed has such zeroth order terms; see (2-1).

using suitable modifications of the ideas discussed before. In particular, an appropriate modification of (1-4) implies that $\Omega \to \Omega_0$ in a suitable sense as $|u|, v \to \infty$.

Finally, revisiting the argument for the energy estimates for Maxwell–Klein–Gordon, one notes that it can in fact be used to control solutions to the Maxwell–Klein–Gordon system on a *dynamical* background such that r and $\log \Omega$ approach their Reissner–Nordström values with a sufficiently fast polynomial rate as $|u|, v \to \infty$. In particular, the estimates we described above for the metric components are sufficient for us to set up a bootstrap argument to simultaneously control the scalar field and the geometric quantities.

Note that in terms of regularity, we have closed the problem at the level of the (nondegenerate) L^2 norm of first derivatives of the metric components and scalar field. As long as $r > 0$, this is the level of regularity for which well-posedness holds in spherical symmetry. It follows that we can also construct an extension which is a solution to (1-1).

1C. *Structure of the paper.* The remainder of the paper is structured as follows. In Section 2, we will introduce the geometric setup and discuss (1-1) in spherical symmetry. In Section 3, we discuss the geometry of the interior of the extremal Reissner–Nordström black hole. In Section 4, we introduce the assumptions on the characteristic initial data. In Section 5, we give the statement of the main theorem (Theorem 5.1, see also Theorem 5.5). In Section 6, we begin the proof of Theorem 5.1 and set up the bootstrap argument. In Section 7, we prove the pointwise estimates. In Section 8, we prove the energy estimates. In Section 9, we close the bootstrap argument and show that the solution extends up to the Cauchy horizon. In Section 10, we complete the proof of Theorem 5.1 by constructing a spherically symmetric solution which extends beyond the Cauchy horizon. In Section 11, we prove additional estimates in the case $\mathfrak{m} = \mathfrak{e} = 0$.

2. Geometric preliminaries

2A. *Class of spacetimes.* In this paper, we consider *spherically symmetric spacetimes* $(\mathcal{M}, g)$ with $\mathcal{M} = \mathcal{Q} \times \mathbb{S}^2$ such that the metric g takes the form

$$g = g_{\mathcal{Q}} + r^2(d\theta^2 + \sin^2\theta\, d\varphi^2),$$

where $(\mathcal{Q}, g_{\mathcal{Q}})$ is a smooth (1+1)-dimensional Lorentzian spacetime and $r : \mathcal{Q} \to \mathbb{R}_{>0}$ is smooth and can geometrically be interpreted as the area radius of the orbits of spherical symmetry. We assume that $(\mathcal{Q}, g_{\mathcal{Q}})$ admits a global double null foliation,[14] so that we write the metric g in double null coordinates as

$$g = -\Omega^2(u, v)\, du\, dv + r^2(u, v)(d\theta^2 + \sin^2\theta\, d\varphi^2),$$

for some smooth and strictly positive function Ω^2 on $\mathcal{Q}$.

[14]Note that for sufficiently regular $g_{\mathcal{Q}}$, the metric can always be put into double null coordinates *locally*. Hence the assumption is only relevant for global considerations. We remark that the interior of extremal Reissner–Nordström spacetimes can be written (globally) in such a system of coordinates (see Section 3) and so can spacetimes that arise from spherically symmetric perturbations of the interior of extremal Reissner–Nordström, which we consider in this paper.

2B. ***The Maxwell field and the scalar field.*** We will assume that both the Maxwell field F and the scalar field ϕ in (1-1) are spherically symmetric. For ϕ, this means that ϕ is constant on each spherical orbit, and can be thought of as a function on $\mathcal{Q}$.

For the Maxwell field, spherical symmetry means that there exists a function Q on $\mathcal{Q}$, so that the Maxwell field F takes the following form

$$F = \frac{Q}{2(\boldsymbol{\pi}^* r)^2}\boldsymbol{\pi}^*(\Omega^2\, du \wedge dv),$$

where $\boldsymbol{\pi}$ denotes the projection map $\boldsymbol{\pi} : \mathcal{M} \to \mathcal{Q}$. We will call Q the *charge* of the Maxwell field.

2C. ***The system of equations.*** In this subsection, we write down the symmetry-reduced equations in a double null coordinate system as in Section 2A (see [Kommemi 2013] for details). Before we write down the equations, we introduce the following notation for the covariant derivative operator with respect to the 1-form A:

$$D_\mu \phi = \partial_\mu \phi + i\mathfrak{e} A_\mu \phi.$$

2C1. *Propagation equations for the metric components.*

$$r\partial_u\,\partial_v r = -\tfrac{1}{4}\Omega^2 - \partial_u r\,\partial_v r + \mathfrak{m}^2\pi r^2\Omega^2|\phi|^2 + \tfrac{1}{4}\Omega^2 r^{-2}Q^2, \tag{2-1}$$

$$r^2\partial_u\,\partial_v \log\Omega = -2\pi r^2(D_u\phi\overline{D_v\phi} + \overline{D_u\phi}D_v\phi) - \tfrac{1}{2}\Omega^2 r^{-2}Q^2 + \tfrac{1}{4}\Omega^2 + \partial_u r\,\partial_v r. \tag{2-2}$$

2C2. *Propagation equations for the scalar field and electromagnetic tensor.*

$$D_u D_v\phi + D_v D_u\phi = -\tfrac{1}{2}\mathfrak{m}^2\Omega^2\phi - 2r^{-1}(\partial_u r\, D_v\phi + \partial_v r\, D_u\phi), \tag{2-3}$$

$$D_u D_v\phi - D_v D_u\phi = \tfrac{1}{2}r^{-2}\Omega^2 i\mathfrak{e}Q\cdot\phi, \tag{2-4}$$

$$\partial_u Q = 2\pi i r^2\mathfrak{e}(\phi\overline{D_u\phi} - \bar{\phi}D_u\phi), \tag{2-5}$$

$$\partial_v Q = -2\pi i r^2\mathfrak{e}(\phi\overline{D_v\phi} - \bar{\phi}D_v\phi). \tag{2-6}$$

Furthermore, we can write

$$Q = 2r^2\Omega^{-2}(\partial_u A_v - \partial_v A_u). \tag{2-7}$$

2C3. *Raychaudhuri's equations.*

$$\partial_u(\Omega^{-2}\,\partial_u r) = -4\pi r\Omega^{-2}|D_u\phi|^2, \tag{2-8}$$

$$\partial_v(\Omega^{-2}\,\partial_v r) = -4\pi r\Omega^{-2}|D_v\phi|^2. \tag{2-9}$$

2D. ***Hawking mass.*** Define the Hawking mass m by

$$m := \frac{r}{2}(1 - g_{\mathcal{Q}}(\nabla r, \nabla r)) = \frac{r}{2}\left(1 + \frac{4\partial_u r\,\partial_v r}{\Omega^2}\right). \tag{2-10}$$

By (2-1), (2-8) and (2-9),

$$\partial_u m = -8\pi \frac{r^2(\partial_v r)}{\Omega^2}|D_u\phi|^2 + 2(\partial_u r)\mathfrak{m}^2\pi r^2|\phi|^2 + \frac{1}{2}\frac{(\partial_u r)Q^2}{r^2}, \tag{2-11}$$

$$\partial_v m = -8\pi \frac{r^2(\partial_u r)}{\Omega^2}|D_v\phi|^2 + 2(\partial_v r)\mathfrak{m}^2\pi r^2|\phi|^2 + \frac{1}{2}\frac{(\partial_v r)Q^2}{r^2}. \tag{2-12}$$

2E. ***Global gauge transformations.*** Consider the following global gauge transformation induced by the function $\chi : \mathcal{D} \to \mathbb{R}$, $\mathcal{D} \subset \mathbb{R}^2$:

$$\tilde{\phi}(u, v) = e^{-i\mathfrak{e}\chi(u,v)}\phi(u, v),$$
$$\tilde{A}_\mu(u, v) = A_\mu(u, v) + \partial_\mu\chi(u, v),$$

with $\mu = u, v$. Let us define $\widetilde{D} = d + i\mathfrak{e}\tilde{A}$. Then,

$$\widetilde{D}_\mu\tilde{\phi} = e^{-i\mathfrak{e}\chi}D_\mu\phi.$$

As a result we conclude that the norms $|\phi| = |\tilde{\phi}|$ and $|D_\mu\phi| = |\widetilde{D}_\mu\tilde{\phi}|$ are (globally) *gauge-invariant*.

In most of this paper, the choice of gauge will not be important. We will only explicitly choose a gauge when discussing local existence or when we need to construct an extension of the solution. Instead, most of the time we will estimate the gauge-invariant quantities $|\phi|$ and $|D_\mu\phi|$. For this purpose, let us note that we have the following estimates regarding these quantities:

Lemma 2.1. *The following estimates hold*:

$$|\phi|(u, v) \le |\phi|(u_1, v) + \int_{u_1}^{u} |D_u\phi|(u', v)\, du', \tag{2-13}$$

$$|\phi|(u, v) \le |\phi|(u, v_1) + \int_{v_1}^{v} |D_v\phi|(u, v')\, dv'. \tag{2-14}$$

Proof. We can always pick χ such that $A_u = 0$ and $\widetilde{D}_u\tilde{\phi} = \partial_u\tilde{\phi}$. This fact, together with the fundamental theorem of calculus and the gauge-invariance property above, imply

$$|\phi|(u, v) = |\tilde{\phi}|(u, v) \le |\tilde{\phi}|(u_1, v) + \int_{u_1}^{u} |\widetilde{D}_u\tilde{\phi}|(u', v)\, du' = |\phi|(u_1, v) + \int_{u_1}^{u} |D_u\phi|(u', v)\, du',$$

which implies (2-13).

Similarly, by choosing χ such that $A_v = 0$, we obtain (2-14). □

3. Interior of extremal Reissner–Nordström black holes

The *interior region of the extremal Reissner–Nordström solution* with mass $M > 0$ is the Lorentzian manifold $(\mathcal{M}_{\mathrm{eRN}}, g_{\mathrm{eRN}})$, where $\mathcal{M}_{\mathrm{eRN}} = (0, M)_r \times (-\infty, \infty)_t \times \mathbb{S}^2$ and the metric g_{eRN} in the (t, r, θ, φ)-coordinate system is given by

$$g_{\mathrm{eRN}} = -\Omega_0^2 dt^2 + \Omega_0^{-2} dr^2 + r_0^2(d\theta^2 + \sin^2\theta\, d\varphi^2),$$

where

$$\Omega_0 = \left(1 - \frac{M}{r_0}\right).$$

We define the Eddington–Finkelstein r^*-coordinate (as a function of r) by

$$r^* = \frac{M^2}{M-r} + 2M \log(M-r) + r, \tag{3-1}$$

and define the Eddington–Finkelstein double-null coordinates by

$$u = t - r^*, \quad v = t + r^*. \tag{3-2}$$

In Eddington–Finkelstein double-null coordinates (u, v, θ, φ), the metric takes the form as in Section 2A:

$$g_{\mathrm{eRN}} = -\Omega_0^2(u, v)\, du\, dv + r_0^2(u, v)(d\theta^2 + \sin^2\theta\, d\varphi^2),$$

where r_0 is defined implicitly by (3-1) and (3-2) and $\Omega_0^2(u, v) = (1 - M/(r_0(u, v)))^2$.

For the purpose of this paper, we do not need the explicit expressions for r_0 and Ω_0 as functions of (u, v), but it suffices to have some simple estimates. Since we will only be concerned with the region of the spacetime close to timelike infinity i^+ (see Figure 1),[15] we will assume $v \geq 1$ and $u \leq -1$. In this region, we have the following estimates (the proof is simple and will be omitted):

Lemma 3.1. *For $v \geq 1$ and $u \leq -1$, there exists $C > 0$ (depending on M) such that for $v \geq 1$ and $u \leq -1$,*

$$|r_0 - M|(u, v) \leq \frac{C}{(v + |u|)}, \quad |\partial_v r_0|(u, v) + |\partial_u r_0|(u, v) \leq \frac{C}{(v + |u|)^2}.$$

Given any $\beta > 0$, we can find a constant $C_\beta > 0$ (depending on M and β) such that for $v \geq 1$ and $u \leq -1$,

$$\left|\Omega_0 - \frac{2M}{v + |u|}\right|(u, v) \leq C_\beta (v + |u|)^{-2+\beta}, \tag{3-3}$$

$$|\partial_v(v^2\Omega_0^2) + \partial_u(u^2\Omega_0^2)|(u, v) \leq C_\beta (v + |u|)^{-2+\beta}. \tag{3-4}$$

3A. ***Regular coordinates.*** We would like to think of $\mathcal{M}_{\mathrm{eRN}}$ as having the "event horizon" and the "Cauchy horizon" as null boundaries, which are formally the boundaries $\{u = -\infty\}$ and $\{v = \infty\}$ respectively. To properly define them, we will introduce double null coordinate systems which are regular at the event horizon and at the Cauchy horizon respectively. We will also use these coordinate systems later in the paper

- to pose the characteristic initial value problem near the event horizon, and
- to extend the solution up to the Cauchy horizon.

[15] Formally, it is the "2-sphere at $u = -\infty$, $v = \infty$".

3A1. *Regular coordinates at the event horizon.* Define U by the relation

$$\frac{dU}{du} = \Omega_0^2(u,1) = \left(1 - \frac{M}{r_0(u,1)}\right)^2, \quad U(-\infty) = 0. \tag{3-5}$$

By Lemma 3.1, there exists a constant C (depending on M), so that we can estimate

$$0 \le \frac{dU}{du} \le C(1+|u|)^{-2}. \tag{3-6}$$

Define the *event horizon* as the boundary $\{U = 0\}$. We will abuse notation to denote the event horizon as both the boundary in the quotient manifold $\{(U,v) : U = 0\} \subset \mathcal{Q}$ and the original manifold $\{(U,v) : U = 0\} \times \mathbb{S}^2 \subset \mathcal{M}_{\mathrm{eRN}}$ (see Section 2).

After defining $u(U)$ as the inverse of $u \mapsto U$, we abuse notation to write $r_0(U,v) = r_0(u(U),v)$ and $\widehat{\Omega}_0$ is defined by

$$\widehat{\Omega}_0^2(U,v) = \Omega_0^{-2}(u(U),1)\Omega_0^2(u(U),v),$$

and the extremal Reissner–Nordström metric takes the following form in the (U,v,θ,φ)-coordinate system:

$$g_{\mathrm{eRN}} = -\widehat{\Omega}_0^2(U,v)\,dU\,dv + r_0^2(U,v)(d\theta^2 + \sin^2\theta\,d\varphi^2).$$

In particular, by (3-3), it holds that

$$\widehat{\Omega}_0(0,v) = 1 \tag{3-7}$$

for all v. Additionally, we have, for all v,

$$r_0(0,v) = M.$$

Hence, in the (U,v,θ,φ)-coordinate system, $\widehat{\Omega}_0(U,v)$ and $r_0(U,v)$ extend continuously (in fact smoothly) to the event horizon. Moreover, for every $v \ge 1$ and $u(U) \le -1$, $\widehat{\Omega}_0^2(U,v)$ is bounded above and below as follows:

$$\frac{2}{v+1} \le \widehat{\Omega}_0(U,v) \le 1. \tag{3-8}$$

3A2. *Regular coordinates at the Cauchy horizon.* Define V by the relation

$$\frac{dV}{dv} = \Omega_0^2(-1,v) = \left(1 - \frac{M}{r_0(-1,v)}\right)^2, \quad V(\infty) = 0. \tag{3-9}$$

By Lemma 3.1, there exists a constant C (depending on M), so that we can estimate

$$0 \le \frac{dV}{dv} \le C(1+v)^{-2}. \tag{3-10}$$

Define the *Cauchy horizon* as the boundary $\{V = 0\}$. (Again, this is to be understood either as $\{(u,V) : V = 0\} \subset \mathcal{Q}$ or the original manifold $\{(u,V) : V = 0\} \times \subset \mathcal{M}_{\mathrm{eRN}}$.) After defining $v(V)$ as the inverse of $v \mapsto V$, we abuse notation to write $r_0(u,v(V)) = r_0(u,v(v))$ and $\widetilde{\Omega}_0$ is defined by

$$\widetilde{\Omega}_0^2(u,v(V)) = \Omega_0^{-2}(-1,v(V))\Omega_0^2(u,v(V)),$$

and the extremal Reissner–Nordström metric takes the following form in the (u, V, θ, φ)-coordinate system:

$$g_{\mathrm{eRN}} = -\widetilde{\Omega}_0^2(u, V)\, du\, dV + r_0^2(u, V)(d\theta^2 + \sin^2\theta\, d\varphi^2).$$

In analogy with Section 3A1, it is easy to see that $\widetilde{\Omega}_0^2$ and r_0 extend smoothly to the Cauchy horizon.

4. Initial data assumptions

We will consider the characteristic initial value problem for (1-1) with initial data given on two transversally intersecting null hypersurfaces, which in the double null coordinates (U, v) are denoted by

$$H_0 := \{(U, v) : U = 0\}, \quad \underline{H}_{v_0} := \{(U, v) : v = v_0\}.$$

Here, the (U, v)-coordinates should be thought of as comparable to the Reissner–Nordström (U, v)-coordinates in Section 3A1; see Section 4A for further comments.

The initial data consist of (ϕ, r, Ω, Q) on both H_0 and $\underline{H}_{v_0}$, subject to (2-5) and (2-8) on $\underline{H}_{v_0}$, as well as (2-6) and (2-9) on H_0.

We impose the following *gauge conditions* on the initial hypersurfaces $\underline{H}_{v_0}$ and H_0:

$$\widehat{\Omega}(U, v_0) = \widehat{\Omega}_0(U, v_0) \quad \text{for } U \in [0, U_0], \qquad \widehat{\Omega}(0, v) = \widehat{\Omega}_0(0, v) = 1 \quad \text{for } v \in [v_0, \infty), \tag{4-1}$$

which can be thought of as a normalization condition for the null coordinates.

The initial data for (ϕ, r, Ω, Q) will be prescribed in Sections 4C–4F, but before that, we will give some remarks in Sections 4A and 4B: In Section 4A, we discuss our conventions on null coordinates; in Section 4B, we discuss which parts of the data are freely prescribable and which parts are determined by the constraints. We then proceed to discuss the initial data and the bounds that they satisfy. In Section 4C, we discuss the data for ϕ; in Section 4D, we discuss the data for r; in Section 4E, we discuss the data for Q; in Section 4F, we discuss the data for $\partial_U r$ on H_0.

4A. ***A comment about the use of the null coordinates.*** In the beginning of Section 4, we normalized the null coordinates (U, v) on the initial hypersurfaces by the condition (4-1) so that they play a similar role to the (U, v)-coordinates on extremal Reissner–Nordström spacetimes introduced in Section 3A1. This set of null coordinates has the advantage of being *regular near the event horizon* and therefore it is easy to see that the Einstein–Maxwell–Klein–Gordon system is locally well-posed with the prescribed initial data.

However, in the remainder of the paper, it will be useful to pass to other sets of null coordinates. For this we introduce the following convention. *We use all of the coordinate systems* (U, v)*,* (u, v) *and* (u, V)*, where* u *and* V *are defined* (*as functions of* U *and* v *respectively*) *by* (3-5) *and* (3-9)*.*

All the data will be prescribed in the (U, v)-coordinate system and we will prove estimates for ϕ, r and Q in these coordinates. Nevertheless, using (3-5), they imply immediately also estimates in the (u, v)-coordinate system, and it is those estimates that will be used in the later parts of the paper.

4B. ***A comment about freely prescribable data.*** Since the initial data need to satisfy (2-5), (2-6), (2-8) and (2-9), not all of the data are freely prescribed. Instead, we have freely prescribable and constrained data:

- A normalization condition for u and v can be specified. In our case, we specify the condition (4-1).
- ϕ on H_0 and $\underline{H}_0$ can be prescribed freely.
- r and Q can then be obtained by solving (2-5), (2-6), (2-8) and (2-9) with appropriate initial conditions, namely,
  - r and Q are to approach their corresponding values in extremal Reissner–Nordström with mass $M > 0$; i.e.,
  $$\lim_{v\to\infty} r(0, v) = \lim_{v\to\infty} Q(0, v) = M.$$
  - $(\partial_U r)(0, v_0)$ can be freely prescribed; see (4-7).

We remark that in order to fully specify the initial data, it only remains to pick a gauge condition for A. For this purpose, it will be most convenient to set $A_U(U, v_0) = 0$ and $A_v(0, v) = 0$. (This can always be achieved as each of these are only set to vanish on *one hypersurface*; see the discussions following (9-6).) Nevertheless, the choice of gauge will not play a role in the rest of this subsection, since all the estimates we will need for ϕ and its derivatives can be phrased in terms of the *gauge-invariant* quantities $|\phi|$, $|D_v\phi|$ and $|D_u\phi|$.

4C. ***Initial data for*** $\boldsymbol{\phi}$. We assume that there exist constants $\mathcal{D}_{\mathrm{i}}$ and $\mathcal{D}_{\mathrm{o}}$ such that

$$\int_0^{U_0} |D_U\phi|^2(U, v_0)\, dU \le \mathcal{D}_{\mathrm{i}}, \tag{4-2}$$

$$\int_{v_0}^{\infty} v'^{2+\alpha}|D_v\phi|^2(0, v')\, dv' \le \mathcal{D}_{\mathrm{o}}, \tag{4-3}$$

where we will take $\alpha > 0$. We additionally assume that

$$\lim_{v\to\infty} \phi(0, v) = 0. \tag{4-4}$$

Lemma 4.1. *The following estimate holds*:

$$|\phi|(0, v) \le \sqrt{\mathcal{D}_{\mathrm{o}}}\, v^{-\frac{1}{2}-\frac{\alpha}{2}}. \tag{4-5}$$

Proof. By (4-4), (2-14) and the Cauchy–Schwarz inequality, we have

$$|\phi|(0, v) \le \int_v^{\infty} |D_v\phi|(0, v')\, dv' \le \sqrt{\int_v^{\infty} v'^{-2-\alpha}\, dv'} \cdot \sqrt{\int_v^{\infty} v'^{2+\alpha}|D_v\phi|(0, v')\, dv'},$$

so we can conclude using (4-3). □

4D. ***Initial data for*** $\boldsymbol{r}$. We assume that

$$\lim_{v\to\infty} r(0, v) = M \tag{4-6}$$

and we prescribe freely $\partial_U r(0, v_0)$. Let us assume that

$$\partial_U r(0, v_0) < 0, \quad |\partial_U r|(0, v_0) \le M\mathcal{D}_{\mathrm{i}}. \tag{4-7}$$

We use (2-8) and (2-9) as constraint equations for the variable r along $H_0 = \{U = 0\}$ and $\underline{H}_{v_0} = \{v = v_0\}$.

4D1. *Initial data for r on H_0.* We obtain along H_0

$$\partial_v^2 r(0, v) = -4\pi r(0, v)|D_v\phi|^2. \tag{4-8}$$

The above ODE can be solved to obtain $r(0, v)$.

Lemma 4.2. *There exists a unique smooth solution to* (4-8) *satisfying* (4-6)*. Moreover, if v_0 satisfies the inequality*

$$\mathcal{D}_{\mathrm{o}} v_0^{-1} \le \tfrac{1}{8\pi}, \tag{4-9}$$

then the following estimates hold for $v \ge v_0$:

$$\tfrac{1}{2}M \le r(0, v) \le M, \quad |r - M|(0, v) \le 4\pi M\mathcal{D}_{\mathrm{o}} v^{-1}, \quad |\partial_v r|(0, v) \le 4\pi M\mathcal{D}_{\mathrm{o}} v^{-2}.$$

Proof. Existence and uniqueness can be obtained using a standard ODE argument. We will focus on proving the estimates.

First, observe that by integrating (4-8), and using the assumptions $r(0, v) \to M$ and (4-3), it follows that $\lim_{v\to\infty}(\partial_v r)(0, v)$ exists. Now using again the assumption $r(0, v) \to M$, we deduce that

$$\lim_{v\to\infty}(\partial_v r)(0, v) = 0. \tag{4-10}$$

Together with (4-8) this implies

$$\partial_v r(0, v) \ge 0.$$

Since $r(0, v) \to M$, we can then bound

$$r(0, v) \le M. \tag{4-11}$$

By (4-8) and (4-10),

$$|\partial_v r(0, v)| \le 4\pi \sup_{v_0 \le v < \infty} r(0, v) \cdot \int_v^\infty |D_v\phi|^2(u, v')\, dv'.$$

We deduce, using (4-3) and (4-11), that

$$|\partial_v r(0, v)| \le 4\pi M\mathcal{D}_{\mathrm{o}} v^{-2-\alpha}, \tag{4-12}$$

and therefore

$$|r(0, v) - M| \le \frac{4\pi M}{1+\alpha}\mathcal{D}_{\mathrm{o}} v^{-1-\alpha} \tag{4-13}$$

for all $v_0 \le v < \infty$. In particular, given (4-9), it holds that for all $v \in [v_0, \infty)$,

$$r(0, v) \ge \tfrac{1}{2}M. \tag{4-14}$$

The estimates stated in the lemma hence follow from (4-11)–(4-14). ☐

4D2. *Initial data for r on $\underline{H}_0$.* We similarly obtain along $\underline{H}_0$

$$\partial_U(\widehat{\Omega}^{-2}(U, v_0)\,\partial_U r(U, v_0)) = -4\pi\widehat{\Omega}^{-2}(U, v_0)r(U, v_0)|D_U\phi|^2. \tag{4-15}$$

The above ODE can be solved to obtain $r(U, v_0)$.

Lemma 4.3. *There exists a unique smooth solution to* (4-15) *satisfying* (4-6). *Moreover, if U_0, v_0 satisfy the inequality*

$$\mathcal{D}_{\mathrm{o}} v_0^{-1} \le \tfrac{1}{8\pi}, \quad M\mathcal{D}_{\mathrm{i}} v_0^2 U_0 \le \tfrac{1}{36\pi}, \tag{4-16}$$

then the following estimates hold for $U \in [0, U_0]$:

$$\tfrac{1}{4}M \le r(U, v_0) \le \tfrac{5}{4}M, \quad |\partial_U r|(U, v_0) \le 9\pi M\mathcal{D}_{\mathrm{i}} v_0^2.$$

Proof. As in Lemma 4.3, since existence and uniqueness is standard, we focus on the estimates. To this end, we introduce a bootstrap argument, starting with the assumption

$$r(U, v_0) \le 2M. \tag{4-17}$$

Integrating (4-15) and using (4-1),

$$|\widehat{\Omega}^{-2}(U, v_0)\,\partial_U r(U, v_0) - \partial_U r(0, v_0)| \le 4\pi \sup_{0\le U'\le U_0} \widehat{\Omega}^{-2}(U', v_0)\, r(U', v_0)\cdot \int_0^U |D_U\phi|^2(U'', v_0)\, dU''.$$

By (3-8), (4-2) and (4-7), this implies

$$|\partial_U r(U, v_0)| \le M\mathcal{D}_{\mathrm{i}} + 8\pi M\cdot\left(\frac{v_0+1}{2}\right)^2\cdot\mathcal{D}_{\mathrm{i}} = M\mathcal{D}_{\mathrm{i}}(1+2\pi(v_0+1)^2) \le 9\pi M\mathcal{D}_{\mathrm{i}} v_0^2. \tag{4-18}$$

Integrating in U, this yields (for $U \in [0, U_0]$),

$$|r(U, v_0) - r(0, v_0)| \le 9\pi M\mathcal{D}_{\mathrm{i}} v_0^2 U_0,$$

which implies, using Lemma 4.2 (or more precisely (4-11) and (4-14)),

$$\tfrac{1}{2}M - 9\pi M\mathcal{D}_{\mathrm{i}} v_0^2 U_0 \le r(U, v_0) \le M + 9\pi M\mathcal{D}_{\mathrm{i}} v_0^2 U_0.$$

Hence, by (4-16), it holds that

$$\tfrac{1}{4}M \le r(U, v_0) \le \tfrac{5}{4}M, \tag{4-19}$$

and we have improved the bootstrap assumption (4-17). This closes the bootstrap argument, and the desired estimates follow from (4-18) and (4-19). □

4E. ***Initial data for Q.*** In view of (2-5) and (2-6) which have to be satisfied on the initial hypersurfaces, it suffices to impose Q on one initial sphere. We assume that

$$\lim_{v\to\infty} Q(0, v) = M. \tag{4-20}$$

Lemma 4.4. *Assume* (4-9) *holds. Then the following estimate holds on H_0*:

$$|Q(0, v) - M|(0, v) \le 4\pi|\mathfrak{e}|M\mathcal{D}_{\mathrm{o}} v^{-1-\alpha}. \tag{4-21}$$

Proof. Using (2-6), (4-11) and the Cauchy–Schwarz inequality we estimate

$$|Q(0,v)-M|(0,v) \le 4\pi|\mathfrak{e}| \sup_{v''\in[v_0,\infty)} r^2(0,v'')\cdot\int_v^\infty |\phi|\cdot|D_v\phi|(0,v')\,dv'$$
$$\le 4\pi|\mathfrak{e}|M^2 \sup_{v\le v'<\infty}|\phi|(0,v')\cdot\sqrt{\int_v^\infty v'^{-2-\alpha}\,dv'}\cdot\sqrt{\int_v^\infty v'^{2+\alpha}|D_v\phi|^2(0,v')\,dv'},$$

so we can use (4-3) and (4-5) to conclude (4-21). □

4F. $\partial_U r$ *along* H_0. The function $\partial_u r$ along H_0 is not freely prescribable, but is dictated by (2-1) and the freely prescribable data for $(\partial_U r)(0,v_0)$ (which obeys (4-7)). We will need the following estimate for $\partial_U r$ along H_0.

Lemma 4.5. *Suppose* (4-9) *holds. Then there exists a constant* $C>0$ *depending only on* M *and* $\mathfrak{m}$ *such that for every* $v\in[v_0,\infty)$,

$$|\partial_U r(0,v)| \le C(\mathcal{D}_o+\mathcal{D}_i). \tag{4-22}$$

Proof. By (2-1) we have

$$\partial_v(r\,\partial_U r)(0,v) = 4M^2\mathfrak{m}^2\pi r^2|\phi|^2 + M^2r^{-2}(Q^2-r^2)$$
$$= 4M^2\mathfrak{m}^2\pi r^2|\phi|^2 + M^2r^{-2}(Q^2-M^2) + M^2r^{-2}(M^2-r^2).$$

Hence,

$$|(r\,\partial_U r)(0,v)-(r\,\partial_U r)(0,v_0)| \lesssim \left|\int_{v_0}^\infty \mathfrak{m}^2r^2|\phi|^2 + \tfrac{1}{4\pi}M^{-2}(Q^2-M^2) + \tfrac{1}{4\pi}M^{-2}(M^2-r^2)\,dv'\right| \lesssim \mathcal{D}_o,$$

where we have used Lemmas 4.1, 4.2 and 4.4 (and we crucially used that $\alpha>0$). Together with (4-7), we can therefore conclude (4-22). □

5. Statement of the main theorem

We are now ready to give a precise statement of the main theorem. Let us recall (from Section 4A) that we also consider the coordinate system (u,v), where $u(U)$ is defined via the relation (3-5). It will be convenient from this point onwards to use the u-(instead of U-) coordinate.

Theorem 5.1. *Suppose*

- *the parameters* M *and* $\mathfrak{e}$ *obey*[16]

$$1-(10+5\sqrt{6}-3\sqrt{9+4\sqrt{6}})|\mathfrak{e}|M>0. \tag{5-1}$$

- *the initial data are smooth and satisfy* (4-1), (4-2), (4-3), (4-4), (4-6), (4-7) *and* (4-20) *for some finite* $\mathcal{D}_o$ *and* $\mathcal{D}_i$.

Then for $|u_0|$ *sufficiently large depending on* M, $\mathfrak{m}$, $\mathfrak{e}$, α, $\mathcal{D}_o$ *and* $\mathcal{D}_i$ *and* v_0 *sufficiently large depending on* M, $\mathfrak{m}$, $\mathfrak{e}$, α *and* $\mathcal{D}_o$ (*but not* $\mathcal{D}_i$!), *the following hold*:

[16]Note that $(10+5\sqrt{6}-3\sqrt{9+4\sqrt{6}})\sim 9.24\ldots$.

• (*existence of solution*) *There exists a unique smooth*, *spherically symmetric solution to* (1-1) *in the double null coordinate system in* $(u, v) \in (-\infty, u_0] \times [v_0, \infty)$.

• (*extendibility to the Cauchy horizon*) *In an appropriate coordinate system*, *a Cauchy horizon can be attached to the solution so that the metric*, *the scalar field and the Maxwell field extend continuously to it.*

• (*quantitative estimates*) *The following estimates hold for all* $(u, v) \in (-\infty, u_0) \times [v_0, \infty)$ *for some implicit constant depending on* M, $\mathfrak{m}$ *and* $\mathfrak{e}$ (*which shows that the solution is close to extremal Reissner–Nordström in an appropriate sense*):

$$|\phi|(u, v) \lesssim \mathcal{D}_{\mathrm{o}} v^{-\frac{1}{2}-\frac{\alpha}{2}} + (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}})|u|^{-\frac{1}{2}}, \quad |r - M|(u, v) \lesssim \mathcal{D}_{\mathrm{o}} v^{-1} + (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}})|u|^{-1},$$
$$|\Omega^2 - \Omega_0^2|(u, v) \lesssim |u|^{-\frac{1}{2}}(|u| + v)^{-2},$$
$$|\partial_u r|(u, v) \lesssim (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}})|u|^{-2}, \quad |\partial_v r|(u, v) \lesssim (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}) v^{-2},$$
$$\int_{v_0}^{\infty} v^2 |\partial_v \phi|^2(u, v)\, dv + \int_{-\infty}^{u_0} u^2 |\partial_u \phi|^2(u, v)\, du \lesssim \mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}},$$
$$\int_{-\infty}^{u_0} u^2 \Big(\partial_u \Big(\log \frac{\Omega}{\Omega_0}\Big)\Big)^2 (u, v)\, du + \int_{v_0}^{v_\infty} v^2 \Big(\partial_v \Big(\log \frac{\Omega}{\Omega_0}\Big)\Big)^2 (u, v)\, dv \le \tfrac{1}{2}.$$

• (*extendibility as a spherically symmetric solution*) *The solution can be extended nonuniquely in* (*space-time*) $C^{0,\frac{1}{2}} \cap W^{1,2}_{\mathrm{loc}}$ *beyond the Cauchy horizon as a spherically symmetric solution to the Einstein–Maxwell–Klein–Gordon system.*

Remark 5.2 ($v_0 \ge 1,\ u_0 \le -1.$). Without loss of generality, we will from now on assume that $v_0 \ge 1$ and $u_0 \le -1$.

Remark 5.3 (validity of the estimates in Section 4). Recall that in Section 4, some of the estimates that were proven depend on the assumptions (4-9) and (4-16). From now on, we take v_0 sufficiently large and u_0 sufficiently negative (in a manner allowed by Theorem 5.1) so that (4-9) and (4-16) hold.

Remark 5.4 (relaxing the largeness of v_0). Note that v_0 is assumed to be large depending on M, $\mathfrak{m}$, $\mathfrak{e}$, α and $\mathcal{D}_{\mathrm{o}}$ so that we restrict our attention to a region where the geometry is close to that of extremal Reissner–Nordström. However, in general, if we are given data with $v_{0,i} = 1$ (say) and $\mathcal{D}_{\mathrm{o}}$ not necessarily small, we can do the following:

(1) First, find a v_0 (sufficiently large) such that v_0 is sufficiently large depending on M, $\mathfrak{m}$, $\mathfrak{e}$, α and $\mathcal{D}_{\mathrm{o}}$ in a way that is required by Theorem 5.1.

(2) Solve a *finite* characteristic initial value problem in $(-\infty, u_0] \times [v_{0,i}, v_0]$ for some u_0 sufficiently negative. (Such a problem can always be solved for u_0 sufficiently negative. This can be viewed as a restatement of the fact that for *local* characteristic initial value problems, one only needs the smallness of *one* characteristic length, as long as the other characteristic length is *finite*; see [Luk 2012].)

(3) Now, let $\mathcal{D}_{\mathrm{i}}$ be the size of the *new data* on $\{v = v_0\}$ which is obtained from the previous step. By choosing u_0 smaller if necessary, it can be arranged so that $|u_0|$ is large in terms of M, $\mathfrak{m}$, $\mathfrak{e}$ and $\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}$ in a way consistent with Theorem 5.1.

(4) Theorem 5.1 can now be applied to obtain a solution in $(-\infty, u_0]\times[v_0, \infty)$ such that the conclusions of Theorem 5.1 hold.

In the case $\mathfrak{e}=\mathfrak{m}=0$, we obtain the following additional regularity of the scalar field:

Theorem 5.5. *In the case* $\mathfrak{e}=\mathfrak{m}=0$, *suppose that in addition to the assumptions of Theorem 5.1*, *the following pointwise bounds hold for the initial data*:

$$\sup_{u\in(-\infty,u_0]} |u|^2|\partial_u\phi|(u, v_0)+\sup_{v\in[v_0,\infty)} v^2|\partial_v\phi|(-\infty, v)<\infty. \tag{5-2}$$

Then, *taking* u_0 *more negative if necessary*, *in the* (u, V)*-coordinate system*, *see* (9-1), *the scalar field is Lipschitz up to the Cauchy horizon.*

6. The main bootstrap argument

6A. ***Setup of the bootstrap.*** We will assume that

- there exists a smooth solution (ϕ, Ω, r, A) to the system of (2-1)–(2-9) in the rectangle $D_{U_0,[v_0,v_\infty)}=\{(U, v)\mid 0\le U\le U_0,\ v_0\le v<v_\infty\}$, such that
- the initial gauge conditions are satisfied, i.e., $\widehat{\Omega}^2(U, v_0)=\widehat{\Omega}_0^2(U, v_0)$ and $\widehat{\Omega}^2(0, v)=\widehat{\Omega}_0^2(0, v)$, and
- the initial conditions for ϕ, r, Q are attained.

On this region, we will moreover assume that certain *bootstrap assumptions* hold (see Section 6B). Our goal will then be to improve these bootstrap assumptions, which then by continuity, implies that the above three properties hold for all $v\ge v_0$, i.e., in the region $D_{U_0,v_0}=D_{U_0,[v_0,\infty)}$.

Recall again that we often use the (u, v)- instead the (U, v)-coordinates. Abusing notation, we will also write

$$D_{u_0,[v_0,v_\infty)}=D_{U_0,[v_0,v_\infty)}=\{(u, v)\mid -\infty<u\le u_0:=u(U_0),\ v_0\le v\le v_\infty\}.$$

6B. ***Bootstrap assumptions.*** Fix $\eta>0$ sufficiently small (depending only on $\mathfrak{e}$ and M) so that

$$1-(10+5\sqrt{6}-3\sqrt{9+4\sqrt{6}})(1+\eta)|\mathfrak{e}|M>0. \tag{6-1}$$

(Such an η exists in view of (5-1).) Define

$$\mu=\big(1-(10+5\sqrt{6}-3\sqrt{9+4\sqrt{6}})(1+\eta)|\mathfrak{e}|M\big). \tag{6-2}$$

Let us make the following bootstrap assumptions for the quantities (ϕ, Ω, r) in D_{U_0,v_∞}, for some $\mathcal{A}_\phi\ge 1$ to be chosen later:

$$\sup_{v\in[v_0,v_\infty]}\int_{-\infty}^{u_0} u'^2\Big(\partial_u\Big(\log\frac{\Omega}{\Omega_0}\Big)\Big)^2(u', v)\,du'+\sup_{u\in(-\infty,u_0]}\int_{v_0}^{v_\infty} v'^2\Big(\partial_v\Big(\log\frac{\Omega}{\Omega_0}\Big)\Big)^2(u, v')\,dv'\le M, \tag{A1}$$

$$\sup_{v\in[v_0,v_\infty]}\int_{-\infty}^{u_0} u'^2|D_u\phi|^2(u', v)\,du'+\sup_{u\in(-\infty,u_0]}\int_{v_0}^{v_\infty} v'^2|D_v\phi|^2(u, v')\,dv'\le\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}}), \tag{A2}$$

$$\sup_{u\in(-\infty,u_0],\ v\in[v_0,v_\infty]}|r-M|(u, v)\le\tfrac{1}{2}M. \tag{A3}$$

Our goal will be to show that under these assumptions, for $|u_0|$ sufficiently large depending on M, $\mathfrak{m}$, $\mathfrak{e}$, α, η, $\mathcal{D}_{\mathrm{o}}$ and $\mathcal{D}_{\mathrm{i}}$ and v_0 sufficiently large depending on M, $\mathfrak{m}$, $\mathfrak{e}$, α, η and $\mathcal{D}_{\mathrm{o}}$,

- the estimate (A1) can be improved so that the right-hand side can be replaced by $\frac{1}{2}M$;
- the estimate (A2) can be improved so that the right-hand side can be replaced by $C(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})$, where C is a constant depending only on M, $\mathfrak{m}$, $\mathfrak{e}$, α and η;
- the estimate (A3) can be improved to $|r-M|\le\frac{1}{4}M$.

6C. ***Conventions regarding constants.*** In closing the bootstrap argument, the main source of smallness will come from choosing $|u_0|$ and v_0 appropriately large. We remark on our conventions regarding the constants that will be used in the bootstrap argument:

• All the implicit constants (either in the form of C or $\lesssim$) are allowed to depend on the parameters M, $\mathfrak{m}$, $\mathfrak{e}$ and α. In particular, they are allowed to depend on η, defined in (6-1), and μ, defined in (6-2). There will be places where the exact values of these parameters matter (hence the corresponding restriction in Theorem 5.1): at those places the constants will be explicitly written.

• $|u_0|$ is taken to be large depending on M, $\mathfrak{m}$, $\mathfrak{e}$, α, η, $\mathcal{D}_{\mathrm{o}}$ and $\mathcal{D}_{\mathrm{i}}$, and v_0 is taken to be large depending on M, $\mathfrak{m}$, $\mathfrak{e}$, α, η and $\mathcal{D}_{\mathrm{o}}$. In particular, we will use

$$\mathcal{D}_{\mathrm{o}}v_0^{-\frac{1}{10}}\ll 1,\quad (\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u_0|^{-\frac{1}{10}}\ll 1$$

without explicit comments, where by $\ll 1$ we mean that it is small with respect to the constants appearing in the argument that depend on M, $\mathfrak{m}$, $\mathfrak{e}$, α and η.

• $\mathcal{A}_\phi\ge 1$ will eventually be chosen to be large depending M, $\mathfrak{m}$, $\mathfrak{e}$ and α, *but not on* $\mathcal{D}_{\mathrm{o}}$ *and* $\mathcal{D}_{\mathrm{i}}$. In particular, we will also use

$$\mathcal{A}_\phi^3\mathcal{D}_{\mathrm{o}}v_0^{-\frac{1}{10}}\ll 1,\quad \mathcal{A}_\phi^3(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u_0|^{-\frac{1}{10}}\ll 1 \tag{6-3}$$

without explicit comments.

7. Pointwise estimates

Proposition 7.1. *For all* $-\infty<u\le u_0$, $v_0\le v\le v_\infty$ *we have*

$$|\phi|(u,v)\lesssim\sqrt{\mathcal{D}_{\mathrm{o}}}v^{-\frac{1}{2}-\frac{\alpha}{2}}+\mathcal{A}_\phi^{\frac{1}{2}}\sqrt{\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}}}|u|^{-\frac{1}{2}}, \tag{7-1}$$

$$|Q-M|(u,v)\lesssim\mathcal{D}_{\mathrm{o}}v^{-1-\alpha}+\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-1}, \tag{7-2}$$

$$|\Omega-\Omega_0|(u,v)\lesssim|u|^{-\frac{1}{2}}(v+|u|)^{-1}, \tag{7-3}$$

$$|\Omega^2-\Omega_0^2|(u,v)\lesssim|u|^{-\frac{1}{2}}(v+|u|)^{-2}, \tag{7-4}$$

$$\left|\Omega-\frac{2M}{(v+|u|)}\right|(u,v)\lesssim|u|^{-\frac{1}{2}}(v+|u|)^{-1}, \tag{7-5}$$

$$\left|\Omega^2-\frac{4M^2}{(v+|u|)^2}\right|(u,v)\lesssim|u|^{-\frac{1}{2}}(v+|u|)^{-2}. \tag{7-6}$$

In particular,

$$\tfrac{1}{2}M \le |Q|(u,v) \le \tfrac{3}{2}M, \tag{7-7}$$

$$2M^2(v+|u|)^{-2} \le \Omega^2(u,v) \le 6M^2(v+|u|)^{-2}. \tag{7-8}$$

Proof. Proof of (7-1). By (2-13) and the Cauchy–Schwarz inequality, we obtain

$$|\phi|(u,v) \le |\phi|(-\infty,v) + |u|^{-\frac{1}{2}}\sqrt{\int_{-\infty}^{u} u'^2 |D_u\phi|^2(u',v)\,du'}. \tag{7-9}$$

Using (4-5) and the bootstrap assumption (A2) to control the first and second term respectively, we obtain (7-1).

Proof of (7-2). Using the estimate (7-1) for ϕ, the bootstrap assumption (A3) for r together with (2-5), we obtain a pointwise estimate for $|Q-M|$:

$$\begin{aligned}|Q-M|(u,v) &\le |Q-M|(-\infty,v) + \int_{-\infty}^{u} |\partial_u Q|(u',v)\,du' \\ &\le |Q-M|(-\infty,v) + 4\pi|\mathfrak{e}| \int_{-\infty}^{u} r^2|\phi||D_u\phi|(u',v)\,du' \\ &\le |Q-M|(-\infty,v) + 4\pi|\mathfrak{e}||u|^{-\frac{1}{2}} \sup_{-\infty<u'\le u} r^2|\phi|(u',v)\cdot\sqrt{\int_{-\infty}^{u} u^2|D_u\phi|^2(u',v)\,du'} \\ &\le |Q-M|(-\infty,v) + C\sqrt{\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})}|u|^{-\frac{1}{2}}\big(|u|^{-\frac{1}{2}}\sqrt{\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})} + v^{-\frac{1}{2}-\frac{\alpha}{2}}\sqrt{\mathcal{D}_{\mathrm{o}}}\big).\end{aligned}$$

Using (4-21) and Young inequality, we therefore conclude that

$$|Q-M|(u,v) \lesssim \mathcal{D}_{\mathrm{o}} v^{-1-\alpha} + \mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-1}.$$

Proof of (7-3), (7-4), (7-5) and (7-6). By our choice of initial gauge (4-1), we have

$$\log\frac{\Omega}{\Omega_0}(-\infty,v) = \log\frac{\widehat{\Omega}}{\widehat{\Omega}_0}(U=0,v) = 0,$$

so we can estimate using (A1)

$$\left|\log\frac{\Omega}{\Omega_0}\right|(u,v) \le |u|^{-\frac{1}{2}}\sqrt{\int_{-\infty}^{u} u'^2\Big(\partial_u\Big(\log\frac{\Omega}{\Omega_0}\Big)\Big)^2(u',v')\,du'} \le M^{\frac{1}{2}}|u|^{-\frac{1}{2}}.$$

Using (A1) and the simple inequality $|e^{\vartheta}-1| \le |\vartheta|e^{|\vartheta|}$, we have

$$\left|\frac{\Omega}{\Omega_0}-1\right|(u,v) \le M^{\frac{1}{2}}|u|^{-\frac{1}{2}}\max\Big\{\frac{\Omega}{\Omega_0},\frac{\Omega_0}{\Omega}\Big\}(u,v), \qquad \left|\frac{\Omega_0}{\Omega}-1\right|(u,v) \le M^{\frac{1}{2}}|u|^{-\frac{1}{2}}\max\Big\{\frac{\Omega}{\Omega_0},\frac{\Omega_0}{\Omega}\Big\}(u,v).$$

We now consider two cases. Suppose $(\Omega/\Omega_0)(u,v) > 1$ for some (u,v); we have

$$\left|\frac{\Omega}{\Omega_0}-1\right|(u,v) \le M^{\frac{1}{2}}|u|^{-\frac{1}{2}}\Big(\frac{\Omega}{\Omega_0}-1\Big)(u,v) + M^{\frac{1}{2}}|u|^{-\frac{1}{2}},$$

which, after choosing u_0 to satisfy $M^{\frac{1}{2}}|u_0|^{-\frac{1}{2}} \le \frac{1}{2}$, implies

$$\left|\frac{\Omega}{\Omega_0}-1\right|(u,v) \le 2M^{\frac{1}{2}}|u|^{-\frac{1}{2}}. \tag{7-10}$$

Multiplying (7-10) by Ω_0 in particular implies

$$|\Omega-\Omega_0|(u,v)\le 4M^{\frac12}|u|^{-\frac12}\Omega_0(u,v) \tag{7-11}$$

in this case. On the other hand, if $(\Omega/\Omega_0)(u,v)<1$ for some (u,v), we have by a similar argument that for $M^{\frac12}|u_0|^{-\frac12}\le\frac12$,

$$\left|\frac{\Omega_0}{\Omega}-1\right|(u,v)\le 2M^{\frac12}|u|^{-\frac12}.$$

This then implies

$$|\Omega_0-\Omega|(u,v)\le 2M^{\frac12}|u|^{-\frac12}|\Omega-\Omega_0|(u,v)+2M^{\frac12}|u|^{-\frac12}\Omega_0(u,v).$$

Choosing $M^{\frac12}|u_0|^{-\frac12}\le\frac14$ implies that we also have (7-11) in this case. Using (7-11) and (3-3), we conclude (7-3).

For (7-4), we use (7-11) twice to obtain

$$|\Omega^2-\Omega_0^2|(u,v)\le 4M^{\frac12}|u|^{-\frac12}\Omega_0(\Omega+\Omega_0)\le 16M|u|^{-1}\Omega_0^2+8M^{\frac12}|u|^{-\frac12}\Omega_0^2,$$

which, after choosing $|u_0|$ to be sufficiently large and using (3-3), implies (7-4).

Finally, (7-5) and (7-6) follow from (7-3), (7-4) and (3-3), with $\beta=\frac12$.

Proof of (7-7) and (7-8). The bound (7-7) is an immediate consequence of (7-2), while (7-8) is an immediate consequence of (7-6). □

Proposition 7.2. *The following estimates hold*:

$$|\partial_u r|(u,v)\lesssim \mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-2}, \tag{7-12}$$

$$|\partial_v r|(u,v)\lesssim \mathcal{D}_{\mathrm{o}}v^{-2}+\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})\min\{v^{-2},|u|^{-2}\}, \tag{7-13}$$

$$|r(u,v)-M|\lesssim \mathcal{D}_{\mathrm{o}}v^{-1}+\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-1}, \tag{7-14}$$

$$|r(u,v)-r_0(u,v)|\lesssim \mathcal{D}_{\mathrm{o}}v^{-1}+\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-1}+(v+|u|)^{-1}. \tag{7-15}$$

In particular,

$$|r(u,v)-M|\le\tfrac14 M, \tag{7-16}$$

which improves the bootstrap assumption (A3).

Proof. Proof of (7-12). By (2-8), (A3), (7-8) and (4-22), we can estimate

$$\begin{aligned}|\partial_u r|(u,v)&\le \Omega^2(u,v)|\partial_U r|(-\infty,v)+C\Omega^2(u,v)\int_{-\infty}^{u}\Omega^{-2}(u',v)|D_u\phi|^2(u',v)\,du'\\ &\le C(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-2}+C(v+|u|)^{-2}\int_{-\infty}^{u}\frac{(v+|u'|)^2}{|u'|^2}|u'|^2|D_u\phi|^2(u',v)\,du'.\end{aligned}$$

Note that for $|u'| \geq |u|$, we have

$$\left(\frac{v+|u'|}{|u'|}\right)^2 = \left(1+\frac{v}{|u'|}\right)^2 \leq \left(1+\frac{v}{|u|}\right)^2 = \left(\frac{v+|u|}{|u|}\right)^2,$$

which we can use to further estimate

$$|\partial_u r|(u,v) \leq C(\mathcal{D}_o+\mathcal{D}_i)|u|^{-2} + C|u|^{-2}\int_{-\infty}^{u} |u'|^2 |D_u\phi|^2(u',v)\,du'$$

and hence, by (A2),

$$|\partial_u r|(u,v) \leq C\mathcal{A}_\phi(\mathcal{D}_o+\mathcal{D}_i)|u|^{-2}.$$

<u>Proof of (7-16)</u>. Using the fundamental theorem of calculus and integrating (7-12) in u, we obtain

$$|r(u,v)-M| \leq |r(-\infty,v)-M| + \int_{-\infty}^{u} |\partial_u r|(u',v)'\,du' \lesssim \mathcal{D}_o v^{-1} + \mathcal{A}_\phi(\mathcal{D}_o+\mathcal{D}_i)|u|^{-1},$$

where in the last inequality we have used Lemma 4.2 and (7-12). Combining this with the estimates for r_0 in Lemma 3.1, we thus obtain the estimate for $r-r_0$ in (7-15). In particular, for $\mathcal{D}_o v_0^{-1}$, $(\mathcal{D}_o+\mathcal{D}_i)|u_0|^{-1}$ suitably small, we obtain

$$|r(u,v)-M| < \tfrac{1}{4}M$$

for all $(u,v) \in D_{u_0,v_\infty}$, which is the estimate (7-14).

<u>Proof of (7-13): the region $\{v \leq |u|\}$</u>. We first rewrite (2-1) as

$$\partial_u(r\,\partial_v r) = \tfrac{1}{4}\Omega^2 r^{-2}(Q^2-M^2) + \tfrac{1}{4}\Omega^2 r^{-2}(M^2-r^2) + \mathfrak{m}^2\pi r^2\Omega^2|\phi|^2.$$

By (7-1) (for ϕ), (7-14) (for $r-M$) and (7-2) (for $Q-M$), the u-integral of the right-hand side of the above equation can be estimated (up to a constant) by

$$\int_{-\infty}^{u} \Omega^2(\mathcal{D}_o v^{-1} + \mathcal{A}_\phi(\mathcal{D}_o+\mathcal{D}_i)|u'|^{-1})\,du'.$$

Using (7-6), we have, in the region $\{v \leq |u|\}$,

$$\int_{-\infty}^{u} \Omega^2\mathcal{D}_o v^{-1}\,du' \lesssim \mathcal{D}_o v^{-1}\int_{-\infty}^{u}(v+|u'|)^{-2}\,du' \lesssim \mathcal{D}_o v^{-1}(v+|u|)^{-1}$$

and

$$\begin{aligned}\int_{-\infty}^{u} \Omega^2\mathcal{A}_\phi(\mathcal{D}_o+\mathcal{D}_i)|u'|^{-1}\,du' &\lesssim \mathcal{A}_\phi(\mathcal{D}_o+\mathcal{D}_i)\int_{-\infty}^{u}(v+|u'|)^{-2}|u'|^{-1}\,du' \\ &\lesssim \mathcal{A}_\phi(\mathcal{D}_o+\mathcal{D}_i)|u|^{-2}.\end{aligned}$$

Together with the bound on $\partial_v r$ on the event horizon in Lemma 4.2, this implies that when $v \leq |u|$, we have the estimate

$$|\partial_v r|(u,v) \lesssim \mathcal{D}_o v^{-2} + \mathcal{A}_\phi(\mathcal{D}_o+\mathcal{D}_i)\min\{v^{-2}, |u|^{-2}\}.$$

<u>Proof of (7-13): the region $\{v \geq |u|\}$</u>. Notice that if we estimate in this region in the same manner as before, we lose a factor of $\log v$ in the bound. So instead of (2-1), we will use the Raychaudhuri's

equation (2-9).[17] More precisely, given (u, v) with $v \geq |u|$, we integrate (2-9) along a constant-u curve starting from its intersection with the curve $\{|u| = v\}$ to obtain

$$\left|\frac{\partial_v r}{\Omega^2}\right|(u, v) \lesssim \left|\frac{\partial_v r}{\Omega^2}\right|(u, -u) + \int_{-u}^{v} \Omega^{-2}|D_v\phi|^2(u, v')\,dv'.$$

By the estimates for $\partial_v r$ in the previous step and (7-4), we have

$$\left|\frac{\partial_v r}{\Omega^2}\right|(u, -u) \lesssim \mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}).$$

Since $v' \geq |u|$ in the domain of integration, we have, after using (7-4) and (A2), that

$$\int_{-u}^{v} \Omega^{-2}|D_v\phi|^2(u, v')\,dv' \lesssim \int_{-u}^{v} (v' + |u|)^2|D_v\phi|^2(u, v')\,dv' \lesssim \int_{-u}^{v} v^2|D_v\phi|^2(u, v')\,dv' \lesssim \mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}).$$

Combining the three estimates above with (7-6) yields that when $v \geq |u|$,

$$|\partial_v r|(u, v) \lesssim \mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}) \min\{v^{-2}, |u|^{-2}\}.$$

Together with the previous step, we have thus completed the proof of (7-13). □

8. Energy estimates

In this section, we prove the energy estimates for (derivatives of) ϕ and Ω. In particular, we will improve our bootstrap assumptions (A1) and (A2). As we discussed in the Introduction, the argument leading to energy estimates for ϕ will go through the introduction of a *renormalized energy*, the analysis of which forms the most technical part of the paper.

In Section 8A, we will motivate the introduction of our renormalized energy for the matter field by considering the stress-energy-momentum tensor associated to the matter field. In Section 8B, we show that the renormalized energy we introduce is coercive; and in Section 8C, we show that one can bound this renormalized energy. Combining these facts yields the desired control for the matter field.

Finally, in Section 8D, we prove the energy estimates for (Ω/Ω_0).

8A. ***The stress energy tensor and the renormalized energy fluxes.*** The null components of the stress-energy-momentum tensor $\mathbb{T}_{\mu\nu}$ corresponding to the scalar field and electromagnetic tensor are given by

$$\mathbb{T}_{uv} = \tfrac{1}{4}\Omega^2\big(\mathfrak{m}^2|\phi|^2 + \tfrac{1}{4\pi}r^{-4}Q^2\big), \quad \mathbb{T}_{uu} = |D_u\phi|^2, \quad \mathbb{T}_{vv} = |D_v\phi|^2.$$

The above expressions suggest that the natural energy fluxes along the null hypersurfaces of constant u and v are obtained by integrating the contraction $\mathbb{T}(X, \partial_v)$ and $\mathbb{T}(X, \partial_u)$, respectively. With the choice

[17] On the other hand, in the region $\{v \leq |u|\}$ that we considered above, it also does not seem that Raychaudhuri can give the desired bound.

$X = u^2\,\partial_u + v^2\,\partial_v$, this gives

$$\int_{v_1}^{v_2} v^2 r^2 |D_v\phi|^2 + \tfrac{1}{4} u^2 r^2 \Omega^2 \big(\mathfrak{m}^2|\phi|^2 + \tfrac{1}{4\pi} r^{-4} Q^2\big)\, dv,$$
$$\int_{u_1}^{u_2} u^2 r^2 |D_u\phi|^2 + \tfrac{1}{4} v^2 r^2 \Omega^2 \big(\mathfrak{m}^2|\phi|^2 + \tfrac{1}{4\pi} r^{-4} Q^2\big)\, du,$$

with $-\infty < u_1 < u_2 \le u_0,\ v_0 \le v_1 < v_2 < \infty$.

However, with the above energy fluxes, the initial energy flux is not finite even initially on the event horizon with the chosen initial data. We therefore introduce the following *renormalized* energy fluxes.[18]

$$E_v(u) := \int_{v_0}^{v_\infty} v^2 M^2 |D_v\phi|^2(u,v) + \tfrac{1}{4} u^2 M^2 \Omega^2 \big(\mathfrak{m}^2|\phi|^2 + \tfrac{1}{4\pi} M^{-4}(Q^2 - M^2)\big)(u,v)\, dv, \tag{8-1}$$

$$E_u(v) := \int_{-\infty}^{u_0} u^2 M^2 |D_u\phi|^2(u,v) + \tfrac{1}{4} v^2 M^2 \Omega^2 \big(\mathfrak{m}^2|\phi|^2 + \tfrac{1}{4\pi} M^{-4}(Q^2 - M^2)\big)(u,v)\, du. \tag{8-2}$$

8B. *Coercivity of the renormalized energy flux.* Our goal in this subsection is to prove that the renormalized energy flux we defined in (8-1) and (8-2) is coercive and controls the quantity on the left-hand side of (A2). The statement of the main result can be found in Proposition 8.7 at the end of the subsection. This will be achieved in a number of steps. We will first need the following preliminary results:

(1) We need an improved version of (7-2), which keeps track of the constants appearing in the leading-order terms (Lemma 8.1).

(2) We then show that $\int_{v_0}^{v} (|u|/(v' + |u|))^2 |\phi|^2(u, v')\, dv'$ can be controlled by the left-hand side of (A2) (Lemma 8.3).

(3) Similarly, we show that $\int_{-\infty}^{u_0} (v/(v + |u'|))^2 |\phi|^2(u', v)\, du'$ can be controlled by the left-hand side of (A2) (Lemma 8.4).

Both (2) and (3) above are based on a Hardy-type inequality; see Lemma 8.2. After these preliminary steps, we turn to the terms in the renormalized energy (see (8-2), (8-1)) which are not manifestly nonnegative. Precisely, we control

- $\frac{1}{16\pi} \int_{v_0}^{v_\infty} u^2 M^{-2} \Omega^2 (Q^2 - M^2)(u,v)\, dv$ in Proposition 8.5, and
- $\frac{1}{16\pi} \int_{-\infty}^{u_0} v^2 M^{-2} \Omega^2 (Q^2 - M^2)(u,v)\, du$ in Proposition 8.6.

Putting all these together, we thus obtain the main result in Proposition 8.7.

We now turn to the details, beginning with the following lemma:

Lemma 8.1. *Let $\eta > 0$ be as in* (6-1)*. Then there exists $C > 0$ such that*

$$|Q^2 - M^2|(u,v) \le 8\pi M |\mathfrak{e}|(1+\eta)|u|^{-1} \int_{-\infty}^{u} u'^2 M^2 |D_u\phi|^2(u',v)\, du' + C\mathcal{D}_{\mathrm{o}} v^{-1} + C\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}})|u|^{-2}. \tag{8-3}$$

[18] Notice that in the renormalization, not only have we "added an infinity term" to each of the fluxes, we have also "replaced several factors of r by factors of M". The replacement of r by M is strictly speaking not necessary to make the renormalized energy fluxes finite, but this simplifies the computations below.

Proof. We compute

$$(Q^2-M^2)(u,v)=(Q(u,v)+M)(Q(u,v)-M)=(Q(u,v)+M)\Big(Q(-\infty,v)-M+\int_{-\infty}^{u}\partial_u Q(u',v)\,du'\Big)$$

and use (2-5) to estimate

$$|Q^2-M^2|(u,v)\le|Q(u,v)+M|\Big(|Q(-\infty,v)-M|+4\pi|\mathfrak{e}|\int_{-\infty}^{u}r^2|\phi||D_u\phi|\,du'\Big).$$

We further use (7-9) to estimate

$$\begin{aligned}
&\int_{-\infty}^{u}r^2|\phi||D_u\phi|(u',v)\,du'\\
&\quad\le\big[M^2+\sup_{-\infty<u'\le u}(r^2-M^2)\big]\cdot\sup_{-\infty<u'\le u}|\phi|(u',v)\cdot\int_{-\infty}^{u}|D_u\phi|(u',v)\,du'\\
&\quad\le\big[M^2+\sup_{-\infty<u'\le u}(r^2-M^2)\big]\cdot|u|^{-\frac12}|\phi|(-\infty,v)\sqrt{\int_{-\infty}^{u}u'^2|D_u\phi|^2(u',v)\,du'}\\
&\qquad+\big[M^2+\sup_{-\infty<u'\le u}(r^2-M^2)\big]\cdot|u|^{-\frac12}\int_{-\infty}^{u}|D_u\phi|(u',v)\,du'\cdot\sqrt{\int_{-\infty}^{u}u'^2|D_u\phi|^2(u',v)\,du'}\\
&\quad\le\big[M^2+\sup_{-\infty<u'\le u}(r^2-M^2)\big]\cdot|u|^{-\frac12}|\phi|(-\infty,v)\sqrt{\int_{-\infty}^{u}u'^2|D_u\phi|^2(u',v)\,du'}\\
&\qquad\qquad+\big[M^2+\sup_{-\infty<u'\le u}(r^2-M^2)\big]\cdot|u|^{-1}\int_{-\infty}^{u}u'^2|D_u\phi|^2(u',v)\,du'. \qquad (8\text{-}4)
\end{aligned}$$

Using (7-14), it follows that

$$|r^2-M^2|(u,v)=|r-M+2M|\cdot|r-M|\lesssim\mathcal{D}_{\mathrm{o}}v^{-1}+\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-1},$$

where we have taken $\mathcal{D}_{\mathrm{o}}v_0^{-1}$ and $(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u_0|^{-1}$ to be suitably small.

Therefore, we can further estimate the right-hand side of (8-4) to obtain

$$\begin{aligned}
\int_{-\infty}^{u}r^2|\phi||D_u\phi|(u',v)\,du'\le\tfrac14\eta^{-1}M^2|\phi|^2(-\infty,v)+(1+\eta)M^2|u|^{-1}\int_{-\infty}^{u}u'^2|D_u\phi|^2(u',v)\,du'\\
+C\mathcal{D}_{\mathrm{o}}v^{-1}|u|^{-1}+C\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-2}, \qquad (8\text{-}5)
\end{aligned}$$

where we moreover applied Young's inequality with an η-weight, where $\eta>0$ is as in the statement of the proposition.

By applying (7-2) and (8-5) together with the initial data estimate (4-5) and (4-21), we therefore obtain

$$\begin{aligned}
&|Q^2-M^2|(u,v)\\
&\le|Q(u,v)+M|\Big(|Q(-\infty,v)-M|+\pi\eta^{-1}M^2|\mathfrak{e}||\phi|^2(-\infty,v)\\
&\qquad+4\pi|\mathfrak{e}|(1+\eta)|u|^{-1}\int_{-\infty}^{u}u'^2M^2|D_u\phi|^2(u',v)\,du'+C\mathcal{D}_{\mathrm{o}}v^{-1}|u|^{-1}+C\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-2}\Big)\\
&\le(2M+C\mathcal{D}_{\mathrm{o}}v^{-1-\alpha}+C\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-1})\\
&\qquad\cdot\Big(4\pi|\mathfrak{e}|(1+\eta)|u|^{-1}\int_{-\infty}^{u}u'^2M^2|D_u\phi|^2(u',v)\,du'+C\mathcal{D}_{\mathrm{o}}v^{-1}+C\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-2}\Big)\\
&\le8\pi M|\mathfrak{e}|(1+\eta)|u|^{-1}\int_{-\infty}^{u}u'^2M^2|D_u\phi|^2(u',v)\,du'+C\mathcal{D}_{\mathrm{o}}v^{-1}+C\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-2}. \qquad \square
\end{aligned}$$

In order to estimate the $|\phi|^2$ integral, we will make use of a Hardy inequality:

Lemma 8.2. *Let $f:\mathbb{R}\to\mathbb{R}$ be in $H^1_{\mathrm{loc}}(\mathbb{R})$ and let $c\geq 0$ be a constant. Then for any $x_1, x_2\in\mathbb{R}$ with $0<x_1<x_2<\infty$,*

$$\int_{x_1}^{x_2}(x+c)^p f^2(x)\,dx \leq 2(x_2+c)^{p+1}f^2(x_2)+\frac{4}{(p+1)^2}\int_{x_1}^{x_2}(x+c)^{p+2}f'^2(x)\,dx \quad \textit{if } p>-1,$$

$$\int_{x_1}^{x_2}(x+c)^p f^2(x)\,dx \leq 2(x_1+c)^{p+1}f^2(x_1)+\frac{4}{(p+1)^2}\int_{x_1}^{x_2}(x+c)^{p+2}f'^2(x)\,dx \quad \textit{if } p<-1.$$

Proof. We will only prove the inequality in the case $p>-1$. The other inequality is similar. We compute

$$\begin{aligned}
0 &\leq \int_{x_1}^{x_2}(x+c)^p\left(\frac{p+1}{2}f+(x+c)f'\right)^2(x)\,dx \\
&= \int_{x_1}^{x_2}\frac{(p+1)^2}{4}(x+c)^p f^2+\frac{p+1}{2}(x+c)^{p+1}\frac{d}{dx}(f^2)+(x+c)^{p+2}f'^2(x)\,dx \\
&= -\frac{(p+1)^2}{4}\int_{x_1}^{x_2}(x+c)^p f^2(x)\,dx+\frac{p+1}{2}(x_2+c)^{p+1}f^2(x_2) \\
&\qquad\qquad -\frac{p+1}{2}(x_1+c)^{p+1}f^2(x_1)+\int_{x_1}^{x_2}(x+c)^{p+2}f'^2(x)\,dx.
\end{aligned}$$

Rearranging and dropping a manifestly nonnegative term yield the conclusion. □

Using Lemma 8.2, we prove a Hardy-type estimate on a constant-u hypersurface in our setting.

Lemma 8.3. *Given $\eta>0$ as in (6-1), there exists $C>0$ independent of $\mathcal{A}_\phi$ such that the following holds:*

$$\int_{v_0}^{v}\left(\frac{|u|}{v'+|u|}\right)^2|\phi|^2(u,v')\,dv' \leq C\mathcal{D}_{\mathrm{o}}+4\int_{v_0}^{v}v'^2|D_v\phi|^2(u,v')\,dv'+3(1+\eta)\int_{-\infty}^{u}|u'|^2|D_u\phi|^2(u',|u|)\,du'.$$

Proof. We will apply the Hardy inequality Lemma 8.2 on a fixed constant-u hypersurface. For this purpose, it is useful to choose an auxiliary gauge for A (see Section 2E and proof of Lemma 2.1) where $|\partial_v\phi|=|D_v\phi|$ (and we will perform all estimates in terms of the gauge-invariant quantities $|\phi|$ and $|D_v\phi|$). Let $\gamma>0$ be a constant to be chosen. If $v>|u|$, we also partition the integration interval, $[v_0,v]=[v_0,\gamma|u|]\cup[\gamma|u|,v]$, so we can estimate

$$\begin{aligned}
&\int_{v_0}^{v}\left(\frac{|u|}{v'+|u|}\right)^2|\phi|^2(u,v')\,dv' \\
&\quad= \int_{v_0}^{\gamma|u|}\left(\frac{|u|}{v'+|u|}\right)^2|\phi|^2(u,v')\,dv'+\int_{\gamma|u|}^{v}\left(\frac{|u|}{v'+|u|}\right)^2|\phi|^2(u,v')\,dv' \\
&\quad\leq \int_{v_0}^{\gamma|u|}|\phi|^2\,dv'+|u|^2\int_{\gamma|u|}^{v}(v'+|u|)^{-2}|\phi|^2(u,v')\,dv' \\
&\quad\leq 4\int_{v_0}^{\gamma|u|}v'^2|D_v\phi|^2(u,v')\,dv'+4|u|^2\int_{\gamma|u|}^{v}|D_v\phi|^2(u,v')\,dv'+2\gamma|u||\phi|^2(u,\gamma|u|)+\frac{2|u|}{(\gamma+1)}|\phi|^2(u,\gamma|u|) \\
&\quad\leq 4\max\{1,\gamma^{-2}\}\int_{v_0}^{v}v'^2|D_v\phi|^2(u,v')\,dv'+\left(2\gamma+\frac{2}{\gamma+1}\right)|u||\phi|^2(u,\gamma|u|), \qquad (8\text{-}6)
\end{aligned}$$

where we applied Lemma 8.2 with $p=0$ and $p=-2$ respectively in the two intervals. By (7-9), Young's inequality and (4-5) (to control the initial data), it moreover holds that for any $\eta>0$, there exists $C_\eta>0$ so that the following is satisfied:

$$|u|\,|\phi|^2(u,v)\le C_\eta\mathcal{D}_{\mathrm{o}}\frac{|u|}{v}+(1+\eta)\int_{-\infty}^{u}|u'|^2\,|D_u\phi|^2(u',v)\,du'. \tag{8-7}$$

Using this to control the last term in (8-6), and setting $\gamma=1$, we obtain the desired conclusion. □

We have a similar Hardy-type estimate on a constant-v hypersurface, with appropriate modifications of the weights.

Lemma 8.4. *Let $\eta>0$ be as in* (6-1). *Then there exists $C>0$ independent of $\mathcal{A}_\phi$ such that the following holds*:

$$\int_{-\infty}^{u_0}\left(\frac{v}{v+|u'|}\right)^2|\phi|^2(u',v)\,du'\le C\mathcal{D}_{\mathrm{o}}+6(1+\eta)\int_{-\infty}^{u_0}u'^2|D_u\phi|^2(u',v)\,du'.$$

Proof. Choose a gauge so that $|D_u\phi|=|\partial_u\phi|$. (As in Lemma 8.3, we will only estimate the gauge-invariant quantities.)

Let $\sigma>0$ be a constant that will be chosen suitably later on. We partition the integration interval: $[-\infty,u_0]=[-\infty,\sigma v]\cup[\sigma v,u_0]$. For the sake of convenience, we will change our integration variable from u to $-u$ and we will denote $-u$ by $|u|$, so we can estimate

$$\begin{aligned}
&\int_{|u_0|}^{\infty}\left(\frac{v}{v+|u'|}\right)^2|\phi|^2(u',v)\,d|u'|\\
&\quad=\int_{|u_0|}^{\sigma v}\left(\frac{v}{v+|u'|}\right)^2|\phi|^2(u',v)\,d|u'|+\int_{\sigma v}^{\infty}\left(\frac{v}{v+|u'|}\right)^2|\phi|^2\,d|u'|\\
&\quad\le\int_{|u_0|}^{\sigma v}|\phi|^2(u',v)\,d|u'|+v^2\int_{\sigma v}^{\infty}(v+|u'|)^{-2}|\phi|^2(u',v)\,d|u'|\\
&\quad\le 4\int_{|u_0|}^{\sigma v}|u'|^2\,|D_u\phi|^2(u',v)\,d|u'|+4v^2\int_{\sigma v}^{\infty}|D_u\phi|^2(u',v)\,d|u'|+2\sigma v|\phi|^2(\sigma v,v)+2\frac{v^2}{\sigma v+v}|\phi|^2(\sigma v,v)\\
&\quad\le 4\max\{1,\sigma^{-2}\}\int_{-\infty}^{u_0}u'^2|D_u\phi|^2(u',v)\,du'+\left(2+\frac{2}{\sigma(1+\sigma)}\right)\sigma v|\phi|^2(\sigma v,v),
\end{aligned}$$

where we applied Lemma 8.2 with $p=0$ and $p=-2$ in the two intervals. We apply (8-7) to conclude that for any η', $\sigma>0$, there exists $C_{\eta',\sigma}>0$ such that

$$\int_{u}^{u_0}\left(\frac{v}{v+|u'|}\right)^2|\phi|^2\,du'\le\left(4\max\{1,\sigma^{-2}\}+(1+\eta')\left(2+\frac{2}{\sigma(1+\sigma)}\right)\right)\int_{-\infty}^{u_0}u'^2|D_u\phi|^2\,du'+C_{\eta',\sigma}\mathcal{D}_{\mathrm{o}}.$$

Finally, choosing η' sufficiently small and σ sufficiently large, we can choose

$$4\max\{1,\sigma^{-2}\}+4\sigma^{-2}+(1+\eta')\left(2+\frac{2}{\sigma(1+\sigma)}\right)\le 6(1+\eta),$$

which then gives the desired conclusion. □

With Lemmas 8.3 and 8.4 in place, we are now ready to control the terms in $E_v(u)$ and $E_u(v)$ which are not manifestly nonnegative. These are the terms

$$\frac{1}{16\pi}\int_{v_0}^{v_\infty} u^2 M^{-2}\Omega^2(Q^2-M^2)(u,v)\,dv, \qquad \frac{1}{16\pi}\int_{-\infty}^{u_0} v^2 M^{-2}\Omega^2(Q^2-M^2)(u,v)\,du$$

in (8-1) and (8-2), which will be handled in Propositions 8.5 and 8.6 respectively.

Proposition 8.5. *For $\eta>0$ as in* (6-1) *and for $\kappa>0$ arbitrary, there exists a constant $C>0$ independent of $\mathcal{A}_\phi$ (but dependent on κ in addition to M, $\mathfrak{e}$, $\mathfrak{m}$, α and η) such that*

$$\begin{aligned}&\left|\frac{1}{16\pi}\int_{v_0}^{v} u^2M^{-2}\Omega^2(Q^2-M^2)(u,v')\,dv'\right|\\ &\quad\le(\kappa+4\kappa^{-1})|\mathfrak{e}|M^3\int_{v_0}^{v} v'^2|D_v\phi|^2\,dv'+(2+3\kappa^{-1})(1+\eta)|\mathfrak{e}|M^3\int_{-\infty}^{u}|u'|^2|D_u\phi|^2\,du'+C(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}}).\end{aligned}$$

Proof. The main integration by parts. We begin the argument by a simple integration by parts:

$$\begin{aligned}&\left|\frac{1}{16\pi}\int_{v_0}^{v} u^2M^{-2}\Omega^2(Q^2-M^2)(u,v')\,dv'\right|\\ &\quad\le\left|-\frac{1}{16\pi}\int_{v_0}^{v}\left(\int_{v_0}^{v'}u^2M^{-2}\Omega^2(u,v')\,dv''\right)\partial_v(Q^2-M^2)(u,v')\,dv'\right|\\ &\qquad\qquad+\left|\frac{1}{16\pi}\left(\int_{v_0}^{v'}u^2M^{-2}\Omega^2(u,v'')\,dv''\right)(Q^2-M^2)(u,v')\Big|_{v'=v_0}^{v'=v}\right|\\ &\quad\le\frac{1}{16\pi}\left|\int_{v_0}^{v}u^2M^{-2}\Omega^2(u,v')\,dv'\right||Q^2-M^2|(u,v)\\ &\qquad\qquad+\frac{1}{8\pi}\int_{v_0}^{v}\left|\int_{v_0}^{v'}u^2M^{-2}\Omega^2(u,v'')\,dv'''\right||Q||\partial_vQ|(u,v')\,dv'.\end{aligned}\tag{8-8}$$

Note that there are two terms that we need to estimate.

An auxiliary computation. Before we proceed, we first estimate the integral

$$\int_{v_0}^{v}u^2M^{-2}\Omega^2(u,v')\,dv',$$

which appears in (8-8). From (7-6) it follows that

$$M^{-2}\Omega^2\le 4(v+|u|)^{-2}+C|u|^{-\frac{1}{2}}(v+|u|)^{-2},\tag{8-9}$$

and hence,

$$\int_{v_0}^{v}u^2M^{-2}\Omega^2(u,v')\,dv'\le 4\int_{v_0}^{v}\left(\frac{|u|}{v'+|u|}\right)^2dv'+C|u|^{-\frac{1}{2}}\int_{v_0}^{v}\left(\frac{|u|}{v'+|u|}\right)^2dv'.$$

Note that

$$\partial_v(|u|v(v+|u|)^{-1})=\left(\frac{|u|}{v+|u|}\right)^2.\tag{8-10}$$

Hence,

$$\int_{v_0}^{v} u^2 M^{-2}\Omega^2(u,v')\,dv' \le 4|u|v(v+|u|)^{-1} + C|u|^{\frac12} v(v+|u|)^{-1}. \tag{8-11}$$

Estimating the boundary term. We first estimate the boundary term in (8-8) above by using (8-3) and (8-11):

$$\begin{aligned}\frac{1}{16\pi}\left|\int_{v_0}^{v} u^2 M^{-2}\Omega^2(u,v')\,dv'\right| |Q^2-M^2|(u,v)\\ \le 2(1+\eta)M|\mathfrak{e}|\int_{-\infty}^{u} u^2|D_u\phi|^2(u',v)M^2\,du' + C\mathcal{D}_{\mathrm{o}} + C\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-1} + C(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-\frac12}.\end{aligned} \tag{8-12}$$

Estimating the remaining integral, I: the error term. Now, we estimate the remaining integral on the very right-hand side of (8-8) by applying (2-6) and (8-11):

$$\begin{aligned}\frac{1}{8\pi}\int_{v_0}^{v}\left|\int_{v_0}^{v'} u^2M^{-2}\Omega^2(u,v'')\,dv''\right| |Q||\partial_v Q|(u,v')\,dv'\\ \le \underbrace{2M^3|\mathfrak{e}|\int_{v_0}^{v} |u|v'(v'+|u|)^{-1}|\phi||D_v\phi|\,dv'}_{\text{main term}} + \mathrm{Err},\end{aligned} \tag{8-13}$$

where

$$\begin{aligned}\mathrm{Err} = C\int_{v_0}^{v} |u|v'(v'+|u|)^{-1}|Q-M||\phi||D_v\phi|(u,v')\,dv'\\ + C\int_{v_0}^{v} |M+(Q-M)||u|^{\frac12}v'(v'+|u|)^{-1}|\phi||D_v\phi|(u,v')\,dv'\\ + C\int_{v_0}^{v} |u|v'(v'+|u|)^{-1}|r^2-M^2||\phi||D_v\phi|(u,v')\,dv'.\end{aligned} \tag{8-14}$$

Let us start with the error term, beginning with the second term (8-14), which is the hardest since the decay is the weakest. By (7-1),

$$\begin{aligned}&\int_{v_0}^{v} |M+(Q-M)||u|^{\frac12}v(v+|u|)^{-1}|\phi||D_v\phi|(u,v')\,dv'\\ &\lesssim \sqrt{\mathcal{D}_{\mathrm{o}}}\int_{v_0}^{v} |u|^{\frac12}v^{\frac12-\frac{\alpha}{2}}(v+|u|)^{-1}|D_v\phi|(u,v')\,dv' + \sqrt{\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})}\int_{v_0}^{v} v(v+|u|)^{-1}|D_v\phi|(u,v')\,dv'\\ &\lesssim \sqrt{\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})}(v_0+|u|)^{-\frac14}\left(\int_{v_0}^{v} v'^{-\frac32}\,dv'\right)^{\frac12}\left(\int_{v_0}^{v} v'^2|D_v\phi|^2(u,v')\,dv'\right)^{\frac12}\\ &\lesssim \mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})(v_0+|u|)^{-\frac14}v_0^{-\frac14}.\end{aligned}$$

The first term in (8-14) can be treated similarly, with the only caveat that there is a contribution where $|\phi|$ and $|Q-M|$ only give v-decay, and therefore one does not get any smallness in $(v_0+|u|)^{-\frac14}$. Nevertheless, this term has a coefficient that depends only on $\mathcal{D}_{\mathrm{o}}$ (and not on $\mathcal{D}_{\mathrm{i}}$). More precisely, using

(7-1) and (7-2), we have

$$\begin{aligned}\int_{v_0}^{v} &|u|v'(v'+|u|)^{-1}|Q-M||\phi||D_v\phi|(u,v')\,dv'\\ &\lesssim \mathcal{D}_{\rm o}^{\frac{3}{2}}\int_{v_0}^{v} v'^{-\frac{1}{2}}|D_v\phi|(u,v')\,dv' + \mathcal{A}_\phi^2(\mathcal{D}_{\rm o}+\mathcal{D}_{\rm i})^2(v_0+|u|)^{-\frac{1}{4}}v_0^{-\frac{1}{4}}\\ &\lesssim \mathcal{D}_{\rm o}^{\frac{3}{2}}v_0^{-\frac{1}{2}}\left(\int_{v_0}^{v} v'^2|D_v\phi|^2(u,v')\,dv'\right)^{\frac{1}{2}} + \mathcal{A}_\phi^2(\mathcal{D}_{\rm o}+\mathcal{D}_{\rm i})^2(v_0+|u|)^{-\frac{1}{4}}v_0^{-\frac{1}{4}}\\ &\lesssim \mathcal{A}_\phi^{\frac{1}{2}}\mathcal{D}_{\rm o}^2 v_0^{-\frac{1}{2}} + \mathcal{A}_\phi^2(\mathcal{D}_{\rm o}+\mathcal{D}_{\rm i})^2(v_0+|u|)^{-\frac{1}{4}}v_0^{-\frac{1}{4}}.\end{aligned}$$

Finally, the third term in (8-14) can be handled in an identical manner as the first term, except for using (7-14) instead of (7-2), so that we have

$$\int_{v_0}^{v} |u|v'(v'+|u|)^{-1}|r^2-M^2||\phi||D_v\phi|(u,v')(u,v')\,dv' \lesssim \mathcal{A}_\phi^{\frac{1}{2}}\mathcal{D}_{\rm o}^2 v_0^{-\frac{1}{2}} + \mathcal{A}_\phi^2(\mathcal{D}_{\rm o}+\mathcal{D}_{\rm i})^2(v_0+|u|)^{-\frac{1}{4}}v_0^{-\frac{1}{4}}.$$

Putting all these together, choosing $|u_0|$ and v_0 appropriately large (where the largeness of v_0 does *not* depend on $\mathcal{D}_{\rm i}$), and returning to (8-14), we thus obtain

$$\mathrm{Err} \lesssim \mathcal{D}_{\rm o}+\mathcal{D}_{\rm i}. \tag{8-15}$$

Estimating the remaining integral, II: the main term. Now for the main term in (8-13), we have, using Young's inequality,

$$\begin{aligned}2M^3|\mathfrak{e}|&\int_{v_0}^{v} |u|v'(v'+|u|)^{-1}|\phi||D_v\phi|\,dv'\\ &\leq \kappa|\mathfrak{e}|M^3\int_{v_0}^{v} v'^2|D_v\phi|^2\,dv' + \kappa^{-1}|\mathfrak{e}|M^3\int_{v_0}^{v}\left(\frac{|u|}{v'+|u|}\right)^2|\phi|^2\,dv'\\ &\leq (\kappa+4\kappa^{-1})|\mathfrak{e}|M^3\int_{v_0}^{v} v'^2|D_v\phi|^2\,dv' + 3(1+\eta)\kappa^{-1}|\mathfrak{e}|M^3\int_{-\infty}^{u}|u'|^2|D_u\phi|^2\,du' + C_\kappa(\mathcal{D}_{\rm o}+\mathcal{D}_{\rm i}),\end{aligned} \tag{8-16}$$

where in the last line we have used Lemma 8.3.

Putting everything together. Combining (8-8), (8-12), (8-13), (8-15) and (8-16), we obtain the desired conclusion. □

We now turn to the analogue of Proposition 8.5 on constant-v hypersurfaces.

Proposition 8.6. *For $\eta > 0$ as in* (6-1), *there exists a constant $C > 0$ independent of $\mathcal{A}_\phi$ such that*

$$\begin{aligned}&\left|\frac{1}{16\pi}\int_{-\infty}^{u_0} v^2 M^{-2}\Omega^2(Q^2-M^2)(u',v)\,du'\right|\\ &\qquad\leq 2(1+\sqrt{6})|\mathfrak{e}|M^3(1+\eta)\int_{-\infty}^{u_0}|u'|^2|D_u\phi|^2(u',v)\,du' + C(\mathcal{D}_{\rm o}+\mathcal{D}_{\rm i}).\end{aligned}$$

Proof. We will consider the integral

$$\frac{1}{16\pi}\int_u^{u_0} v^2 M^{-2}\Omega^2(Q^2-M^2)(u',v)\,du'$$

and take the limit $u\downarrow -\infty$.

The main integration by parts. We integrate by parts as in (8-8)

$$\begin{aligned}
&\left|\frac{1}{16\pi}\int_u^{u_0} v^2M^{-2}\Omega^2(Q^2-M^2)(u',v)\,du'\right|\\
&\quad\le\left|\frac{1}{16\pi}\int_u^{u_0}\left(\int_{u'}^{u_0} v^2M^{-2}\Omega^2\,du''\right)\partial_u(Q^2-M^2)(u',v)\,du'\right|\\
&\qquad\qquad+\left|\frac{1}{16\pi}\left(\int_{u'}^{u_0} v^2M^{-2}\Omega^2(u'',v)\,du''\right)(Q^2-M^2)(u',v)\Big|_{u'=u}^{u'=u_0}\right|\\
&\quad\le\frac{1}{16\pi}\int_u^{u_0} v^2M^{-2}\Omega^2(u',v)\,du'\cdot|Q^2-M^2|(u,v)\\
&\qquad\qquad+\frac{1}{8\pi}\int_u^{u_0}\left[\int_\infty^{u'} v^2M^{-2}\Omega^2(u'',v)\,du''\right]|Q||\partial_uQ|(u',v)\,du'. \qquad (8\text{-}17)
\end{aligned}$$

An auxiliary computation. By (8-9) and

$$-\partial_u(|u|v(v+|u|)^{-1})=\left(\frac{v^2}{v+|u'|}\right)^2,$$

we obtain

$$\begin{aligned}
\int_u^{u_0} v^2M^{-2}\Omega^2(u',v)\,du' &\le 4\int_u^{u_0}\left(\frac{v^2}{v+|u'|}\right)^2du'+Cv^2\int_u^{u_0}\frac{1}{|u'|^{\frac12}(v+|u'|)^2}\,du' \qquad (8\text{-}18)\\
&\le 4|u|v(v+|u|)^{-1}+C|u|^{\frac12}v^2(v+|u|)^{-2}.
\end{aligned}$$

Estimating the boundary term. We now control the boundary term in (8-17). By (8-18) combined with (8-3), we obtain

$$\begin{aligned}
&\frac{1}{16\pi}\left|\int_u^{u_0} v^2M^{-2}\Omega^2(u',v)\,du'\right||Q^2-M^2|(u,v)\\
&\le 2(1+\eta)M^3|\mathfrak{e}|\int_{-\infty}^u u'^2|D_u\phi|^2(u',v)\,du'+C\mathcal{D}_{\mathrm{o}}+C\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-1}+C(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u|^{-\frac12}. \qquad (8\text{-}19)
\end{aligned}$$

Estimating the remaining integral. The remaining integral in (8-17) can be controlled as follows:

$$\begin{aligned}
&\frac{1}{8\pi}\int_u^{u_0}\left|\int_{u'}^{u_0} v^2M^{-2}\Omega^2(u'',v)\,du''\right||Q||\partial_uQ|(u',v)\,du'\\
&\qquad\le\underbrace{2M^3|\mathfrak{e}|\int_u^{u_0}|u'|v(v+|u'|)^{-1}|\phi||D_u\phi|(u',v)\,du'}_{\text{main term}}+\mathrm{Err},
\end{aligned}$$

where

$$\begin{aligned}\mathrm{Err} = C\int_u^{u_0} |u'|v(v+|u'|)^{-1}|Q-M||\phi||D_u\phi|(u',v)\,du' \\ + C\int_u^{u_0} |M+(Q-M)||u'|^{\frac{1}{2}}v(v+|u'|)^{-1}|\phi||D_u\phi|(u',v)\,du' \\ + C\int_u^{u_0} |u'|v(v+|u'|)^{-1}|r^2-M^2||\phi||D_u\phi|(u',v)\,du'.\end{aligned}$$

The error term can be estimated in essentially the same manner as the error term in the proof of Proposition 8.5, except we use (A2) for $\int_u^{u_0} u'^2|D_u\phi|^2(u',v)\,du'$ instead of $\int_{v_0}^{v} v'^2|D_v\phi|^2(u,v')\,dv'$. We omit the details and just record the estimate

$$\mathrm{Err} \lesssim \mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}. \tag{8-20}$$

For the main term in (8-17), we apply Hölder's inequality, Lemma 8.4 and Young's inequality to obtain

$$\begin{aligned}&2M^3|\mathfrak{e}|\int_u^{u_0} |u'|v(v+|u'|)^{-1}|\phi||D_u\phi|(u',v)\,du' \\ &\qquad\le 2|\mathfrak{e}|M^3\biggl(\int_u^{u_0} |u'|^2|D_u\phi|^2(u',v)\,du'\biggr)^{\frac{1}{2}}\biggl(\int_u^{u_0}\Bigl(\frac{v}{v+|u'|}\Bigr)^2|\phi|^2(u',v)\,du'\biggr)^{\frac{1}{2}} \\ &\qquad\le 2|\mathfrak{e}|M^3\sqrt{6}(1+\eta)\int_u^{u_0} |u'|^2|D_u\phi|^2(u',v)\,du' + C\mathcal{D}_{\mathrm{o}}.\end{aligned} \tag{8-21}$$

<u>Putting everything together</u>. Putting together (8-17), (8-19), (8-20) and (8-21), and taking the limit $u \downarrow -\infty$, we obtain the desired conclusion. □

We can now prove the main result of this subsection, namely, the coercivity of the renormalized energy flux (up to controllable error terms).

Proposition 8.7. *We can estimate*

$$\int_{-\infty}^{u_0} |u|^2M^2|D_u\phi|^2\,du + \int_{v_0}^{v_\infty} v^2M^2|D_v\phi|^2\,dv \le \mu^{-1}(E_u(v)+E_v(u)) + C(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}}), \tag{8-22}$$

with μ as in (6-2).

Proof. Plugging in the estimates in Propositions 8.5 and 8.6 into (8-1) and (8-2) respectively, and using $\mathfrak{m} \ge 0$, we deduce that

$$\begin{aligned}E_u(v)+E_v(u) \ge \bigl(1-(4+2\sqrt{6}+3\kappa^{-1})(1+\eta)|\mathfrak{e}|M\bigr)\int_{-\infty}^{u_0} |u|^2r^2|D_u\phi|^2\,du' \\ + (1-(\kappa+4\kappa^{-1})|\mathfrak{e}|M)\int_{v_0}^{v_\infty} v^2M^2|D_v\phi|^2\,dv' - C(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}}).\end{aligned}$$

Now we choose $\kappa = 2+\sqrt{6}+\sqrt{9+4\sqrt{6}}$ to obtain the conclusion. □

8C. ***Energy estimates for ϕ.*** We define

$$E_u(v;u) := \int_{-\infty}^{u} u^2M^2|D_u\phi|^2(u',v) + \tfrac{1}{4}v^2M^2\Omega^2\big(\mathfrak{m}^2|\phi|^2 + \tfrac{1}{4\pi}M^{-4}(Q^2-M^2)\big)(u',v)\,du',$$
$$E_v(u;v) := \int_{v_0}^{v} v^2M^2|D_v\phi|^2(u,v') + \tfrac{1}{4}u^2M^2\Omega^2\big(\mathfrak{m}^2|\phi|^2 + \tfrac{1}{4\pi}M^{-4}(Q^2-M^2)\big)(u,v')\,dv'.$$

With the above definitions, we have $E_u(v) = E_u(v;u_0)$ and $E_v(u) = E_v(u;v_\infty)$.

Proposition 8.8. *$E_u(v;u)$ and $E_v(u;v)$ obey the estimate*

$$\sup_{v_0\le v\le v_\infty} E_u(v;u) + \sup_{-\infty<u<u_0} E_v(u;v) \le C(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}}).$$

Proof. In order to simplify the notation, in this proof, we omit the arguments in the integrals, which will typically be taken as (u',v'). For any $u\in(-\infty,u_0]$ and $v\in[v_0,v_\infty]$, we have the decomposition

$$\begin{aligned}[E_u(v;u)-E_u(v_0;u)]+[E_v(u;v)-E_v(-\infty;v)] &= \int_{v_0}^{v}\partial_v E_u(v';u)\,dv' + \int_{-\infty}^{u}\partial_u E_v(u';v)\,du' \\ &= J_1+J_2+J_3+J_4+J_5+J_6,\end{aligned}$$

where

$$\begin{aligned}
J_1 &= M^2\int_{v_0}^{v}\int_{-\infty}^{u} u'^2\,\partial_v(|D_u\phi|^2)\,du'\,dv',\\
J_2 &= \tfrac{1}{4}M^2\mathfrak{m}^2\int_{v_0}^{v}\int_{-\infty}^{u} v'^2\Omega^2\,\partial_v(|\phi|^2) + \partial_v(v'^2\Omega^2)\cdot|\phi|^2\,du'\,dv',\\
J_3 &= \tfrac{1}{16\pi}M^{-2}\int_{v_0}^{v}\int_{-\infty}^{u} 2v'^2\Omega^2Q\,\partial_vQ + \partial_v(v'^2\Omega^2)(Q^2-M^2)\,du'\,dv',\\
J_4 &= M^2\int_{v_0}^{v}\int_{-\infty}^{u} v'^2M^2\,\partial_u(|D_v\phi|^2)\,du'\,dv',\\
J_5 &= \tfrac{1}{4}M^2\mathfrak{m}^2\int_{v_0}^{v}\int_{-\infty}^{u} u'^2\Omega^2\,\partial_u(|\phi|^2) + \partial_u(u'^2\Omega^2)\cdot|\phi|^2\,du'\,dv',\\
J_6 &= \tfrac{1}{16\pi}M^{-2}\int_{v_0}^{v}\int_{-\infty}^{u} 2u'^2\Omega^2Q\,\partial_uQ + \partial_u(u'^2\Omega^2)(Q^2-M^2)\,du'\,dv'.
\end{aligned}$$

We first use (2-3) and (2-4) to rewrite the integral J_1 in terms of expressions that are zeroth- or first-order derivatives of the variables ϕ,Ω,r. For this, we use that we have the following identity for complex-valued functions f:

$$\partial_v(|f|^2) = (D_vf - i\mathfrak{e}A_vf)\bar f + f\,\overline{(D_vf - i\mathfrak{e}A_vf)} = \bar f D_vf + f\,\overline{D_vf}$$

and similarly

$$\partial_u(|f|^2) = \bar f D_uf + f\,\overline{D_uf}.$$

We therefore obtain

$$\begin{aligned}J_1 &= \int_{v_0}^{v}\int_{-\infty}^{u} u'^2 M^2(\overline{D_u\phi}D_vD_u\phi + D_u\phi\overline{D_vD_u\phi})\,du'\,dv'\\ &= -\tfrac{1}{2}\int_{v_0}^{v}\int_{-\infty}^{u} \tfrac{1}{2}u'^2M^2\mathfrak{m}^2\Omega^2(\phi\overline{D_u\phi}+\bar\phi D_u\phi)+2M^2r^{-1}u'^2\,\partial_u r(\overline{D_u\phi}D_v\phi+\overline{D_v\phi}D_u\phi)\\ &\qquad\qquad + 4M^2r^{-1}u'^2\,\partial_v r|D_u\phi|^2+\tfrac{1}{2}i\mathfrak{e}M^2r^{-2}u'^2\Omega^2Q(\phi\overline{D_u\phi}-\bar\phi D_u\phi)\,du'\,dv'\end{aligned}$$

and similarly,

$$\begin{aligned}J_4 &= \int_{v_0}^{v}\int_{-\infty}^{u} v'^2 M^2(\overline{D_v\phi}D_uD_v\phi + D_v\phi\overline{D_uD_v\phi})\,du'\,dv'\\ &= -\tfrac{1}{2}\int_{v_0}^{v}\int_{-\infty}^{u} \tfrac{1}{2}v'^2M^2\mathfrak{m}^2\Omega^2(\phi\overline{D_v\phi}+\bar\phi D_v\phi)+2M^2r^{-1}v'^2\,\partial_v r(\overline{D_u\phi}D_v\phi+\overline{D_v\phi}D_u\phi)\\ &\qquad\qquad + 4M^2r^{-1}v'^2\,\partial_u r|D_v\phi|^2-\tfrac{1}{2}i\mathfrak{e}M^2r^{-2}\Omega^2v'^2Q(\phi\overline{D_v\phi}-\bar\phi D_v\phi)\,du'\,dv'.\end{aligned}$$

We also rewrite J_2 and J_5 to obtain

$$\begin{aligned}J_2 &= \tfrac{1}{4}M^2\mathfrak{m}^2\int_{v_0}^{v}\int_{-\infty}^{u} v'^2\Omega^2(\bar\phi D_v\phi+\phi\overline{D_v\phi})+\partial_v(v'^2\Omega^2)\cdot|\phi|^2\,du'\,dv',\\ J_5 &= \tfrac{1}{4}M^2\mathfrak{m}^2\int_{v_0}^{v}\int_{-\infty}^{u} u'^2\Omega^2(\bar\phi D_u\phi+\phi\overline{D_u\phi})+\partial_u(u'^2\Omega^2)\cdot|\phi|^2\,du'\,dv'.\end{aligned}$$

Finally, we use (2-5) and (2-6) to rewrite J_3 and J_6:

$$\begin{aligned}J_3 &= \int_{v_0}^{v}\int_{-\infty}^{u} -\tfrac{1}{4}i\mathfrak{e}M^{-2}r^2v'^2\Omega^2Q(\phi\overline{D_v\phi}-\bar\phi D_v\phi)+\tfrac{1}{16\pi}M^{-2}\,\partial_v(v'^2\Omega^2)(Q^2-M^2)\,du'\,dv',\\ J_6 &= \int_{v_0}^{v}\int_{-\infty}^{u} \tfrac{1}{4}i\mathfrak{e}M^{-2}r^2u'^2\Omega^2Q(\phi\overline{D_u\phi}-\bar\phi D_u\phi)+\tfrac{1}{16\pi}M^{-2}\,\partial_u(u'^2\Omega^2)(Q^2-M^2)\,du'\,dv'.\end{aligned}$$

By incorporating the cancellations in the terms in J_i, we can write

$$[E_u(v;u)-E_u(v_0;u)]+[E_v(u;v)-E_v(-\infty;v)]=\sum_{i=1}^{7}F_i, \tag{8-23}$$

with

$$\begin{aligned}F_1 &= -M^2\int_{v_0}^{v}\int_{-\infty}^{u} r^{-1}(u'^2\,\partial_u r+v'^2\,\partial_v r)(\overline{D_u\phi}D_v\phi+\overline{D_v\phi}D_u\phi)\,du'\,dv',\\ F_2 &= -2M^2\int_{v_0}^{v}\int_{-\infty}^{u} r^{-1}\,\partial_v r\cdot u'^2|D_u\phi|^2+r^{-1}\,\partial_u r\cdot v'^2|D_v\phi|^2\,du'\,dv',\\ F_3 &= \tfrac{1}{4}M^2\mathfrak{m}^2\int_{v_0}^{v}\int_{-\infty}^{u}[\partial_v(v'^2\Omega_0^2)+\partial_u(u'^2\Omega_0^2)]|\phi|^2\,du'\,dv',\\ F_4 &= \tfrac{1}{16\pi}M^{-2}\int_{v_0}^{v}\int_{-\infty}^{u}[\partial_v(v'^2\Omega_0^2)+\partial_u(u'^2\Omega_0^2)](Q^2-M^2)\,du'\,dv',\\ F_5 &= \tfrac{1}{4}\int_{v_0}^{v}\int_{-\infty}^{u}[\partial_v(v'^2\cdot(\Omega^2-\Omega_0^2))+\partial_u(u'^2\cdot(\Omega^2-\Omega_0^2))](M^2\mathfrak{m}^2|\phi|^2+\tfrac{1}{4\pi}M^{-2}(Q^2-M^2))\,du'\,dv',\end{aligned}$$

$$F_6 = \tfrac{1}{4} i\mathfrak{e} M^{-2} \int_{v_0}^{v} \int_{-\infty}^{u} r^{-2}(r^4 - M^4) u'^2 Q\Omega^2 (\phi \overline{D_u \phi} - \bar{\phi} D_u \phi)\, du'\, dv',$$
$$F_7 = \tfrac{1}{4} i\mathfrak{e} M^{-2} \int_{v_0}^{v} \int_{-\infty}^{u} r^{-2}(M^4 - r^4) v'^2 Q\Omega^2 (\phi \overline{D_v \phi} - \bar{\phi} D_v \phi)\, du'\, dv'.$$

We estimate using Cauchy–Schwarz inequality, Young's inequality, Proposition 7.2 and (A2)

$$\begin{aligned}
|F_1| &\lesssim \int_{v_0}^{v} \int_{-\infty}^{u} (u'^2 |\partial_u r| + v'^2 |\partial_v r|) |D_u \phi| |D_v \phi|\, du'\, dv' \\
&\lesssim \int_{v_0}^{v} \int_{-\infty}^{u} \mathcal{A}_\phi (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}) |D_u \phi| |D_v \phi|\, du'\, dv' \\
&\lesssim \int_{v_0}^{v} \int_{-\infty}^{u} \mathcal{A}_\phi (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}) v'^{-2} u'^{\frac{3}{2}} |D_u \phi|^2\, du'\, dv' + \int_{v_0}^{v} \int_{-\infty}^{u} \mathcal{A}_\phi (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}) u'^{-\frac{3}{2}} v'^2 |D_v \phi|^2\, du'\, dv' \\
&\lesssim \mathcal{A}_\phi (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}) v_0^{-1} |u_0|^{-\frac{1}{2}} \cdot \sup_{v_0 \le v \le v_\infty} \int_{-\infty}^{u} u'^2 |D_u \phi|^2\, du' \\
&\qquad + \mathcal{A}_\phi (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}) |u_0|^{-\frac{1}{2}} \cdot \sup_{-\infty < u < u_0} \int_{v_0}^{v_\infty} v'^2 |D_v \phi|^2\, dv' \\
&\lesssim \mathcal{A}_\phi^2 (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}})^2 |u_0|^{-\frac{1}{2}}.
\end{aligned}$$

We can similarly estimate

$$\begin{aligned}
|F_2| &\lesssim \int_{v_0}^{v} \int_{-\infty}^{u} |\partial_v r| \cdot u'^2 |D_u \phi|^2\, du'\, dv' + \int_{v_0}^{v} \int_{-\infty}^{u} |\partial_u r| \cdot v'^2 |D_v \phi|^2\, du'\, dv' \\
&\lesssim \mathcal{A}_\phi (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}) \biggl(\int_{v_0}^{v} \int_{-\infty}^{u} v'^{-\frac{3}{2}} \cdot u'^{\frac{3}{2}} |D_u \phi|^2\, du'\, dv' + \int_{v_0}^{v} \int_{-\infty}^{u} u'^{-2} \cdot v'^2 |D_v \phi|^2\, du'\, dv' \biggr) \\
&\qquad + \mathcal{D}_{\mathrm{o}} \int_{v_0}^{v} \int_{-\infty}^{u} v'^{-2} \cdot u'^2 |D_u \phi|^2\, du'\, dv' \\
&\lesssim [\mathcal{D}_{\mathrm{o}} v_0^{-1} + \mathcal{A}_\phi (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}) (v_0^{-\frac{1}{2}} |u_0|^{-\frac{1}{2}} + |u_0|^{-1})] \mathcal{A}_\phi (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}).
\end{aligned}$$

In order to estimate $|F_3|$, we use (3-4) (with a constant depending on $\beta > 0$) and (7-1) to get

$$\begin{aligned}
|F_3| &\lesssim \int_{v_0}^{v} \int_{-\infty}^{u} |\partial_v (v^2 \Omega_0^2) + \partial_u (u^2 \Omega_0^2)| \cdot |\phi|^2\, du'\, dv' \\
&\lesssim \int_{v_0}^{v} \int_{-\infty}^{u} (v' + |u'|)^{-2+\beta} (\mathcal{D}_{\mathrm{o}} v'^{-1} + \mathcal{A}_\phi (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}) |u'|^{-1})\, du'\, dv' \\
&\lesssim \mathcal{A}_\phi (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}) (v_0 + |u_0|)^{-1+2\beta}.
\end{aligned}$$

Similarly, using (3-4) and (7-2),

$$\begin{aligned}
|F_4| &\lesssim \int_{v_0}^{v} \int_{-\infty}^{u} |\partial_v (v^2 \Omega_0^2) + \partial_u (u^2 \Omega_0^2)| \cdot |Q - M| |Q + M|\, du'\, dv' \\
&\lesssim \int_{v_0}^{v} \int_{-\infty}^{u} (v' + |u'|)^{-2+\beta} (\mathcal{D}_{\mathrm{o}} v'^{-1} + \mathcal{A}_\phi (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}) |u'|^{-1})\, du'\, dv' \\
&\lesssim \mathcal{A}_\phi (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}) (v_0 + |u_0|)^{-1+2\beta}.
\end{aligned}$$

Before we estimate $|F_5|$, it is convenient to rewrite the following expression:

$$\begin{aligned}
&\partial_v(v^2(\Omega^2-\Omega_0^2))+\partial_u(u^2(\Omega^2-\Omega_0^2))\\
&\qquad=\partial_v\biggl(v^2\Omega_0^2\biggl(\frac{\Omega^2}{\Omega_0^2}-1\biggr)\biggr)+\partial_u\biggl(u^2\Omega_0^2\biggl(\frac{\Omega^2}{\Omega_0^2}-1\biggr)\biggr)\\
&\qquad=(\partial_v(v^2\Omega_0^2)+\partial_u(u^2\Omega_0^2))\biggl(\frac{\Omega^2}{\Omega_0^2}-1\biggr)+v^2\Omega_0^2\,\partial_v\biggl(\frac{\Omega^2}{\Omega_0^2}-1\biggr)+u^2\Omega_0^2\,\partial_u\biggl(\frac{\Omega^2}{\Omega_0^2}-1\biggr)\\
&\qquad=(\partial_v(v^2\Omega_0^2)+\partial_u(u^2\Omega_0^2))\biggl(\frac{\Omega^2}{\Omega_0^2}-1\biggr)+2v^2\Omega^2\,\partial_v\biggl(\log\frac{\Omega}{\Omega_0}\biggr)+2u^2\Omega^2\,\partial_u\biggl(\log\frac{\Omega}{\Omega_0}\biggr).
\end{aligned}$$

Therefore,

$$\begin{aligned}
|F_5|\lesssim{}&\int_{v_0}^{v}\int_{-\infty}^{u}|\partial_v(v'^2\Omega_0^2)+\partial_u(u'^2\Omega_0^2)|\biggl|\frac{\Omega^2}{\Omega_0^2}-1\biggr|\cdot(|\phi|^2+|Q-M||Q+M|)\,du'\,dv'\\
&+\int_{v_0}^{v}\int_{-\infty}^{u}v'^2\Omega^2\biggl|\partial_v\biggl(\log\frac{\Omega}{\Omega_0}\biggr)\biggr|\cdot(|\phi|^2+|Q-M||Q+M|)\,du'\,dv'\\
&\quad+\int_{v_0}^{v}\int_{-\infty}^{u}u'^2\Omega^2\biggl|\partial_u\biggl(\log\frac{\Omega}{\Omega_0}\biggr)\biggr|\cdot(|\phi|^2+|Q-M||Q+M|)\,du'\,dv'=:F_{5,1}+F_{5,2}+F_{5,3}.
\end{aligned}$$

Using (3-4), (7-1), (7-2), (7-3), we can estimate $|F_{5,1}|$ in the same way as $|F_3|$ and $|F_4|$ to obtain

$$|F_{5,1}|\lesssim\mathcal{A}_\phi(\mathcal{D}_\mathrm{o}+\mathcal{D}_\mathrm{i})|u_0|^{-\frac{1}{2}}(v_0+|u_0|)^{-1+2\beta}.$$

For $|F_{5,2}|$, we use (7-1), (7-2) and (A1) to estimate

$$\begin{aligned}
|F_{5,2}|&\lesssim\int_{v_0}^{v}\int_{-\infty}^{u}(\mathcal{D}_\mathrm{o}v'^{-1}+\mathcal{A}_\phi(\mathcal{D}_\mathrm{o}+\mathcal{D}_\mathrm{i})|u'|^{-1})v'^2\Omega^2\biggl|\partial_v\biggl(\log\frac{\Omega}{\Omega_0}\biggr)\biggr|\,du'\,dv'\\
&\lesssim\mathcal{D}_\mathrm{o}\biggl(\sup_{u'\in(-\infty,u_0]}\int_{v_0}^{v}v'^2\Bigl(\partial_v\Bigl(\log\frac{\Omega}{\Omega_0}\Bigr)\Bigr)^2(u',v')\,dv'\biggr)^{\frac{1}{2}}\int_{-\infty}^{u}\biggl(\int_{v_0}^{v}(v'+|u'|)^{-4}\,dv'\biggr)^{\frac{1}{2}}du'\\
&\quad+\mathcal{A}_\phi(\mathcal{D}_\mathrm{o}+\mathcal{D}_\mathrm{i})\biggl(\sup_{u'\in(-\infty,u_0]}\int_{v_0}^{v}v'^2\Bigl(\partial_v\Bigl(\log\frac{\Omega}{\Omega_0}\Bigr)\Bigr)^2(u',v')\,dv'\biggr)^{\frac{1}{2}}\int_{-\infty}^{u}\biggl(\int_{v_0}^{v}\frac{v'^2}{|u'|^2(v'+|u'|)^4}\,dv'\biggr)^{\frac{1}{2}}du'\\
&\lesssim\mathcal{D}_\mathrm{o}(v_0+|u_0|)^{-\frac{1}{2}}+\mathcal{A}_\phi(\mathcal{D}_\mathrm{o}+\mathcal{D}_\mathrm{i})|u_0|^{-\frac{1}{2}},
\end{aligned}$$

where in the last line we have evaluated an integral as follows (we only include this estimate for completeness; in what follows, we will bound similar integrals in analogous manner without spelling out the full details):

$$\begin{aligned}
\int_{-\infty}^{u}\biggl(\int_{v_0}^{v}\frac{v'^2}{|u'|^2(v'+|u'|)^4}\,dv'\biggr)^{\frac{1}{2}}du'&\lesssim\int_{-\infty}^{u}\biggl(\int_{v_0}^{|u|}\frac{v'^2}{|u'|^2(v'+|u'|)^4}\,dv'+\int_{|u|}^{v}\frac{v'^2}{|u'|^2(v'+|u'|)^4}\,dv'\biggr)^{\frac{1}{2}}du'\\
&\lesssim\int_{-\infty}^{u}\biggl(\int_{v_0}^{|u|}\frac{v'^2}{|u'|^6}\,dv'+\int_{|u|}^{v}\frac{1}{|u'|^2v'^2}\,dv'\biggr)^{\frac{1}{2}}du'\\
&\lesssim\int_{-\infty}^{u}|u'|^{-\frac{3}{2}}\,du'\lesssim|u_0|^{-\frac{1}{2}}.
\end{aligned}$$

For $|F_{5,3}|$, we similarly use (7-1), (7-2) and (A1) to estimate

$$\begin{aligned}
|F_{5,3}| &\lesssim \int_{v_0}^{v}\int_{-\infty}^{u}(\mathcal{D}_{\mathrm{o}}v'^{-1}+\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u'|^{-1})u'^2\Omega^2\Big|\partial_u\Big(\log\frac{\Omega}{\Omega_0}\Big)\Big|\,du'\,dv' \\
&\lesssim \mathcal{D}_{\mathrm{o}}\bigg(\sup_{u'\in(-\infty,u_0]}\int_{-\infty}^{u}u'^2\Big(\partial_u\Big(\log\frac{\Omega}{\Omega_0}\Big)\Big)^2(u',v')\,du'\bigg)^{\frac12}\int_{v_0}^{v}\bigg(\int_{-\infty}^{u}\frac{u'^2}{v'^2(v'+|u'|)^4}\,du'\bigg)^{\frac12}dv' \\
&\quad+\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})\bigg(\sup_{u'\in(-\infty,u_0]}\int_{-\infty}^{u}u'^2\Big(\partial_u\Big(\log\frac{\Omega}{\Omega_0}\Big)\Big)^2(u',v')\,du'\bigg)^{\frac12}\int_{v_0}^{v}\bigg(\int_{-\infty}^{u}(v'+|u'|)^{-4}\,du'\bigg)^{\frac12}dv' \\
&\lesssim \mathcal{D}_{\mathrm{o}}v_0^{-\frac12}+\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})(v_0+|u_0|)^{-\frac12}.
\end{aligned}$$

Thus, combining the estimates for $F_{5,1}$, $F_{5,2}$ and $F_{5,3}$, we obtain

$$|F_5|\lesssim \mathcal{D}_{\mathrm{o}}v_0^{-\frac12}+\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u_0|^{-\frac12}.$$

We are left with $|F_6|$ and $|F_7|$, which are slightly easier because more decay is available. For F_6, we use the Cauchy–Schwarz inequality, (7-1), (7-6), (7-14), and (A2) to obtain

$$\begin{aligned}
|F_6| &\lesssim \int_{v_0}^{v}\int_{-\infty}^{u}|r-M|u'^2\Omega^2|\phi|\,|D_u\phi|\,du'\,dv' \\
&\lesssim \int_{v_0}^{v}\int_{-\infty}^{u}(\mathcal{D}_{\mathrm{o}}v'^{-1}+\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u'|^{-1})(\sqrt{\mathcal{D}_{\mathrm{o}}}v'^{-\frac12}+\sqrt{\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})}|u'|^{-\frac12})u'^2\Omega^2|D_u\phi|\,du'\,dv' \\
&\lesssim \mathcal{D}_{\mathrm{o}}^{\frac32}\bigg(\sup_{v'\in[v_0,v)}\int_{-\infty}^{u}u'^2|D_u\phi|^2(u',v')\,du'\bigg)^{\frac12}\int_{v_0}^{v}\bigg(\int_{-\infty}^{u}v'^{-3}u'^2(v'+|u'|)^{-4}\,du'\bigg)^{\frac12}dv' \\
&\quad+\mathcal{A}_\phi^{\frac32}(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})^{\frac32}\bigg(\sup_{v'\in[v_0,v)}\int_{-\infty}^{u}u'^2|D_u\phi|^2(u',v')\,du'\bigg)^{\frac12}\int_{v_0}^{v}\bigg(\int_{-\infty}^{u}|u'|^{-1}(v'+|u'|)^{-4}\,du'\bigg)^{\frac12}dv' \\
&\lesssim \mathcal{A}_\phi^{\frac12}\mathcal{D}_{\mathrm{o}}^{\frac32}(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})^{\frac12}v_0^{-\frac12}|u_0|^{-\frac12}+\mathcal{A}_\phi^2(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})^2|u_0|^{-\frac12}(v_0+|u_0|)^{-\frac12}.
\end{aligned}$$

Similarly, we use the Cauchy–Schwarz inequality, (7-1), (7-6), (7-14), and (A2) to obtain

$$\begin{aligned}
|F_7| &\lesssim \int_{v_0}^{v}\int_{-\infty}^{u}|r-M|v'^2\Omega^2|\phi|\,|D_v\phi|\,du'\,dv' \\
&\lesssim \int_{v_0}^{v}\int_{-\infty}^{u}(\mathcal{D}_{\mathrm{o}}v'^{-1}+\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u'|^{-1})(\sqrt{\mathcal{D}_{\mathrm{o}}}v'^{-\frac12}+\sqrt{\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})}|u'|^{-\frac12})v'^2\Omega^2|D_v\phi|\,du'\,dv' \\
&\lesssim \mathcal{D}_{\mathrm{o}}^{\frac32}\bigg(\sup_{u'\in(-\infty,u_0]}\int_{v_0}^{v}v'^2|D_v\phi|^2(u',v')\,dv'\bigg)^{\frac12}\int_{-\infty}^{u}\bigg(\int_{v_0}^{v}v'^{-1}(v'+|u'|)^{-4}\,dv'\bigg)^{\frac12}du' \\
&\quad+\mathcal{A}_\phi^{\frac32}(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})^{\frac32}\bigg(\sup_{u'\in(-\infty,u_0]}\int_{v_0}^{v}v'^2|D_v\phi|^2(u',v')\,dv'\bigg)^{\frac12}\int_{-\infty}^{u}\bigg(\int_{v_0}^{v}v'^2|u'|^{-3}(v'+|u'|)^{-4}\,dv'\bigg)^{\frac12}du' \\
&\lesssim \mathcal{A}_\phi^{\frac12}\mathcal{D}_{\mathrm{o}}^{\frac32}(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})^{\frac12}v_0^{-\frac12}(v_0+|u_0|)^{-\frac12}+\mathcal{A}_\phi^2(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})^2|u_0|^{-\frac12}(v_0+|u_0|)^{-\frac12}.
\end{aligned}$$

Choosing v_0 and $|u_0|$ large in a manner allowed by (6-3), we obtain

$$|F_1| + \cdots + |F_7| \lesssim \mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}.$$

Finally, noting that the initial data contributions $E_u(v_0; u)$ and $E_v(-\infty; v)$ are by definition bounded by $\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}$, and returning to (8-23), we obtain

$$\sup_{v_0 \le v < v_\infty} E_u(v; u) + \sup_{-\infty < u < u_0} E_v(u; v) \lesssim \mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}},$$

which is to be proved. □

Combining Propositions 8.7 and 8.8, we obtain the following estimate. In particular, this is an improvement over the bootstrap assumption (A2) for $\mathcal{A}_\phi$ sufficiently large depending on M, $\mathfrak{m}$, $\mathfrak{e}$ and η.

Corollary 8.9. *Choosing $\mathcal{A}_\phi$ sufficiently large (depending on M, $\mathfrak{m}$ and $\mathfrak{e}$), the following estimate holds*:

$$\sup_{v \in [v_0, v_\infty)} \int_{-\infty}^{u_0} u^2 |D_u \phi|^2(u, v)\, du + \sup_{u \in (-\infty, u_0)} \int_{v_0}^{v_\infty} v^2 |D_v \phi|^2(u, v)\, dv \le C(\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}) \le \tfrac{1}{2} A_\phi (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}).$$

At this point we fix $\mathcal{A}_\phi$ so that Corollary 8.9 holds.

8D. *Energy estimates for* $\log(\Omega/\Omega_0)$. Finally, we carry out the energy estimates for $\log(\Omega/\Omega_0)$. As we noted in the Introduction, the essential point is to establish that $\log(\Omega/\Omega_0)$ obeys an equation of the form (1-5) up to lower-order terms. More precisely, starting with (2-2), the estimates that we have obtained so far show that the $D_u\phi\overline{D_v\phi}$ and $\partial_u r\, \partial_v r$ terms have better decay properties, and that r and Q both decay to M. Therefore, (2-2) can indeed be thought of as (1-5).

We split the proof of the energy estimates into two parts. First, in Lemma 8.10, we consider an energy inspired by the form (1-5) and write down the error terms that arise when controlling this energy. Then, in Proposition 8.11, we will bound all the error terms arising in Lemma 8.10 to obtain the desired estimate for $\log(\Omega/\Omega_0)$.

Lemma 8.10. *The following identity holds for any $u \in (-\infty, u_0)$ and $v \in [v_0, v_\infty)$*:

$$\int_{-\infty}^{u} u'^2 \Big(\partial_v \log\Big(\frac{\Omega}{\Omega_0}\Big)\Big)^2 + \tfrac{1}{8} M^{-4} u'^2 \Omega^{-2} (\Omega^2 - \Omega_0^2)^2 (u', v)\, du' \\ + \int_{v_0}^{v} v'^2 \Big(\partial_v \log\Big(\frac{\Omega}{\Omega_0}\Big)\Big)^2 + \tfrac{1}{8} M^{-4} v'^2 \Omega^{-2} (\Omega^2 - \Omega_0^2)^2 (u, v')\, dv' = \sum_{i=1}^{6} O_i,$$

where

$$O_1 = -4\pi \int_{v_0}^{v} \int_{-\infty}^{u} (D_u\phi \overline{D_v\phi} + \overline{D_u\phi} D_v\phi) \Big(v'^2 \partial_v \log\Big(\frac{\Omega}{\Omega_0}\Big) + u'^2\, \partial_u \log\Big(\frac{\Omega}{\Omega_0}\Big)\Big)\, du'\, dv',$$

$$O_2 = \tfrac{1}{8} M^{-4} \int_{v_0}^{v} \int_{-\infty}^{u} [\partial_v (v'^2 \Omega_0^2) + \partial_u (u'^2 \Omega_0^2)] \frac{\Omega_0^2}{\Omega^2} \Big(\frac{\Omega^2}{\Omega_0^2} - 1\Big)^2\, du'\, dv',$$

$$O_3 = -\tfrac{1}{4} M^{-4} \int_{v_0}^{v} \int_{-\infty}^{u} \Omega^{-2} (\Omega^2 - \Omega_0^2)^2 \Big(v'^2\, \partial_v \log\Big(\frac{\Omega}{\Omega_0}\Big) + u'^2\, \partial_u \log\Big(\frac{\Omega}{\Omega_0}\Big)\Big)\, du'\, dv',$$

$$O_4=\int_{v_0}^{v}\int_{-\infty}^{u}\Omega_0^2\big[Q^2(r_0^{-4}-r^{-4})+r_0^{-4}(M^2-Q^2)-\tfrac{1}{2}(r_0^{-2}-r^{-2})\big]\cdot\Big(v'^2\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)+u'^2\,\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big)\,du'\,dv',$$

$$O_5=\int_{v_0}^{v}\int_{-\infty}^{u}(\Omega^2-\Omega_0^2)\big[r^{-4}(M^2-Q^2)+\tfrac{1}{2}(r^{-2}-M^{-2})-M^2(r^{-4}-M^{-4})\big]\cdot\Big(v'^2\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)+u'^2\,\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big)\,du'\,dv',$$

$$O_6=2\int_{v_0}^{v}\int_{-\infty}^{u}(r^{-2}\,\partial_ur\,\partial_vr-r_0^{-2}\,\partial_ur_0\,\partial_vr_0)\Big(v'^2\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)+u'^2\,\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big)\,du'\,dv',$$

where, as in Proposition 8.8, we have suppressed the argument (u',v') *in the integrand in the* O_i *terms.*

Proof. By (2-2) we have

$$\begin{aligned}\partial_u\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)&=-2\pi(D_u\phi\overline{D_v\phi}+\overline{D_u\phi}D_v\phi)+r^{-2}\partial_ur\,\partial_vr-r_0^{-2}\partial_ur_0\,\partial_vr_0\\&\quad-\tfrac{1}{2}\Omega^2r^{-4}Q^2+\tfrac{1}{2}\Omega_0^2r_0^{-4}M^2+\tfrac{1}{4}\Omega^2r^{-2}-\tfrac{1}{4}\Omega_0^2r_0^{-2}\\&=-2\pi(D_u\phi\overline{D_v\phi}+\overline{D_u\phi}D_v\phi)+r^{-2}\,\partial_u(r-r_0)\,\partial_vr+r^{-2}\,\partial_ur_0\,\partial_v(r-r_0)\\&\quad+\partial_ur_0\,\partial_vr_0(r^{-2}-r_0^{-2})-\tfrac{1}{2}(\Omega^2-\Omega_0^2)r^{-4}M^2+\tfrac{1}{2}(\Omega^2-\Omega_0^2)r^{-4}(M^2-Q^2)\\&\quad+\tfrac{1}{4}(\Omega^2-\Omega_0^2)M^{-2}+\tfrac{1}{4}(\Omega^2-\Omega_0^2)(r^{-2}-M^{-2})\\&\quad+\tfrac{1}{2}\Omega_0^2Q^2(r_0^{-4}-r^{-4})+\tfrac{1}{2}\Omega_0^2r_0^{-4}(M^2-Q^2)-\tfrac{1}{4}\Omega_0^2(r_0^{-2}-r^{-2})\\&=-2\pi(D_u\phi\overline{D_v\phi}+\overline{D_u\phi}D_v\phi)+r^{-2}\partial_u(r-r_0)\,\partial_vr+r^{-2}\,\partial_ur_0\,\partial_v(r-r_0)\\&\quad+\partial_ur_0\,\partial_vr_0(r^{-2}-r_0^{-2})-\tfrac{1}{2}(\Omega^2-\Omega_0^2)M^{-2}-\tfrac{1}{2}(\Omega^2-\Omega_0^2)M^2(r^{-4}-M^{-4})\\&\quad+\tfrac{1}{2}(\Omega^2-\Omega_0^2)r^{-4}(M^2-Q^2)+\tfrac{1}{4}(\Omega^2-\Omega_0^2)M^{-2}+\tfrac{1}{4}(\Omega^2-\Omega_0^2)(r^{-2}-M^{-2})\\&\quad+\tfrac{1}{2}\Omega_0^2Q^2(r_0^{-4}-r^{-4})+\tfrac{1}{2}\Omega_0^2r_0^{-4}(M^2-Q^2)-\tfrac{1}{4}\Omega_0^2(r_0^{-2}-r^{-2}).\end{aligned}$$

Using the above equation, we obtain

$$\begin{aligned}&\partial_u\Big(v^2\Big(\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big)^2\Big)\\&\quad=2v^2\,\partial_u\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\cdot\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\\&\quad=-4\pi v^2(D_u\phi\overline{D_v\phi}+\overline{D_u\phi}D_v\phi)\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)+2r^{-2}\,\partial_u(r-r_0)\,\partial_vr\,v^2\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\\&\qquad+2r^{-2}\,\partial_ur_0\,\partial_v(r-r_0)v^2\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)+2\partial_ur_0\,\partial_vr_0(r^{-2}-r_0^{-2})v^2\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\\&\qquad-\tfrac{1}{2}M^{-2}v^2(\Omega^2-\Omega_0^2)\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)-(\Omega^2-\Omega_0^2)M^2(r^{-4}-M^{-4})v^2\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\\&\qquad+(\Omega^2-\Omega_0^2)r^{-4}(M^2-Q^2)v^2\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)+\tfrac{1}{2}(\Omega^2-\Omega_0^2)(r^{-2}-M^{-2})v^2\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\\&\qquad+\Omega_0^2Q^2(r_0^{-4}-r^{-4})v^2\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)+\Omega_0^2r_0^{-4}(M^2-Q^2)v^2\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\\&\qquad-\tfrac{1}{2}\Omega_0^2(r_0^{-2}-r^{-2})v^2\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big).\end{aligned}$$

Note that we can write

$$(\Omega^2-\Omega_0^2)\,\partial_v \log\Big(\frac{\Omega}{\Omega_0}\Big)=\tfrac{1}{2}(\Omega^2-\Omega_0^2)\,\partial_v\Big(\frac{\Omega^2}{\Omega_0^2}-1\Big)\frac{\Omega_0^2}{\Omega^2}=\frac{1}{4}\frac{\Omega_0^4}{\Omega^2}\,\partial_v\bigg(\Big(\frac{\Omega^2}{\Omega_0^2}-1\Big)^2\bigg).$$

Hence,

$$\begin{aligned}-\tfrac{1}{2}M^{-4}v^2(\Omega^2-\Omega_0^2)\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)&=-\tfrac{1}{8}v^2M^{-4}\frac{\Omega_0^4}{\Omega^2}\,\partial_v\bigg(\Big(\frac{\Omega^2}{\Omega_0^2}-1\Big)^2\bigg)\\&=-\,\partial_v\big(\tfrac{1}{8}M^{-4}v^2\Omega^{-2}(\Omega^2-\Omega_0^2)^2\big)+\tfrac{1}{8}M^{-4}\,\partial_v\Big(v^2\Omega_0^2\frac{\Omega_0^2}{\Omega^2}\Big)\Big(\frac{\Omega^2}{\Omega_0^2}-1\Big)^2\\&=-\partial_v\big(\tfrac{1}{8}M^{-4}v^2\Omega^{-2}(\Omega^2-\Omega_0^2)^2\big)+\tfrac{1}{8}M^{-4}\,\partial_v(v^2\Omega_0^2)\frac{\Omega_0^2}{\Omega^2}\Big(\frac{\Omega^2}{\Omega_0^2}-1\Big)^2\\&\qquad-\tfrac{1}{4}M^{-4}v^2\Omega^{-2}\,\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)(\Omega^2-\Omega_0^2)^2.\end{aligned}$$

We similarly consider $\partial_v(u^2(\partial_u\log(\Omega/\Omega_0))^2)$ and use the Leibniz rule (with u replacing the role of v). Noting also that by the gauge condition (4-1), $\log(\Omega/\Omega_0)=0$ on the initial hypersurfaces, this yields the statement of the lemma. □

Proposition 8.11. *The following estimate holds*:

$$\sup_{v\in[v_0,v_\infty]}\int_{-\infty}^{u_0}u'^2\Big(\partial_u\Big(\log\frac{\Omega}{\Omega_0}\Big)\Big)^2(u',v)\,du'+\sup_{u\in(-\infty,u_0]}\int_{v_0}^{v_\infty}v'^2\Big(\partial_v\Big(\log\frac{\Omega}{\Omega_0}\Big)\Big)^2(u,v')\,dv'\le\tfrac{1}{2}M.$$

Proof. In order to obtain the stated estimates, we need to bound each of the terms in Lemma 8.10. The basic idea is to use the bootstrap assumption (A1) to control $\partial_v\log(\Omega/\Omega_0)$ and $\partial_u\log(\Omega/\Omega_0)$ and to use the estimates that we have previously obtained to deduce the decay and smallness of these terms.

We begin with the estimates for O_1. This turns out to be the most difficult term since we do not have any kind of pointwise estimates for $|D_v\phi|$, $|D_u\phi|$, $|\partial_v\log(\Omega/\Omega_0)|$ and $|\partial_u\log(\Omega/\Omega_0)|$. We bound it as follows using (A1):

$$\begin{aligned}|O_1|&\lesssim\int_{v_0}^{v}\int_{-\infty}^{u}|D_u\phi|\cdot|D_v\phi|\cdot\Big(v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|+u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|\Big)\,du'\,dv'\\&\lesssim\Big(\int_{v_0}^{v}v'^2\sup_{u'\in(-\infty,u]}|D_v\phi|^2(u',v')\,dv'\Big)^{\frac12}\cdot\Big(\int_{-\infty}^{u}u'^2\sup_{v'\in[v_0,v]}|D_u\phi|^2(u',v')\,du'\Big)^{\frac12}\\&\quad\times\bigg(|u_0|^{-\frac12}\Big(\sup_{u'\in(-\infty,u]}\int_{v_0}^{v}v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|^2(u',v')\,dv'\Big)^{\frac12}\\&\qquad\qquad+v_0^{-\frac12}\Big(\sup_{v'\in[v_0,v]}\int_{-\infty}^{u}u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|^2(u',v')\,du'\Big)^{\frac12}\bigg)\\&\lesssim(|u_0|^{-\frac12}+v_0^{-\frac12})\Big(\int_{v_0}^{v}\sup_{u'\in(-\infty,u]}\Big[\int_{-\infty}^{u'}v'^2\,\partial_u(|D_v\phi|^2)(u'',v')\,du''\Big]dv'\Big)^{\frac12}\\&\quad\times\Big(\int_{-\infty}^{u}\sup_{v'\in[v_0,v]}\Big[\int_{v_0}^{v'}|u'|^2\,\partial_v(|D_u\phi|^2)(u',v'')\,dv''\Big]du'\Big)^{\frac12}.\end{aligned}\tag{8-24}$$

We first consider the last factor in (8-24). From the computation for J_1 in the proof of Proposition 8.8, which used (2-3) and (2-4), it follows that

$$\begin{aligned}\int_{-\infty}^{u} \sup_{v'\in[v_0,v]}\bigg[\int_{v_0}^{v'} |u'|^{\frac{3}{2}}\,\partial_v(|D_u\phi|^2)\,dv''\bigg]\,du' \\ \lesssim \int_{v_0}^{v}\int_{-\infty}^{u} u'^{\frac{3}{2}}\Omega^2|\phi||D_u\phi| + u'^{\frac{3}{2}}|\partial_u r||D_u\phi|D_v\phi| + u'^{\frac{3}{2}}|\partial_v r||D_u\phi|^2\,du'\,dv' \\ =: O_{1,1}+O_{1,2}+O_{1,3}. \end{aligned}\tag{8-25}$$

The terms $O_{1,2}$ and $O_{1,3}$ have already been controlled in the proof of Proposition 8.8. More precisely, estimating as the terms F_1 and F_2 in the proof of Proposition 8.8, and noting that $O_{1,2}$ and $O_{1,3}$ have an additional $u'^{-\frac{1}{2}}$-weight compared to F_1 and F_2, we have

$$O_{1,2}+O_{1,3} \lesssim \mathcal{A}_\phi^2(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})^2|u_0|^{-1} + \mathcal{A}_\phi\mathcal{D}_{\mathrm{o}}(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})v_0^{-1}|u_0|^{-\frac{1}{2}} \lesssim \mathcal{A}_\phi^2(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})^2|u_0|^{-\frac{1}{2}}.$$

It thus remains to bound $O_{1,1}$, which has no analogue in Proposition 8.8. To control this term, we use (7-1), (7-8), the Cauchy–Schwarz inequality and the bootstrap assumption (A2) to obtain

$$\begin{aligned} O_{1,1} &\lesssim \sqrt{\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})}\int_{v_0}^{v}\bigg(\int_{-\infty}^{u} u'^2|D_u\phi|^2\,du'\bigg)^{\frac{1}{2}}\bigg(\int_{-\infty}^{u}(v'+|u'|)^{-4}\,du'\bigg)^{\frac{1}{2}}dv' \\ &\qquad + \sqrt{\mathcal{D}_{\mathrm{o}}}\int_{v_0}^{v}\bigg(\int_{-\infty}^{u} u'^2|D_u\phi|^2\,du'\bigg)^{\frac{1}{2}}\bigg(\int_{-\infty}^{u}\frac{|u'|}{v'^{1+\alpha}}(v'+|u'|)^{-4}\,du'\bigg)^{\frac{1}{2}}dv' \\ &\lesssim \sqrt{\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})}\bigg(\sup_{v'\in[v_0,v]}\int_{-\infty}^{u} u'^2|D_u\phi|^2(u',v')\,du'\bigg)^{\frac{1}{2}} \\ &\qquad \times\bigg(\int_{v_0}^{v}(v'+|u|)^{-\frac{3}{2}}\,dv' + \int_{v_0}^{v} v'^{-\frac{1}{2}-\frac{\alpha}{2}}(v'+|u|)^{-1}\,dv'\bigg) \\ &\lesssim \mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})(v_0+|u_0|)^{-\frac{1}{2}}. \end{aligned}$$

Combining all these and plugging back into (8-25), we obtain

$$\begin{aligned}\int_{-\infty}^{u} \sup_{v'\in[v_0,v]}\bigg[\int_{v_0}^{v'} |u'|^{\frac{3}{2}}\,\partial_v(|D_u\phi|^2)\,dv''\bigg]\,du' &\lesssim \mathcal{A}_\phi^2(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})^2|u_0|^{-\frac{1}{2}} + \mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})(v_0+|u_0|)^{-\frac{1}{2}} \\ &\lesssim \mathcal{A}_\phi^2(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})^2|u_0|^{-\frac{1}{2}}. \end{aligned}\tag{8-26}$$

For the other factor in (8-24), we estimate similarly by

$$\begin{aligned}\int_{v_0}^{v} \sup_{-\infty\le u'\le u}\bigg[\int_{-\infty}^{u'} v'^{\frac{3}{2}}\,\partial_u(|D_v\phi|^2)\,du''\bigg]\,dv' \\ \lesssim \int_{v_0}^{v}\int_{-\infty}^{u} v'^2\Omega^2|\phi||D_v\phi| + v'^2|\partial_v r||D_u\phi|D_v\phi| + v'^2|\partial_u r||D_v\phi|^2\,du'\,dv' =: O_{1,4}+O_{1,5}+O_{1,6}. \end{aligned}$$

The terms $O_{1,5}$ and $O_{1,6}$, just as $O_{1,2}$ and $O_{1,3}$, can be bounded above by $\mathcal{A}_\phi^2(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})^2|u_0|^{-\frac{1}{2}}$ as the terms F_1 and F_2 in the proof of Proposition 8.8. For the term $O_{1,4}$, we have, using (7-1), (7-8), the

Cauchy–Schwarz inequality and the bootstrap assumption (A2),

$$\begin{aligned}
&\int_{v_0}^{v}\int_{-\infty}^{u} v'^{\frac{3}{2}}\Omega^2|\phi||D_v\phi|\,du'\,dv' \\
&\quad\lesssim \sqrt{\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})}\int_{-\infty}^{u}\Big(\int_{v_0}^{v} v'^2|D_v\phi|^2\,dv'\Big)^{\frac{1}{2}}\Big(\int_{v_0}^{v}|u'|^{-1}v'(v'+|u'|)^{-4}\,dv'\Big)^{\frac{1}{2}}\,du' \\
&\qquad\qquad + \sqrt{\mathcal{D}_{\mathrm{o}}}\int_{-\infty}^{u}\Big(\int_{v_0}^{v} v'^2|D_v\phi|^2\,dv'\Big)^{\frac{1}{2}}\Big(\int_{v_0}^{v} v'^{-2\alpha}(v'+|u'|)^{-4}\,dv'\Big)^{\frac{1}{2}}\,du' \\
&\quad\lesssim \sqrt{\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})}\Big(\sup_{u'\in(-\infty,u]}\Big(\int_{v_0}^{v} v'^2|D_v\phi|^2(u',v')\,dv'\Big)^{\frac{1}{2}}\Big) \\
&\qquad\qquad \times\Big(\int_{-\infty}^{u}|u'|^{-\frac{1}{2}}(v_0+|u'|)^{-1}\,du' + \int_{-\infty}^{u}(v_0+|u'|)^{-\frac{3}{2}}\,du'\Big) \\
&\quad\lesssim \mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u_0|^{-\frac{1}{2}}.
\end{aligned}$$

Combining, we obtain

$$\int_{v_0}^{v}\sup_{-\infty\le u'\le u}\Big[\int_{-\infty}^{u'} v'^{\frac{3}{2}}\,\partial_u(|D_v\phi|^2)\,du''\Big]\,dv' \lesssim \mathcal{A}_\phi^2(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})^2|u_0|^{-\frac{1}{2}}. \tag{8-27}$$

Combining (8-24), (8-26) and (8-27), we can therefore conclude that

$$|O_1| \lesssim \mathcal{A}_\phi^2(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})^2|u_0|^{-\frac{1}{2}}(|u_0|^{-\frac{1}{2}}+v_0^{-\frac{1}{2}}).$$

We estimate $|O_2|$ by applying (3-4) and (7-3) (here, as before, the implicit constant may depend on β for $\beta > 0$):

$$\begin{aligned}
|O_2| &\lesssim \int_{v_0}^{v}\int_{-\infty}^{u}|\partial_v(v'^2\Omega_0^2)+\partial_u(u'^2\Omega_0^2)|\frac{\Omega_0^2}{\Omega^2}\Big(\frac{\Omega^2}{\Omega_0^2}-1\Big)^2\,du'\,dv' \\
&\lesssim \int_{v_0}^{v}\int_{-\infty}^{u}(v'+|u'|)^{-2+\beta}\Big(\frac{\Omega^2}{\Omega_0^2}-1\Big)^2\,du'\,dv' \\
&\lesssim \int_{v_0}^{v}\int_{-\infty}^{u}(v'+|u'|)^{-2+\beta}|u'|^{-1}\,du'\,dv' \lesssim v_0^{-1+\beta}+|u_0|^{-1+\beta}.
\end{aligned}$$

It turns out that the remaining terms have a similar structure and is convenient to bound them in the same way. The following are the three basic estimates. First, using the Cauchy–Schwarz inequality and (A1), we have

$$\begin{aligned}
&\int_{v_0}^{v}\int_{-\infty}^{u}(v'+|u'|)^{-2}|u'|^{-1}\Big(v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|+u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|\Big)\,du'\,dv' \\
&\quad\lesssim \Big(\int_{v_0}^{v}\int_{-\infty}^{u}(v'+|u'|)^{-4}|u'|^{-\frac{1}{2}}v'^2\,du'\,dv'\Big)^{\frac{1}{2}}\Big(\int_{v_0}^{v}\int_{-\infty}^{u}|u'|^{-\frac{3}{2}}v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|^2\,du'\,dv'\Big)^{\frac{1}{2}} \\
&\qquad + \Big(\int_{v_0}^{v}\int_{-\infty}^{u}(v'+|u'|)^{-4}v'^{\frac{3}{2}}\,du'\,dv'\Big)^{\frac{1}{2}}\Big(\int_{v_0}^{v}\int_{-\infty}^{u}v'^{-\frac{3}{2}}u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|^2\,du'\,dv'\Big)^{\frac{1}{2}} \\
&\quad\lesssim \big((|u_0|^{-\frac{1}{4}}+v_0^{-\frac{1}{4}})|u_0|^{-\frac{1}{4}}+(v_0+|u_0|)^{-\frac{1}{4}}v_0^{-\frac{1}{4}}\big) \lesssim |u_0|^{-\frac{1}{4}}.
\end{aligned}\tag{8-28}$$

Again, using the Cauchy–Schwarz inequality and (A1), we have

$$\begin{aligned}
&\int_{v_0}^{v}\int_{-\infty}^{u}(v'+|u'|)^{-2}v'^{-1}\Big(v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|+u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|\Big)\,du'\,dv'\\
&\lesssim\Big(\int_{v_0}^{v}\int_{-\infty}^{u}(v'+|u'|)^{-4}|u'|^{\frac32}\,du'\,dv'\Big)^{\frac12}\Big(\int_{v_0}^{v}\int_{-\infty}^{u}|u'|^{-\frac32}v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|^2\,du'\,dv'\Big)^{\frac12}\\
&\qquad+\Big(\int_{v_0}^{v}\int_{-\infty}^{u}(v'+|u'|)^{-4}v'^{-\frac12}|u'|^2\,du'\,dv'\Big)^{\frac12}\Big(\int_{v_0}^{v}\int_{-\infty}^{u}v'^{-\frac32}u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|^2\,du'\,dv'\Big)^{\frac12}\\
&\lesssim\big((v_0+|u_0|)^{-\frac14}|u_0|^{-\frac14}+(v_0^{-\frac14}+|u_0|^{-\frac14})v_0^{-\frac14}\big)\lesssim v_0^{-\frac14}.
\end{aligned}\tag{8-29}$$

Thirdly, we have a another slight variant of the above estimates, for which we again use the Cauchy–Schwarz inequality and (A1):

$$\begin{aligned}
&\int_{v_0}^{v}\int_{-\infty}^{u}v'^{-2}|u'|^{-2}\Big(v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|+u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|\Big)\,du'\,dv'\\
&\lesssim\Big(\int_{v_0}^{v}\int_{-\infty}^{u}v'^{-2}|u'|^{-\frac52}\,du'\,dv'\Big)^{\frac12}\Big(\int_{v_0}^{v}\int_{-\infty}^{u}|u'|^{-\frac32}v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|^2\,du'\,dv'\Big)^{\frac12}\\
&\qquad+\Big(\int_{v_0}^{v}\int_{-\infty}^{u}v'^{-\frac52}|u'|^{-2}\,du'\,dv'\Big)^{\frac12}\Big(\int_{v_0}^{v}\int_{-\infty}^{u}v'^{-\frac32}u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|^2\,du'\,dv'\Big)^{\frac12}\\
&\lesssim(v_0^{-\frac12}|u_0|^{-1}+v_0^{-1}|u_0|^{-\frac12})\lesssim|u_0|^{-\frac14}.
\end{aligned}\tag{8-30}$$

Using these basic estimates, we now estimate $|O_3|,\dots,|O_6|$. Using (7-4) and (7-8) to bound $\Omega^{-2}(\Omega^2-\Omega_0^2)^2$, we bound O_3 via (8-28)

$$\begin{aligned}
|O_3|&\lesssim\int_{v_0}^{v}\int_{-\infty}^{u}\Omega^{-2}(\Omega^2-\Omega_0^2)^2\Big(v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|+u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|\Big)\,du'\,dv'\\
&\lesssim\int_{v_0}^{v}\int_{-\infty}^{u}(v'+|u'|)^{-2}|u'|^{-1}\Big(v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|+u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|\Big)\,du'\,dv'\lesssim|u_0|^{-\frac14}.
\end{aligned}$$

Similarly, using (7-2), (7-14), (7-15), (8-28) and (8-29), we obtain the following estimate for $|O_4|$:

$$\begin{aligned}
|O_4|&\lesssim\int_{v_0}^{v}\int_{-\infty}^{u}\Omega_0^2(|r-M|+|r-r_0|+|Q-M|)\Big(v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|+u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|\Big)\,du'\,dv'\\
&\lesssim\int_{v_0}^{v}\int_{-\infty}^{u}(v'+|u'|)^{-2}(\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})|u'|^{-1}+\mathcal{D}_o v'^{-1}+(v'+|u'|)^{-1})\\
&\qquad\qquad\cdot\Big(v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|+u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|\Big)\,du'\,dv'\\
&\lesssim(\mathcal{A}_\phi(\mathcal{D}_{\mathrm{o}}+\mathcal{D}_{\mathrm{i}})+1)|u_0|^{-\frac14}+\mathcal{D}_o v_0^{-\frac14}.
\end{aligned}$$

By Lemma 3.1 and (7-8), $|\Omega^2-\Omega_0^2|(u',v')\lesssim(v'+|u'|)^{-2}$. Hence $|O_5|$ can be controlled in a similar manner to O_4 as follows:

$$\begin{aligned}|O_5|&\lesssim\int_{v_0}^{v}\int_{-\infty}^{u}|\Omega^2-\Omega_0^2|(|r-M|+|r-r_0|+|Q-M|)\Big(v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|+u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|\Big)\,du'\,dv'\\&\lesssim\int_{v_0}^{v}\int_{-\infty}^{u}(v'+|u'|)^{-2}(\mathcal{A}_\phi(\mathcal{D}_\mathrm{o}+\mathcal{D}_\mathrm{i})|u'|^{-1}+\mathcal{D}_o v'^{-1}+(v'+|u'|)^{-1})\\&\qquad\qquad\cdot\Big(v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|+u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|\Big)\,du'\,dv'\\&\lesssim(\mathcal{A}_\phi(\mathcal{D}_\mathrm{o}+\mathcal{D}_\mathrm{i})+1)|u_0|^{-\frac14}+\mathcal{D}_o v_0^{-\frac14}.\end{aligned}$$

Finally, we estimate $|O_6|$. For this we use Lemma 3.1, (7-12), (7-13) and (8-30) to obtain

$$\begin{aligned}|O_6|&\lesssim\int_{v_0}^{v}\int_{-\infty}^{u}(|\partial_v r||\partial_u r|+|\partial_v r_0||\partial_u r_0|)\Big(v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|+u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|\Big)\,du'\,dv'\\&\lesssim\int_{v_0}^{v}\int_{-\infty}^{u}[(v'+|u'|)^{-4}+\mathcal{A}_\phi^2(\mathcal{D}_\mathrm{o}+\mathcal{D}_\mathrm{i})^2|u'|^{-2}v'^{-2}]\Big(v'^2\Big|\partial_v\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|+u'^2\Big|\partial_u\log\Big(\frac{\Omega}{\Omega_0}\Big)\Big|\Big)\,du'\,dv'\\&\lesssim\mathcal{A}_\phi^2(\mathcal{D}_\mathrm{o}+\mathcal{D}_\mathrm{i})^2|u_0|^{-\frac14}.\end{aligned}$$

Hence, choosing v_0 and $|u_0|$ large in a manner allowed by (6-3), we obtain

$$\sup_{v\in[v_0,v_\infty]}\int_{-\infty}^{u_0}u^2\Big(\partial_u\Big(\log\frac{\Omega}{\Omega_0}\Big)\Big)^2(u,v)\,du+\sup_{u\in(-\infty,u_0]}\int_{v_0}^{v_\infty}v^2\Big(\partial_v\Big(\log\frac{\Omega}{\Omega_0}\Big)\Big)^2(u,v)\,dv\le\tfrac12 M,$$

which is to be proved. □

9. Stability of the Cauchy horizon of extremal Reissner–Nordström

We now conclude the bootstrap argument and show that the solution exists and remains regular for all $v\ge v_0$ and that certain estimates hold. More precisely, we have:

Proposition 9.1. *There exists a smooth solution* (ϕ,r,Ω,A) *to* (2-1)–(2-9) *in the rectangle* (*see Figure 1*)

$$D_{u_0,v_0}=\{(u,v')\mid-\infty\le u\le u_0,\ v_0\le v<\infty\}$$

with the prescribed initial data. Moreover, all the estimates in Sections 7 and 8 hold in D_{u_0,v_0}.

Proof. For every $v\in[v_0,\infty)$, consider the following conditions:

(A) A smooth solution (ϕ,r,Ω,A) to (2-1)–(2-9) exists in the rectangle

$$D_{u_0,[v_0,v)}=\{(u,v')\mid-\infty\le u\le u_0,\ v_0\le v'<v\}$$

with the prescribed initial data.

(B) The estimates (A1), (A2) and (A3) hold in $D_{u_0,[v_0,v)}$.

Consider the set $\mathfrak{I}\subset[v_0,\infty)$ defined by

$$\mathfrak{I}:=\{v\in[v_0,\infty):\text{(A) and (B) are both satisfied for all }v'\in[v_0,v)\}.$$

We will show that $\mathfrak{I}$ is nonempty, closed and open, which implies that $\mathfrak{I} = [v_0, \infty)$. Standard local existence implies that $\mathfrak{I}$ is nonempty. Closedness of $\mathfrak{I}$ follows immediately from the definition of $\mathfrak{I}$. The most difficult property to verify is the openness of $\mathfrak{I}$. For this, suppose $v \in \mathfrak{I}$. We then argue as follows:

- Under the bootstrap assumptions (A1), (A2) and (A3), all the estimates in Sections 7 and 8 hold in $D_{u_0,[v_0,v)}$. A standard propagation of regularity result shows that the solution can be extended smoothly up to
$$D_{u_0,[v_0,v]} = \{(u, v') \mid -\infty \le u \le u_0,\ v_0 \le v' \le v\}.$$
Hence, one can apply a local existence result for the characteristic initial value problem to show that there exists $\delta > 0$ such that a smooth solution (ϕ, r, Ω, A) to (2-1)–(2-9) exists in $D_{u_0,[v_0,v+\delta)}$.
- The estimates in (7-16), Corollary 8.9 and Proposition 8.11 *improve* those in (A1), (A2) and (A3). Hence, by continuity, after choosing $\delta > 0$ smaller if necessary, (A1), (A2) and (A3) hold in $D_{u_0,[v_0,v+\delta)}$.

By combining the two points above, we deduce that after choosing $\delta > 0$ smaller if necessary, $(v - \delta, v + \delta) \subset \mathfrak{I}$. This proves the openness of $\mathfrak{I}$. By the connectedness of $[v_0, \infty)$, we deduce that $\mathfrak{I} = [v_0, \infty)$. This implies the existence of a smooth solution in D_{u_0,v_0}. Moreover, this implies the assumptions (A1), (A2) and (A3) that are used in Sections 7 and 8 in fact hold throughout D_{u_0,v_0}. Therefore, indeed all the estimates in Sections 7 and 8 hold in D_{u_0,v_0}. □

We have therefore shown the existence of a solution in the whole region D_{u_0,v_0}. Since we have now closed our bootstrap argument, *in the remainder of the paper, we will suppress any dependence on* $\mathcal{A}_\phi$ (which in turn depends only on M, $\mathfrak{m}$ and $\mathfrak{e}$).

In the remainder of this section, we show that one can attach a *Cauchy horizon* to the solution and prove regularity of the solution *up to* the Cauchy horizon. More precisely, define V to be a function of v in exactly the same manner as in Section 3A2; i.e.,
$$\frac{dV}{dv} = \Omega_0^2(1, v), \qquad V(\infty) = 0. \tag{9-1}$$
We will use also the convention that
$$V_0 := V(v_0).$$
Define moreover (as in Section 3A2) the *Cauchy horizon* $\mathcal{CH}^+$ as the boundary $\{V = 0\}$ in the (u, V, θ, φ)-coordinate system. Note that this induces a natural differential structure on $D_{u_0,v_0} \cup \mathcal{CH}^+$. In the new coordinate system, in order to distinguish the "new Ω", we follow the convention in Section 3A2 and set $g(\partial_u, \partial_V) = -\frac{1}{2}\widetilde{\Omega}^2$ instead. We show that the solution $(\phi, r, \widetilde{\Omega}, A)$ (after choosing an appropriate gauge for A) extends to the Cauchy horizon continuously, and that in fact their derivatives are in L^2_{loc} up to the Cauchy horizon. (In fact, as we will show in Section 10, there are nonunique extensions as spherically symmetric solutions to (1-1) beyond the Cauchy horizon.)

We begin by restating some of the estimates we have obtained in this new coordinate system.

Lemma 9.2. *In the* (u, V)*-coordinate system,* ϕ, r *and* $\widetilde{\Omega}$ *satisfy the following estimates*:
$$\frac{1}{|u|^2} \lesssim \widetilde{\Omega}^2(u, V) \lesssim 1, \qquad |\partial_V r(u, V)| \lesssim \mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}, \tag{9-2}$$

$$\int_{V_0}^{0} |\partial_V \phi|^2(u, V')\, dV' + \int_{-\infty}^{u_0} u^2 |\partial_u \phi|^2(u', V)\, du' \lesssim \mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}, \tag{9-3}$$

$$\int_{V_0}^{0} |\partial_V \log \widetilde{\Omega}|^2(u, V')\, dV' + \int_{-\infty}^{u_0} u^2 |\partial_u \log \widetilde{\Omega}|^2(u', V)\, du' \lesssim 1, \tag{9-4}$$

$$\int_{V_0}^{0} |\partial_V r|^2(u, V')\, dV' + \int_{-\infty}^{u_0} u^2 |\partial_u r|^2(u', V)\, du' \lesssim \mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}. \tag{9-5}$$

Proof. Proof of estimates for $\widetilde{\Omega}$ in (9-2). By (7-6) and (9-1),

$$\left|\widetilde{\Omega}^2(u, V) - \frac{4M^2}{(v(V) + |u|)^2}\Omega_0^{-2}(-1, v(V))\right| = \Omega_0^{-2}(-1, v(V))\left|\Omega^2(u, v(V)) - \frac{4M^2}{(v + |u|)^2}\right|$$
$$\lesssim |u|^{-\frac{1}{2}}\left(\frac{v(V) + 1}{v(V) + |u|}\right)^2,$$

which implies both the upper and lower bounds for $\widetilde{\Omega}$ in (9-2).

Proof of estimate for $\partial_V r$ in (9-2). The estimate for $\partial_V r$ in (9-2) follows from (7-13) and (9-1).

Proof of (9-3) and (9-4). These follow from Corollary 8.9, Proposition 8.11, (9-1) and (3-3).

Proof of (9-5). Finally, (9-5) can be obtained by directly integrating the pointwise estimates in (7-12) (for $\partial_u r$) and (9-2) (for $\partial_V r$). □

We also have the following $W^{1,2}$ estimate for the charge Q.

Lemma 9.3. *In the (u, V)-coordinate system, Q satisfies the estimate*

$$\int_{V_0}^{0} |\partial_V Q|^2(u, V')\, dV' + \int_{-\infty}^{u_0} u^2 |\partial_u Q|^2(u', V)\, du' \lesssim \mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}.$$

Proof. Estimate for $\partial_V Q$. By (2-6) (adapted to the (u, V)-coordinate system),

$$\partial_V Q = -2\pi i r^2 \mathfrak{e}(\phi \overline{D_V \phi} - \bar{\phi} D_V \phi).$$

Therefore, using (7-1), (7-14) and (7-1),

$$\int_{V_0}^{0} |\partial_V Q|^2(u, V')\, dV' \lesssim \int_{V_0}^{0} |D_V \phi|^2(u, V')\, dV' \lesssim \mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}.$$

Estimate for $\partial_u Q$. By (2-5), we have $\partial_u Q = 2\pi i r^2 \mathfrak{e}(\phi \overline{D_u \phi} - \bar{\phi} D_u \phi)$. The desired estimate hence follows much as above using (7-1), (7-14) and (9-3). □

In order to consider the extension, we will also need to choose a gauge for A_μ. We will fix A such that

$$A_u = 0 \text{ everywhere} \quad \text{and} \quad A_V = 0 \text{ on the null hypersurface } \{u = u_0\}. \tag{9-6}$$

To see that this is an acceptable gauge choice, simply notice that given any $\tilde{A}_u$, $\tilde{A}_V$, we can define

$$\chi(u, V) = \int_{u_0}^{u} \tilde{A}_u(u, V)\, du' + \int_{V_0}^{V} \tilde{A}_V(u_0, V')\, dV',$$

where $V_0 = V(v_0)$. This implies

$$A_u(u, V) = \tilde{A}_u(u, V) - (\partial_u \chi)(u, V) = 0 \qquad \text{for all } u, \text{ for all } V,$$
$$A_V(u_0, V) = \tilde{A}_V(u, V) - (\partial_v \chi)(u_0, V) = 0 \quad \text{for all } V.$$

Now in the gauge (9-6), we have the following estimates:

Lemma 9.4. *Suppose A satisfies the gauge condition above. Then A_V, $\partial_u A_V$ and $\partial_V A_V$ obey the estimates*

$$\sup_{u\in(-\infty,u_0],\, V\in[V_0,0)} |A_V(u, V)| \lesssim (u_0 - u), \qquad \sup_{V\in[V_0,0)} \int_u^{u_0} |\partial_u A_V|^2(u', V)\, du' \lesssim (u_0 - u),$$
$$\sup_{u\in(-\infty,u_0]} \int_{V_0}^0 |\partial_V A_V|^2(u, V')\, dV' \lesssim (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}})(u_0 - u).$$

Proof. Pointwise estimate for A_V. By (2-7) (adapted to the (u, V)-coordinate system),

$$\partial_u A_V = \frac{1}{2} \frac{\widetilde{\Omega}^2 Q}{r^2}. \tag{9-7}$$

Using (7-2), (7-14) and (9-2), and the fact that $A_V(u_0, V) = 0$, we obtain that for any $u \le u_0$,

$$|A_V(u, V)| \lesssim \int_u^{u_0} du' = (u_0 - u).$$

L^2 estimate for $\partial_u A_V$. To obtain the desired L^2_u estimate for $\partial_u A_V$, we simply use the fact that the right-hand side of (9-7) is bounded (as shown above using (7-2), (7-14) and (9-2)) and integrate it up in u.

L^2 estimate for $\partial_V A_V$. To estimate $\partial_V A_V$, we differentiate (9-7) in V to obtain

$$\partial_u \partial_V A_V = \tfrac{1}{2} \partial_V \left(\frac{\widetilde{\Omega}^2 Q}{r^2} \right). \tag{9-8}$$

Using the pointwise bounds in (7-2), (7-14) and (9-2), and the L^2_V estimates in (9-3), (9-5) and (9-4), we obtain

$$\sup_{u\in(-\infty,u_0]} \int_{V_0}^0 \left| \partial_V \left(\frac{\widetilde{\Omega}^2 Q}{r^2} \right) \right|^2 (u, V')\, dV' \lesssim \mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}}.$$

Now since $\partial_V A_V(u_0, V) = 0$ for all V, we have, for any $u \le u_0$,

$$\int_{V_0}^0 |\partial_V A_V|^2(u, V')\, dV' \le \int_u^{u_0} |\partial_u \partial_V A_V|^2(u', V')\, dV'\, du' \lesssim (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}})(u_0 - u). \qquad \square$$

Proposition 9.5. *Let V be as in* (9-1) *and A satisfy the gauge condition* (9-6). *Then in the (u, V)-coordinate system*:

- *ϕ, r, $\widetilde{\Omega}$, A_V and Q (as functions of $(u, V) \in (-\infty, u_0] \times [V_0, 0)$) can be continuously extended to the Cauchy horizon $\{V = 0\}$.*
- *The extensions of ϕ, r, $\widetilde{\Omega}$, A_V and Q (as functions of $(u, V) \in (-\infty, u_0] \times [V_0, 0]$) are all in $C^{0,\frac{1}{2}} \cap W^{1,2}_{\mathrm{loc}}$.*

- *The Hawking mass* m (*as a function of* $(u, V) \in (-\infty, u_0] \times [V_0, 0)$) *can be continuously extended to the Cauchy horizon* $\{V = 0\}$.

Proof. Continuous extendibility and Hölder estimates. Let us first consider in detail the estimates for ϕ. As we will explain, the estimates for r, $\widetilde{\Omega}$, A_V and Q are similar. Consider two points (u', V') and (u'', V''). Set $v' = v(V')$ and $v'' = v(V'')$, where v is the inverse function of $v \mapsto V$ above. Then we have, using the fundamental theorem of calculus and the Cauchy–Schwarz inequality,

$$
\begin{aligned}
&|\phi(u', V') - \phi(u'', V'')| \\
&\leq \left| \int_{u'}^{u''} |\partial_u \phi|(u''', V')\, du''' \right| + \left| \int_{V'}^{V''} |\partial_V \phi|(u'', V''')\, dV''' \right| \\
&\leq \left| \int_{u'}^{u''} |D_u \phi|(u''', V')\, du''' \right| + \left| \int_{V'}^{V''} |D_V \phi|(u'', V''') + |A_V|\,|\phi|(u'', V''')\, dV''' \right| \\
&\lesssim |u' - u''|^{\frac{1}{2}} \left(\int_{u'}^{u''} |D_u \phi|^2(u''', v')\, du''' \right)^{\frac{1}{2}} + |V' - V''|^{\frac{1}{2}} \left(\int_{v'}^{v''} (v''' + 1)^2 |D_v \phi|^2(u'', v''')\, dv''' \right)^{\frac{1}{2}} \\
&\qquad\qquad + (\mathcal{D}_{\mathrm{o}}^{\frac{1}{2}} + \mathcal{D}_{\mathrm{i}}^{\frac{1}{2}})(u_0 - u'')|V' - V''| \\
&\lesssim (\mathcal{D}_{\mathrm{o}} + \mathcal{D}_{\mathrm{i}})(|u' - u''|^{\frac{1}{2}} + |V' - V''|^{\frac{1}{2}}) + (\mathcal{D}_{\mathrm{o}}^{\frac{1}{2}} + \mathcal{D}_{\mathrm{i}}^{\frac{1}{2}})|V' - V''|,
\end{aligned}
\tag{9-9}
$$

where in the last two lines we used (7-1), (9-3) and Lemma 9.4.

In a similar manner, using Lemmas 9.2, 9.3 and 9.4 instead, r, $\widetilde{\Omega}$, A_V and Q can be estimated as follows[19] (to simplify the exposition, we suppress the discussion on the explicit dependence of the constant on $\mathcal{D}_{\mathrm{o}}$ and $\mathcal{D}_{\mathrm{i}}$):

$$
\begin{aligned}
&|r(u', V') - r(u'', V'')| + |\widetilde{\Omega}(u', V') - \widetilde{\Omega}(u'', V'')| \\
&\quad + |A_V(u', V') - A_V(u'', V'')| + |Q(u', V') - Q(u'', V'')| \lesssim_{\mathcal{D}_{\mathrm{o}}, \mathcal{D}_{\mathrm{i}}} (|u' - u''|^{\frac{1}{2}} + |V' - V''|^{\frac{1}{2}}).
\end{aligned}
\tag{9-10}
$$

Define the extension of $(\phi, r, \widetilde{\Omega}, A_V, Q)$ by

$$
\phi(u, V = 0) := \lim_{V \to 0} \phi(u, V), \quad r(u, V = 0) := \lim_{V \to 0} r(u, V),
$$

$$
\widetilde{\Omega}(u, V = 0) := \lim_{V \to 0} \widetilde{\Omega}(u, V), \quad A_V(u, V = 0) := \lim_{V \to 0} A_V(u, V), \quad Q(u, V = 0) := \lim_{V \to 0} Q(u, V).
$$

The estimates in (9-9) and (9-10) above show that the extensions are well-defined and that the extension of $(\phi, r, \widetilde{\Omega}, A_V, Q)$ is indeed $C^{0, \frac{1}{2}}$.

$W^{1,2}_{\mathrm{loc}}$ estimates. Now that we have constructed an extension of $(\phi, r, \widetilde{\Omega}, A_V, Q)$ to $D_{u_0, v_0} \cup \mathcal{CH}^+$, it follows immediately from Lemmas 9.2, 9.4 and 9.3 that the extension is in $W^{1,2}_{\mathrm{loc}}$.

C^0 extendibility of the Hawking mass. Finally, we prove the C^0 extendibility of the Hawking mass, whose definition we recall from (2-10). By (2-11) and (2-12) (appropriately adapted in the (u, V)-coordinate system), we have

$$
\partial_u m = -8\pi \frac{r^2 (\partial_V r)}{\widetilde{\Omega}^2} |D_u \phi|^2 + 2(\partial_u r) \mathfrak{m}^2 \pi r^2 |\phi|^2 + \frac{1}{2} \frac{(\partial_u r) Q^2}{r^2},
\tag{9-11}
$$

[19] In fact, the estimates for r, $\widetilde{\Omega}$ A_V and Q are simpler as we do not need to handle the difference between ∂_V and D_V.

$$\partial_V m = -8\pi \frac{r^2(\partial_u r)}{\widetilde{\Omega}^2} |D_V \phi|^2 + 2(\partial_V r)\mathfrak{m}^2 \pi r^2 |\phi|^2 + \frac{1}{2}\frac{(\partial_V r) Q^2}{r^2}. \tag{9-12}$$

It now follows from (7-2), (7-14), (7-13) and Lemma 9.2 that the right-hand side of (9-11) is bounded in L^1_u and the right-hand side of (9-12) is bounded in L^1_V. This implies the L^1 estimate

$$\int_{-\infty}^{u_0} |\partial_u m|(u', V)\, du' + \int_{V_0}^{0} |\partial_V m|(u, V')\, dV' \lesssim_{\mathcal{D}_o, \mathcal{D}_i} 1. \tag{9-13}$$

On the other hand, by the fundamental theorem of calculus,

$$|m(u', V') - m(u'', V'')| \le \left| \int_{u'}^{u''} |\partial_u m|(u''', V')\, du''' \right| + \left| \int_{V'}^{V''} |\partial_V m|(u'', V''')\, dV''' \right|. \tag{9-14}$$

Combining (9-13) and (9-14), we see that

(1) m can be extended to $\mathcal{CH}^+$ by

$$m(u, 0) = \lim_{V \to 0} m(u, V),$$

(2) the extension is continuous up to $\mathcal{CH}^+$,

which concludes the proof of the proposition. (Let us finally note that since we only have L^1, as opposed to L^2, estimates for $\partial_u m$ and $\partial_V m$, we only show that m is continuous, but do *not* obtain any Hölder estimates.) □

Remark 9.6 ($C^{0,\frac{1}{2}} \cap W^{1,2}_{\mathrm{loc}}$ regularity in the (3+1)-dimensional spacetime). In Proposition 9.5, we proved that the extensions of ϕ, r, $\widetilde{\Omega}$, A_V and Q are $C^{0,\frac{1}{2}} \cap W^{1,2}_{\mathrm{loc}}$ on the (1+1)-dimensional quotient manifold $\mathcal{Q}$ (see the notation in Section 2A). It easily follows that these functions, when considered as functions on $\mathcal{M} = \mathcal{Q} \times \mathbb{S}^2$ are also in $C^{0,\frac{1}{2}} \cap W^{1,2}_{\mathrm{loc}}$. As a consequence, in the coordinate system (u, v, θ, φ), the spacetime metric, the scalar field and the electromagnetic potential all extend to the Cauchy horizon in a manner that is in the (3+1)-dimensional spacetime norm $C^{0,\frac{1}{2}} \cap W^{1,2}_{\mathrm{loc}}$.

10. Constructing extensions beyond the Cauchy horizon

In this section, we prove that the solution can be extended locally beyond the Cauchy horizon *as a spherically symmetric $W^{1,2}$ solution to* (1-1) (in a nonunique manner). Together with Propositions 9.1 and 9.5, this completes the proof of Theorem 5.1.

The idea behind the construction of the extension is that the system (1-1) is *locally well-posed* in spherical symmetry for data such that $\partial_V \phi$, $\partial_V r$ and $\partial_V \log \widetilde{\Omega}$ are merely in L^2 (when r and Ω are bounded away from 0). This follows from the well-known fact that (1+1)-dimensional wave equations are locally well-posed with $W^{1,2}$ data. Related results in the context of general relativity can be found throughout the literature; see for instance [Costa et al. 2015a; Luk and Rodnianski 2017; LeFloch and Stewart 2011]. For completeness, we give a proof in our specific setting.

The section is organized as follows. We first discuss a general local well-posedness result on (1+1)-dimensional wave equation (see Definition 10.1 and Proposition 10.3). We then apply the wave equation result in our setting to construct extensions to our spacetime solutions by solving appropriate characteristic initial value problems. In particular, since we will be able to prescribe data for the construction of the extensions, there are (infinitely many) nonunique extensions.

We begin by considering a general class of (1+1)-dimensional wave equation and introduce the following notion of solution, which makes sense when the derivative of Ψ is only in L^2 in one of the null directions.

Definition 10.1. Let $k \in \mathbb{N}$. Consider a wave equation[20] for $\Psi : [0, \epsilon) \times [0, \epsilon) \to \mathcal{V}$ (where $\mathcal{V} \subset \mathbb{R}^k$ is an open subset) of the form

$$\partial_u \partial_v \Psi_A = f_A(\Psi) + N_A^{BC}(\Psi)\, \partial_u \Psi_B\, \partial_v \Psi_C + K_A^{BC}(\Psi)\, \partial_u \Psi_B\, \partial_u \Psi_C + L_A^B(\Psi)\, \partial_u \Psi_B + R_A^B(\Psi)\, \partial_v \Psi_B, \quad \text{(10-1)}$$

where Ψ_A denotes the components of Ψ, the functions f_A, N_A^{BC}, K_A^{BC}, L_A^B, $R_A^B : \mathcal{V} \to \mathbb{R}$ are smooth, and we sum over all repeated capital Latin indices.

We say that a continuous function $\Psi : [0, \epsilon) \times [0, \epsilon) \to \mathcal{V}$ satisfying $\partial_v \Psi \in L^2_v(C^0_u)$ and $\partial_u \Psi \in C^0_u C^0_v$ is a *solution in the integrated sense* if

$$(\partial_v \Psi_A)(u, v) = (\partial_v \Psi_A)(0, v) + \int_0^u (\text{RHS of (10-1)})(u', v)\, du' \quad \text{for all } u \in [0, \epsilon) \text{ and for a.e. } v \in [0, \epsilon),$$

$$(\partial_u \Psi_A)(u, v) = (\partial_u \Psi_A)(u, 0) + \int_0^v (\text{RHS of (10-1)})(u, v')\, dv' \quad \text{for all } v \in [0, \epsilon) \text{ and for a.e. } u \in [0, \epsilon).$$

Remark 10.2. Given a solution Ψ in the sense of Definition 10.1, it is also a weak solution in the following sense: for any $\chi \in C_c^\infty$,

$$\iint (\partial_u \chi)(u, v)(\partial_v \Psi)(u, v)\, du\, dv = -\iint \chi(u, v)(\text{RHS of (10-1)})(u, v)\, du\, dv,$$

$$\iint (\partial_v \chi)(u, v)(\partial_u \Psi)(u, v)\, du\, dv = -\iint \chi(u, v)(\text{RHS of (10-1)})(u, v)\, du\, dv.$$

The following is a general local existence result for $(1+1)$-dimensional wave equations where $\partial_v \Psi$ is initially only in L^2_v. We construct local solutions in the sense of Definition 10.1. (Let us note that the following wave equation result holds for rougher data where $\partial_v \Psi$ is only in L^1_v. This will however be irrelevant to our problem; see Remark 10.6.)

Proposition 10.3. *Consider the setup in Definition 10.1. Let $\mathcal{K} \subset \mathcal{V}$ be a compact subset. Given initial data to the wave equation* (10-1) *on two transversely intersecting characteristic curves*

$$\{(u, v) : u = 0, v \in [0, v_*]\} \cup \{(u, v) : v = 0, u \in [0, u_*]\}$$

such that

- Ψ *takes value in* $\mathcal{K}$; *and*

[20] For $k > 1$, this should be thought of as a system of wave equations.

- *the following estimates hold for the derivatives of* Ψ *for some* $C_{\mathrm{wave}} > 0$:

$$\int_0^{v_*} |\partial_v \Psi|^2(0, v')\, dv' \le C_{\mathrm{wave}},$$

$$\sup_{u\in[0,u_*]} |\partial_u \Psi|^2(u', 0) \le C_{\mathrm{wave}}.$$

Then, there exist $\epsilon_{\mathrm{wave}} > 0$ *depending on* $\mathcal{K}$ *and* C_{wave} (*and the equation*) *such that there exists a unique solution to* (10-1) *in the sense of Definition 10.1 in the region*

$$(u, v) \in \{(u, v) : u \in [0, \epsilon_{\mathrm{wave}}),\ v \in [0, \epsilon_{\mathrm{wave}})\}$$

which achieves the prescribed initial data.

Proof. We directly work with the formulation in Definition 10.1 and prove the existence and uniqueness of integral solutions. This proposition can be proven via a standard iteration argument. In order to illustrate the main idea and the use of the structure of the nonlinearity, we will only discuss below the proof of a priori estimates.

By a bootstrap argument, we assume that

$$\sup_{u',v'\in[0,\epsilon_{\mathrm{wave}})} |\partial_u \Psi|(u', v') \le 4C_{\mathrm{wave}}. \tag{10-2}$$

Let $\mathcal{K}' \subset \mathcal{V}$ be a fixed compact set such that $\mathcal{K} \subset \mathring{\mathcal{K}}'$. We estimate Ψ using the fundamental theorem of calculus as follows:

$$\begin{aligned}\sup_{u',v'\in[0,\epsilon_{\mathrm{wave}})} |\Psi(u', v') - \Psi(0, v')| &\le \sup_{v'\in[0,\epsilon_{\mathrm{wave}})} \int_0^{\epsilon_{\mathrm{wave}}} |\partial_u \Psi|(u', v')\, du' \\ &\le \epsilon_{\mathrm{wave}} \sup_{u',v'\in[0,\epsilon_{\mathrm{wave}})} |\partial_u \Psi|(u', v') \\ &\le 4C_{\mathrm{wave}}\epsilon_{\mathrm{wave}}.\end{aligned}$$

Using the compactness of $\mathcal{K}$, we can choose ϵ_{wave} sufficiently small so that $\Psi(u, v) \in \mathcal{K}'$ for all $u \in [0, \epsilon)$. Now that we have estimated Ψ, since $\mathcal{K}'$ is compact, it follows that $f_A(\Psi)$, $N_A^{BC}(\Psi)$, $K_A^{BC}(\Psi)$, $L_A^B(\Psi)$, and $R_A^B(\Psi)$ are all bounded. From now on, we will use these bounds and write C for constants that are allowed to depend on $\sup_{x\in\mathcal{K}'} f_A(x)$, etc.

We now turn to the estimates for the derivatives of Ψ. First, we bound $\partial_v \Psi$ using (the integral form of) (10-1) and Hölder's inequality and Young's inequality:

$$\begin{aligned}&\int_0^{\epsilon_{\mathrm{wave}}} \sup_{u'\in[0,\epsilon_{\mathrm{wave}})} |\partial_v \Psi|^2(u', v')\, dv' \\ &\le C_{\mathrm{wave}} + C \int_0^{\epsilon_{\mathrm{wave}}} \int_0^{\epsilon_{\mathrm{wave}}} |\partial_v \Psi|(1 + |\partial_v \Psi| + |\partial_u \Psi| + |\partial_v \Psi||\partial_u \Psi| + |\partial_u \Psi|^2)(u', v')\, du'\, dv' \\ &\le C_{\mathrm{wave}} + C\biggl(1 + \int_0^{\epsilon_{\mathrm{wave}}} \sup_{u'\in[0,\epsilon_{\mathrm{wave}})} |\partial_v \Psi|^2(u', v')\, dv'\biggr)\biggl(\epsilon_{\mathrm{wave}} + \epsilon_{\mathrm{wave}} \sup_{u',v'\in[0,\epsilon_{\mathrm{wave}})} |\partial_u \Psi|(u', v')\biggr) \\ &\qquad + C_{\mathrm{wave}}\epsilon_{\mathrm{wave}}^2 \sup_{u',v'\in[0,\epsilon_{\mathrm{wave}})} |\partial_u \Psi|(u', v').\end{aligned}$$

For $\partial_u \Psi$, we again use (the integral form of) (10-1) and Hölder's inequality and Young's inequality to get

$$
\begin{aligned}
&\sup_{u', v' \in [0, \epsilon_{\text{wave}})} |\partial_u \Psi|(u', v') \\
&\quad \le C_{\text{wave}} + C \sup_{u' \in [0, \epsilon_{\text{wave}})} \int_0^{\epsilon} (1 + |\partial_v \Psi| + |\partial_u \Psi| + |\partial_v \Psi|\,|\partial_u \Psi| + |\partial_u \Psi|^2)(u', v'))(u', v')\, dv' \\
&\quad \le C_{\text{wave}} + C\Big(1 + \int_0^{\epsilon} \sup_{u' \in [0, \epsilon_{\text{wave}}]} |\partial_v \Psi|^2(u', v')\, dv'\Big)\Big(\epsilon_{\text{wave}}^{\frac{1}{2}} + \epsilon_{\text{wave}} \sup_{u', v' \in [0, \epsilon_{\text{wave}})} |\partial_u \Psi|^2(u', v')\Big) \\
&\quad \le C_{\text{wave}} + C\Big(1 + \int_0^{\epsilon} \sup_{u' \in [0, \epsilon_{\text{wave}}]} |\partial_v \Psi|^2(u', v')\, dv'\Big)\Big(\epsilon_{\text{wave}}^{\frac{1}{2}} + \epsilon_{\text{wave}} C_{\text{wave}} \sup_{u', v' \in [0, \epsilon_{\text{wave}})} |\partial_u \Psi|(u', v')\Big).
\end{aligned}
$$

Summing the above two estimates and choosing ϵ_{wave} sufficient small (depending on C_{wave} and $\mathcal{K}'$), it follows that

$$
\int_0^{\epsilon} \sup_{u' \in [0, \epsilon_{\text{wave}})} |\partial_v \Psi|^2(u', v')\, dv' + \sup_{u', v' \in [0, \epsilon_{\text{wave}})} |\partial_u \Psi|(u', v') \le 2C_{\text{wave}}.
$$

This in particular improves the bootstrap assumption (10-2) so that we conclude the argument. □

We now use Proposition 10.3 to solve (1-1). In particular, this allows us to extend the solution in D_{u_0, v_0} (in infinitely many ways!) beyond the Cauchy horizon *as a spherically symmetric strong solution* to (1-1). Before we proceed, let us define a notion of spherically symmetric strong solutions to (1-1) (using Definition 10.1) appropriate for our setting. For simplicity, in our notion of spherically symmetric strong solutions, we will already fix a gauge so that $A_u = 0$.

Definition 10.4. Let $(\phi, \Omega, r, A_v, Q)$ be continuous functions on

$$
\{(u, v) : u \in [u_0, u_0 + \epsilon),\ v \in [v_0, v_0 + \epsilon)\}
$$

for some $\epsilon > 0$ with ϕ complex-valued, (Ω, r, A_v, Q) real-valued and $\Omega,\ r > 0$. We say $(\phi, \Omega, r, A_v, Q)$ is a spherically symmetric strong solution to (1-1) if the following hold:[21]

- $(\phi, \Omega, r, A_v, Q)$ are in the following regularity classes:

$$
\partial_v \phi,\ \partial_v \log \Omega \in L^2_v(C^0_u), \quad \partial_u \phi,\ \partial_u \log \Omega,\ \partial_u r,\ \partial_v r,\ \partial_u A_v \in C^0_u C^0_v.
$$

- (2-1), (2-2) and (2-3) are satisfied as wave equations in the integrated sense as in Definition 10.1 after replacing $D_v \mapsto \partial_v + i\mathfrak{e} A_v,\ D_u \mapsto \partial_u$.

- (2-5), (2-6), (2-8) and (2-9) are all satisfied in the integrated sense as follows, again with the understanding that $D_v \mapsto \partial_v + i\mathfrak{e} A_v,\ D_u \mapsto \partial_u$:

$$
Q(u, v) = Q(0, v) + \int_{u_0}^{u} [2\pi i r^2 \mathfrak{e}(\phi \overline{D_u \phi} - \bar{\phi} D_u \phi)](u', v)\, du', \tag{10-3}
$$

$$
Q(u, v) = Q(u, 0) - \int_{v_0}^{v} [2\pi i r^2 \mathfrak{e}(\phi \overline{D_v \phi} - \bar{\phi} D_v \phi)](u, v')\, dv', \tag{10-4}
$$

[21] We remark that (2-4) is not explicitly featured below. Note however that (2-4) follows as an immediate consequence of (10-7).

$$r\,\partial_u r(u,v) = r\,\partial_u r(0,v) + \int_{u_0}^{u} [2r\,\partial_u r\,\partial_u \log\Omega + (\partial_u r)^2 - 4\pi r^2 |D_u\phi|^2](u',v)\,du', \tag{10-5}$$

$$r\,\partial_v r(u,v) = r\,\partial_v r(u,0) + \int_{v_0}^{v} [2r\,\partial_v r\,\partial_v \log\Omega + (\partial_v r)^2 - 4\pi r^2 |D_v\phi|^2](u,v')\,dv' \tag{10-6}$$

for all $(u,v) \in \{(u,v) : u \in [u_0, u_0+\epsilon),\ v \in [v_0, v_0+\epsilon)\}$.

- (2-7) is satisfied classically everywhere with $A_u = 0$; i.e.,

$$\partial_u A_v = \frac{Q\Omega^2}{2r^2}. \tag{10-7}$$

We emphasize again that a spherically symmetric strong solution to (1-1) in the sense of Definition 10.4 is a fortiori a weak solution to (1-1) in the sense of Remark 1.2.

We now construct extensions to the solutions given by Proposition 9.1 beyond the Cauchy horizon as spherically symmetric strong solutions to (1-1):

Proposition 10.5. *For every $u_{\text{ext}} \in (-\infty, u_0)$, there exists $\epsilon_{\text{ext}} > 0$ such that there are infinitely many inequivalent extensions $(\phi, \widetilde{\Omega}, r, A_V, Q)$ to the region*

$$D_{u_0,v_0} \cup \mathcal{CH}^+ \cup \{(u,V) : u \in [u_{\text{ext}}, u_{\text{ext}}+\epsilon_{\text{ext}}],\ V \in [0, \epsilon_{\text{ext}})\},$$

each of which is a spherically symmetric strong solution to (1-1) (*see Definition 10.4*).

Proof. Let us focus the discussion on constructing *one* such extension. It will be clear at the end that the argument indeed gives infinitely many inequivalent extensions.

Setting up the initial data. Extend the constant-u curve $\{u = u_{\text{ext}}\}$ up to the Cauchy horizon. We will consider a sequence of characteristic initial problems with initial data given on $\{u = u_{\text{ext}}\}$ and $\{V = V_n\}$ where V_n approaches the Cauchy horizon, i.e., $V_n \to 0$. For a fixed $n \in \mathbb{N}$, the data on $\{V = V_n\}$ are simply induced by the solution that we have constructed in Proposition 9.1. On $\{u = u_{\text{ext}}\}$, the data when $V \in [V_n, 0)$ are induced by the solution, but we prescribe data for $V \geq 0$ (i.e., beyond the Cauchy horizon) by the following procedure:

- (*data for* $\widetilde{\Omega}$) As we showed in (9-2), (9-4) and Proposition 9.5, for a fixed u_{ext}, $\widetilde{\Omega}(u_{\text{ext}}, V)$ is continuous up to $\{V = 0\}$, is bounded away from 0, and $\partial_V \widetilde{\Omega}(u_{\text{ext}}, V) \in L^2_V$. We can therefore extend Ω to $\{(u_{\text{ext}}, V) : V \geq 0\}$ so that it is continuous and bounded away from 0 and $\partial_V \widetilde{\Omega}(u_{\text{ext}}, V) \in L^2_V$.

- (*data for* ϕ) As we showed in (9-3) and Proposition 9.5, $\phi(u_{\text{ext}}, V)$ is continuous up to $\{V = 0\}$ and $D_V \phi(u_{\text{ext}}, V) \in L^2_V$. Since by Lemma 9.4, $|A_V|(u_{\text{ext}}, V) \lesssim (u_0 - u_{\text{ext}})$ for $V \leq 0$, this also implies that $\partial_V \phi(u_{\text{ext}}, V) \in L^2_V$. We can therefore extend ϕ to $\{(u_{\text{ext}}, V) : V \geq 0\}$ so that it is continuous and $\partial_V \phi(u_{\text{ext}}, V) \in L^2_V$.

- (*data for* A_V) Next, by Lemma 9.4, $A_V(u_{\text{ext}}, V)$ is continuous up to $\{V = 0\}$ and $\partial_V \phi(u_{\text{ext}}, V) \in L^2_V$. Thus, like $\widetilde{\Omega}$ and ϕ, we can extend A_V to $\{(u_{\text{ext}}, V) : V \geq 0\}$ so that it is continuous and $\partial_V A_V(u_{\text{ext}}, V) \in L^2_V$.

- (*data for* r) Finally, we prescribe r. Note that this is the only piece of the initial data which is not free, but instead is required to satisfy constraints. First we note that by (7-16), (9-5) and Proposition 9.5, for

$V \leq 0$, $r(u_{\text{ext}}, V)$ is continuous up to $\{V=0\}$, bounded away from 0 and $(\partial_V r)(u_{\text{ext}}, V) \in L^2_V$. Moreover, using (2-9) (and the also estimates (9-2) and (9-3)), it can be deduced that $(\partial_V r)(u_{\text{ext}}, V)$ can be extended continuously up to $\{V=0\}$. Now we extend r and $\partial_V r$ beyond the Cauchy horizon $\{V=0\}$ by solving (2-9). Since $\partial_V \phi \in L^2_V$ and $\log \Omega$ is bounded (by the choices above), provided that we only solve slightly beyond the Cauchy horizon (i.e., for V sufficiently small), both r and $|\partial_V r|$ are continuous, bounded above, and r is also bounded away from 0.

Formulating the problem as a system of wave equations. Now apply Proposition 10.3 to solve the following system of wave equations for $\Psi = (r, \log \widetilde{\Omega}, \mathrm{Re}(\phi), \mathrm{Im}(\phi), A_V)$:

$$r\,\partial_u\,\partial_V r = -\tfrac{1}{4}\widetilde{\Omega}^2 - \partial_u r\,\partial_V r + \mathfrak{m}^2\pi r^2\widetilde{\Omega}^2|\phi|^2 + \frac{r^2}{\widetilde{\Omega}^2}(\partial_u A_V)^2, \tag{10-8}$$

$$r^2\,\partial_u\,\partial_V \log\widetilde{\Omega} = -2\pi r^2(\partial_u\phi\overline{(\partial_V + i\mathfrak{e}A_V)\phi} + \overline{\partial_u\phi}(\partial_V + i\mathfrak{e}A_V)\phi) - 2\frac{r^2}{\widetilde{\Omega}^2}(\partial_u A_V)^2 + \tfrac{1}{4}\widetilde{\Omega}^2 + \partial_u r\,\partial_V r, \tag{10-9}$$

$$\partial_u((\partial_V + i\mathfrak{e}A_V)\phi) + (\partial_V + i\mathfrak{e}A_V)\,\partial_u\phi = -\tfrac{1}{2}\mathfrak{m}^2\widetilde{\Omega}^2\phi - 2r^{-1}(\partial_u r(\partial_V + i\mathfrak{e}A_V)\phi + \partial_V r\,\partial_u\phi), \tag{10-10}$$

$$\partial_V\left(\frac{r^2}{\widetilde{\Omega}^2}\,\partial_u A_V\right) = -\pi i r^2\mathfrak{e}(\phi\overline{D_V\phi} - \bar{\phi}D_V\phi). \tag{10-11}$$

It is easy to check that this system of equations indeed has the structure as in (10-1).

Solving the system of wave equations. By Proposition 10.3, there exists $\epsilon_0 > 0$ (independent of n) such that for every V_n, a unique solution to the above system of equation exists for $(u, V) \in \{(u, V) : u \in [u_{\text{ext}}, u_{\text{ext}} + \epsilon_0),\ V \in [V_n, V_n + \epsilon_0)\}$. In particular, since $V_n \to 0$, we can choose $n \in \mathbb{N}$ sufficiently large so that $V_n + \epsilon_0 > 0$. Now fix such an n and choose $\epsilon_{\text{ext}} > 0$ sufficiently small so that $\epsilon_{\text{ext}} < V_n + \epsilon_0$. We have therefore constructed a solution $(r, \log\Omega, \mathrm{Re}(\phi), \mathrm{Im}(\phi), A_V)$ to (10-8)–(10-11) in $D_{u_0,v_0} \cup \mathcal{CH}^+ \cup \{(u, V) : u \in [u_{\text{ext}}, u_{\text{ext}} + \epsilon_{\text{ext}}],\ V \in [0, \epsilon_{\text{ext}})\}$.

Definition of Q and (10-4). Define $Q = 2r^2\widetilde{\Omega}^{-2}\,\partial_u A_V$. By definition Q is continuous and (10-7) is satisfied classically. Moreover, since (10-11) is satisfied in an integrated sense, it also follows that (10-4) is satisfied.

Plugging in the definition of Q into (10-8)–(10-10), we also obtain that r, $\widetilde{\Omega}$ and ϕ respectively satisfy (2-1), (2-2) and (2-3) as wave equations in the integrated sense as in Definition 10.1.

Propagation of constraints and (10-3), (10-5) and (10-6). Next, we check that (10-3), (10-5) and (10-6) are satisfied. This involves a propagation of constraints argument, which is standard except that we need to be slightly careful about regularity issues.

First, we note that since the equations are satisfied classically at (u, V_n) for all $u \in [u_{\text{ext}}, u_{\text{ext}} + \epsilon_0)$, (10-3) and (10-5) are satisfied on $\{V = V_n\}$. Moreover, by the construction of the data for r above, (10-6) is also satisfied on $\{u = u_{\text{ext}}\}$.

Therefore, it follows that (10-3), (10-5) and (10-6) are equivalent respectively to the equations

$$\begin{aligned}(Q(u, V) - Q(u, V_n)) &- (Q(u_{\text{ext}}, V) - Q(u_{\text{ext}}, V_n)) \\ &= \int_{u_{\text{ext}}}^{u} [2\pi i r^2\mathfrak{e}(\overline{D_u\phi} - \bar{\phi}D_u\phi)](u', V)\,du' - \int_{u_{\text{ext}}}^{u} [2\pi i r^2\mathfrak{e}(\overline{D_u\phi} - \bar{\phi}D_u\phi)](u', V_n)\,du',\end{aligned} \tag{10-12}$$

$$
\begin{aligned}
&(r\,\partial_u r(u,V)-r\,\partial_u r(u,V_n))-(r\,\partial_u r(u_{\text{ext}},V)-r\,\partial_u r(u_{\text{ext}},V_n))\\
&\qquad=\int_{u_{\text{ext}}}^{u}\big([2r\,\partial_u r\,\partial_u\log\widetilde{\Omega}+(\partial_u r)^2-4\pi r^2|D_u\phi|^2](u',V)-[\cdots](u',V_n)\big)\,du', \qquad (10\text{-}13)\\
&(r\,\partial_V r(u,V)-r\,\partial_V r(u_{\text{ext}},V))-(r\,\partial_V r(u,V_n)-r\,\partial_V r(u_{\text{ext}},V_n))\\
&\qquad=\int_{V_n}^{V}\big([2r\,\partial_V r\,\partial_V\log\widetilde{\Omega}+(\partial_V r)^2-4\pi r^2|D_V\phi|^2](u,V')-[\cdots](u_{\text{ext}},V')\big)\,dV', \qquad (10\text{-}14)
\end{aligned}
$$

where $[\cdots]$ means that we take exactly the same expression as inside the previous pair of square brackets.

To proceed, observe now that we have the following integrated version of the Leibniz rule: let $f,\ g:[0,T]\to\mathbb{R},\ f\in C^0,\ g\in C^1$. Assume that there exists an $F:[0,T]\to\mathbb{R}$ in L^1 such that $f(t)-f(0)=\int_0^t F(s)\,ds$ for all $t\in[0,T]$. Then by Fubini's theorem and the fundamental theorem of calculus,

$$
\begin{aligned}
\int_0^t F(s)g(s)\,ds &= g(0)\int_0^t F(s)\,ds+\int_0^t\int_0^s F(s)g'(\tau)\,d\tau\,ds\\
&= f(t)g(0)-f(0)g(0)+\int_0^t\int_\tau^t F(s)g'(\tau)\,ds\,d\tau\\
&= f(t)g(0)-f(0)g(0)+\int_0^t[f(t)g'(\tau)-f(\tau)g'(\tau)]\,d\tau\\
&= f(t)g(t)-f(0)g(0)-\int_0^t f(s)g'(s)\,ds. \qquad (10\text{-}15)
\end{aligned}
$$

In other words, assuming Ψ_i satisfies $\partial_u\partial_v\Psi_i=F_i$ (for some $F_i\in L^1_vC^0_u$), the following integrated versions of the Leibniz rule hold:

$$
\partial_u\Psi_i(u,V)\Psi_j(u,V)=\partial_u\Psi_i(u,V_n)\Psi_j(u,V_n)+\int_{V_n}^{V}[\Psi_jF_i+\partial_v\Psi_j\,\partial_u\Psi_i](u,V')\,dV', \qquad (10\text{-}16)
$$

$$
\partial_v\Psi_i(u,V)\Psi_j(u,V)=\partial_u\Psi_i(u_{\text{ext}},V)\Psi_j(u_{\text{ext}},V)+\int_{u_{\text{ext}}}^{u}[\Psi_jF_i+\partial_u\Psi_j\,\partial_v\Psi_i](u',V)\,du'. \qquad (10\text{-}17)
$$

Let us now show that (10-3), or equivalently (10-12), holds. Since we have already established that (10-4) holds, it follows that (10-12) is equivalent to

$$
\begin{aligned}
&-\int_{V_n}^{V}\big([2\pi i r^2\mathfrak{e}(\phi\overline{D_v\phi}-\bar\phi D_v\phi)](u,V')-[\cdots](u_{\text{ext}},V')\big)\,dV'\\
&\qquad\qquad=\int_{u_{\text{ext}}}^{u}\big([2\pi i r^2\mathfrak{e}(\phi\overline{D_u\phi}-\bar\phi D_u\phi)](u',V)-[\cdots](u',V_n)\big)\,du'. \qquad (10\text{-}18)
\end{aligned}
$$

By (10-16) and (10-17) above, it follows that we need to check

$$
\int_{u_{\text{ext}}}^{u}\int_{V_n}^{V}\big(\partial_u(2\pi i r^2\mathfrak{e}(\phi\overline{D_v\phi}-\bar\phi D_v\phi))+\partial_V(2\pi i r^2\mathfrak{e}(\phi\overline{D_u\phi}-\bar\phi D_u\phi))\big)(u',V')\,du'\,dV'=0, \qquad (10\text{-}19)
$$

where expressions such as $\partial_u D_v\phi$ and $\partial_V D_u\phi$ are to be understood *after plugging in the appropriate inhomogeneous terms arising from* (10-10). On the other hand, after plugging in the appropriate expressions from (10-10), it is easy to check that the integrand in (10-19) vanishes almost everywhere. Therefore, (10-19) indeed holds, which then implies that (10-3) holds.

Next, we consider (10-5), or equivalently (10-13). Since we have already established (10-8) in an integrated sense, using the definition of Q above, it follows from (10-16) that (10-13) is equivalent to

$$\int_{V_n}^{V}\Big(\Big[-\frac{1}{4}\widetilde{\Omega}^2+\mathfrak{m}^2\pi r^2\widetilde{\Omega}^2|\phi|^2+\frac{1}{4}\frac{\widetilde{\Omega}^2}{r^2}Q^2\Big](u,V')-[\cdots](u_{\mathrm{ext}},V')\Big)\,dV' \\ =\int_{u_{\mathrm{ext}}}^{u}\big([2r\,\partial_u r\,\partial_u\log\widetilde{\Omega}+(\partial_u r)^2-4\pi r^2|D_u\phi|^2](u',V)-[\cdots](u',V_n)\big)\,du'. \tag{10-20}$$

Using again the integrated Leibniz rule (10-16) and (10-17), it then follows that (10-20) is equivalent to

$$\int_{u_{\mathrm{ext}}}^{u}\int_{V_n}^{V}\partial_u\Big(\Big[-\frac{1}{4}\widetilde{\Omega}^2+\mathfrak{m}^2\pi r^2\widetilde{\Omega}^2|\phi|^2+\frac{1}{4}\frac{\widetilde{\Omega}^2}{r^2}Q^2\Big](u',V')\Big)\,dV'\,du' \\ -\int_{V_n}^{V}\int_{u_{\mathrm{ext}}}^{u}\partial_V\big([2r\,\partial_u r\,\partial_u\log\widetilde{\Omega}+(\partial_u r)^2-4\pi r^2|D_u\phi|^2](u',V')\big)\,du'\,dV'=0, \tag{10-21}$$

where (in a similar manner to (10-19)) expressions $\partial_V\partial_u r$, $\partial_V\partial_u\log\widetilde{\Omega}$ and $\partial_V D_u\phi$ are to be understood *after plugging in the appropriate inhomogeneous terms arising from* (10-8)*,* (10-9) *and* (10-10) *respectively*, and $\partial_u Q$ is to be understood as

$$\partial_u Q=2\pi i r^2\mathfrak{e}(\phi\overline{D_u\phi}-\bar{\phi}D_u\phi);$$

see (10-3). Direct algebraic manipulations (using in particular $Q=2r^2\widetilde{\Omega}^{-2}\,\partial_u A_V$) then show that the integrand in (10-21) vanishes almost everywhere. This verifies (10-5).

Finally, we need to check (10-6), or equivalently (10-14). This can be argued in a very similar manner to (10-5); we omit the details.

Checking the regularity of the functions. We have now checked that all the equations are appropriately satisfied. To conclude that we have a solution in the sense of 10.4, it remains to check that $\partial_V r$ is continuous. (A priori, using Proposition 10.3, we only know that $\partial_V r\in L^2_V(C^0_u)$.) That $\partial_V r$ is continuous is an immediate consequence of (10-14), the fact that the data for $\partial_V r$ are continuous on $\{u=u_{\mathrm{ext}}\}$, and the regularity properties of all the other functions.

We have thus shown how to construct one extension of the solution (as a spherically symmetric strong solution in the sense of Definition 10.4). Since the procedure involves prescribing arbitrary data, one concludes that in fact there are infinitely many inequivalent extensions. □

Remark 10.6. Notice that in spherical symmetry, one can solve the wave equations with data such that one only requires $\partial_V\phi,\ \partial_V r,\ \partial_v\log\widetilde{\Omega}\in L^1_V$. However, if $\partial_V\phi\notin L^2_V$, we have $\partial_V r\to-\infty$ along a constant-u hypersurface, and one cannot make sense of (2-9) beyond the singularity. In other words, if $\partial_V\phi\notin L^2_V$, we cannot find appropriate data to the system of the wave equations so as to guarantee that the solution indeed corresponds to a solution to (1-1).

11. Improved estimates for massless and chargeless scalar field

Proof of Theorem 5.5. We will prove that

$$\sup_{u\in(-\infty,u_0],\, v\in[v_0,\infty)} (|u|^2|\partial_u\phi|(u,v)+v^2|\partial_v\phi|(u,v))<\infty.$$

Recalling the relation between v and the regular coordinate V in (9-1), this then implies the desired conclusion.

We prove the above bounds with a bootstrap argument. Assume that

$$\sup_{u\in(-\infty,u_0],\, v\in[v_0,\infty)} |u|^2|\partial_u\phi|(u,v)\le \mathcal{A}_{\mathrm{imp}}. \tag{11-1}$$

In the following argument, we will allow the implicit constant in $\lesssim$ to depend on all the constants in the previous sections, as well as the size of the left-hand side of (5-2). $\mathcal{A}_{\mathrm{imp}}$ will then be thought of as larger than all these constants. We will show that for appropriate $|u_0|$, the estimate in (11-1) can be improved.

To proceed, note that when $\mathfrak{m}=\mathfrak{e}=0$, (2-3) can be written as

$$\partial_u(r\,\partial_v\phi)=-(\partial_v r)(\partial_u\phi), \tag{11-2}$$

$$\partial_v(r\,\partial_u\phi)=-(\partial_u r)(\partial_v\phi). \tag{11-3}$$

Using (11-2), we estimate

$$v^2|\partial_v\phi|(u,v)\lesssim 1+\mathcal{A}_{\mathrm{imp}}\int_{-\infty}^{u} v^2|u'|^{-2}(v+|u'|)^{-2}\,du'\lesssim 1+\mathcal{A}_{\mathrm{imp}}|u_0|^{-1}. \tag{11-4}$$

Using (11-3) and the estimate (11-4) that we just established, we have

$$|u|^2|\partial_u\phi|(u,v)\lesssim 1+(1+\mathcal{A}_{\mathrm{imp}}|u_0|^{-1})\int_{v_0}^{\infty}|u|^2|v'|^{-2}(v'+|u|)^{-2}\,dv'\lesssim 1+(1+\mathcal{A}_{\mathrm{imp}}|u_0|^{-1})v_0^{-1}. \tag{11-5}$$

Choosing $\mathcal{A}_{\mathrm{imp}}$ sufficiently large and u_0 sufficiently negative (in that order), we have improved the bootstrap assumption (11-1). Then by (11-4) and (11-5),

$$\sup_{u,V}(|\partial_V\phi|(u,V)+|u|^2|\partial_u\phi|(u,V))\lesssim \sup_{u,v}(v^2|\partial_v\phi|(u,v)+|u|^2|\partial_u\phi|(u,v))<\infty,$$

from which the conclusion follows. □

Acknowledgements

Part of this work was carried out when both authors were at the University of Cambridge. Luk is supported by a Sloan fellowship, a Terman fellowship, and the NSF grant DMS-1709458.

References

[Angelopoulos et al. 2018] Y. Angelopoulos, S. Aretakis, and D. Gajic, "Late-time asymptotics for the wave equation on spherically symmetric, stationary spacetimes", *Adv. Math.* **323** (2018), 529–621. MR Zbl

[Aretakis 2015] S. Aretakis, "Horizon instability of extremal black holes", *Adv. Theor. Math. Phys.* **19**:3 (2015), 507–530. MR Zbl

[Costa et al. 2015a] J. L. Costa, P. M. Girão, J. Natário, and J. D. Silva, "On the global uniqueness for the Einstein–Maxwell-scalar field system with a cosmological constant, I: Well posedness and breakdown criterion", *Classical Quantum Gravity* **32**:1 (2015), art. id. 015017. MR Zbl

[Costa et al. 2015b] J. L. Costa, P. M. Girão, J. Natário, and J. D. Silva, "On the global uniqueness for the Einstein–Maxwell-scalar field system with a cosmological constant, II: Structure of the solutions and stability of the Cauchy horizon", *Comm. Math. Phys.* **339**:3 (2015), 903–947. MR Zbl

[Dafermos 2003] M. Dafermos, "Stability and instability of the Cauchy horizon for the spherically symmetric Einstein–Maxwell-scalar field equations", *Ann. of Math.* (2) **158**:3 (2003), 875–928. MR Zbl

[Dafermos 2005] M. Dafermos, "The interior of charged black holes and the problem of uniqueness in general relativity", *Comm. Pure Appl. Math.* **58**:4 (2005), 445–504. MR Zbl

[Dafermos 2014] M. Dafermos, "Black holes without spacelike singularities", *Comm. Math. Phys.* **332**:2 (2014), 729–757. MR Zbl

[Dafermos and Luk 2017] M. Dafermos and J. Luk, "The interior of dynamical vacuum black holes, I: The C^0-stability of the Kerr Cauchy horizon", preprint, 2017. arXiv

[Franzen 2016] A. T. Franzen, "Boundedness of massless scalar waves on Reissner–Nordström interior backgrounds", *Comm. Math. Phys.* **343**:2 (2016), 601–650. MR Zbl

[Gajic 2017a] D. Gajic, "Linear waves in the interior of extremal black holes, I", *Comm. Math. Phys.* **353**:2 (2017), 717–770. MR Zbl

[Gajic 2017b] D. Gajic, "Linear waves in the interior of extremal black holes, II", *Ann. Henri Poincaré* **18**:12 (2017), 4005–4081. MR Zbl

[Geroch and Traschen 1987] R. Geroch and J. Traschen, "Strings and other distributional sources in general relativity", *Phys. Rev. D* (3) **36**:4 (1987), 1017–1031. MR

[Gleeson 2016] E. Gleeson, *Linear instability of the Reissner–Nordström Cauchy horizon*, master's thesis, University of Cambridge, 2016, available at https://arxiv.org/abs/1701.06668.

[Hintz 2017] P. Hintz, "Boundedness and decay of scalar waves at the Cauchy horizon of the Kerr spacetime", *Comment. Math. Helv.* **92**:4 (2017), 801–837. MR Zbl

[Israel 1986] W. Israel, "Third law of black-hole dynamics: a formulation and proof", *Phys. Rev. Lett.* **57**:4 (1986), 397–399. MR

[Kommemi 2013] J. Kommemi, "The global structure of spherically symmetric charged scalar field spacetimes", *Comm. Math. Phys.* **323**:1 (2013), 35–106. MR Zbl

[LeFloch and Stewart 2011] P. G. LeFloch and J. M. Stewart, "The characteristic initial value problem for plane symmetric spacetimes with weak regularity", *Classical Quantum Gravity* **28**:14 (2011), art. id. 145019. MR Zbl

[Luk 2012] J. Luk, "On the local existence for the characteristic initial value problem in general relativity", *Int. Math. Res. Not.* **2012**:20 (2012), 4625–4678. MR Zbl

[Luk 2018] J. Luk, "Weak null singularities in general relativity", *J. Amer. Math. Soc.* **31**:1 (2018), 1–63. MR Zbl

[Luk and Oh 2017a] J. Luk and S.-J. Oh, "Proof of linear instability of the Reissner–Nordström Cauchy horizon under scalar perturbations", *Duke Math. J.* **166**:3 (2017), 437–493. MR Zbl

[Luk and Oh 2017b] J. Luk and S.-J. Oh, "Strong cosmic censorship in spherical symmetry for two-ended asymptotically flat initial data, I: The interior of the black hole region", preprint, 2017. To appear in *Ann. of Math.* (2). arXiv

[Luk and Oh ≥ 2019] J. Luk and S.-J. Oh, "Strong cosmic censorship and generic mass inflation for spherically symmetric charged black holes", in preparation.

[Luk and Rodnianski 2017] J. Luk and I. Rodnianski, "Nonlinear interaction of impulsive gravitational waves for the vacuum Einstein equations", *Camb. J. Math.* **5**:4 (2017), 435–570. MR Zbl

[Luk and Sbierski 2016] J. Luk and J. Sbierski, "Instability results for the wave equation in the interior of Kerr black holes", *J. Funct. Anal.* **271**:7 (2016), 1948–1995. MR Zbl

[Van de Moortel 2018] M. Van de Moortel, “Stability and instability of the sub-extremal Reissner–Nordström black hole interior for the Einstein–Maxwell–Klein–Gordon equations in spherical symmetry”, *Comm. Math. Phys.* **360**:1 (2018), 103–168. MR Zbl

[Murata et al. 2013] K. Murata, H. S. Reall, and N. Tanahashi, “What happens at the horizon(s) of an extreme black hole?”, *Classical Quantum Gravity* **30**:23 (2013), art. id. 235007. MR Zbl

[Penrose 1968] R. Penrose, “Structure of space-time”, in *Battelle Rencontres* (Seattle, 1967), edited by C. DeWitt-Morette and J. A. Wheeler, W. A. Benjamin, New York, 1968. Zbl

[Poisson and Israel 1989] E. Poisson and W. Israel, “Inner-horizon instability and mass inflation in black holes”, *Phys. Rev. Lett.* **63**:16 (1989), 1663–1666. MR

[Sbierski 2015] J. Sbierski, “Characterisation of the energy of Gaussian beams on Lorentzian manifolds: with applications to black hole spacetimes”, *Anal. PDE* **8**:6 (2015), 1379–1420. MR Zbl

Received 12 Jan 2019. Accepted 12 Feb 2019.

DEJAN GAJIC: dejan.gajic@imperial.ac.uk
Department of Mathematics, South Kensington Campus, Imperial College London, London, United Kingdom

JONATHAN LUK: jluk@stanford.edu
Department of Mathematics, Stanford University, Stanford, CA, United States

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.

Figures. Figures must be of publication quality. After acceptance, you will need to submit the original source files in vector graphics format for all diagrams in your manuscript: vector EPS or vector PDF files are the most useful.

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.

Bundle your figure files into a single archive (using zip, tar, rar or other format of your choice) and upload on the link you been provided at acceptance time. Each figure should be captioned and numbered so that it can float. Small figures occupying no more than three lines of vertical space can be kept in the text (“the curve looks like this:”). It is acceptable to submit a manuscript with all figures at the end, if their placement is specified in the text by means of comments such as “Place Figure 1 here”. The same considerations apply to tables.

White Space. Forced line breaks or page breaks should not be inserted in the document. There is no point in your trying to optimize line and page breaks in the original manuscript. The manuscript will be reformatted to use the journal’s preferred fonts and layout.

Proofs. Page proofs will be made available to authors (or to the designated corresponding author) at a Web site in PDF format. Failure to acknowledge the receipt of proofs or to return corrections within the requested deadline may cause publication to be postponed.

PURE and APPLIED ANALYSIS

vol. 1 no. 2 2019

2578-5893 (2019)1:2;1-5