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CONSTANT SIGN AND SIGN CHANGING NLS GROUND STATES ON NONCOMPACT METRIC GRAPHS

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We investigate existence and nonexistence of action ground states and nodal action ground states for the nonlinear Schrödinger equation on noncompact metric graphs with mixed homogeneous Kirchhoff and Dirichlet boundary conditions. We first obtain abstract sufficient conditions for existence, typical of problems with lack of compactness, in terms of "levels at infinity" for the action functional associated with the problems. Then we analyze in detail two relevant classes of graphs. For noncompact graphs with at least one half-line, we detect purely topological sharp conditions preventing the existence of ground states or of nodal ground states. We also investigate analogous conditions of metrical nature. The negative results are complemented by several sufficient conditions to ensure existence, either of topological or metrical nature, or a combination of the two. For graphs with infinitely many edges, all bounded, we focus on periodic graphs and infinite trees. In these cases, our results completely describe the phenomenology. Furthermore, we study nodal domains and nodal sets of nodal ground states and we show that the situation on graphs can be totally different from that on domains of $\mathbb{R}^N$.

1. Introduction

We investigate the existence of constant sign and sign changing solutions of the nonlinear Schrödinger equation

$$u'' + |u|^{p-2}u = \lambda u, \tag{1-1}$$

where $p > 2$ and λ is a real parameter, on noncompact metric graphs under various assumptions.

Throughout this paper we consider the class $\boldsymbol{G}$ of connected metric graphs $\mathcal{G} = (\mathbb{V}, \mathbb{E})$ where the sets $\mathbb{V}$ and $\mathbb{E}$ are at most countable, every vertex $\mathrm{v} \in \mathbb{V}$ has finite degree, and the lengths of the edges $e \in \mathbb{E}$ are bounded away from zero (see Definition 2.1 below). A graph of this type is noncompact if at least one edge is unbounded (i.e., it is a half-line) or if it consists of an infinite number of bounded edges, giving rise to two classes of graphs that behave quite differently and that we will treat separately. Every half-line is considered to end at a "vertex at infinity" of degree 1. The set of all such vertices of $\mathbb{V}$ is denoted by $\mathbb{V}_\infty$.

The analysis of differential equations on metric graphs experienced a massive growth in recent years, in particular motivated by the potential of graphs to serve as simple models for signal propagation in branched structures. In this context, stationary nonlinear Schrödinger equations such as (1-1) gained

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a prominent interest, as it is well known that to any couple (u, λ) satisfying (1-1) there corresponds a standing wave solution $\psi(t, x) := e^{i\lambda t} u(x)$ of the time-dependent nonlinear Schrödinger equation

$$-i\partial_t \psi(t, x) = \partial^2_{xx} \psi(t, x) + |\psi(t, x)|^{p-2} \psi(t, x). \tag{1-2}$$

Nonlinear dispersive equations such as (1-2) are largely studied in view of the role they play in many applications, such as, e.g., in the modeling of quantum mechanical systems in Bose–Einstein condensation or in the modeling of optical fibers.

It is clear however that, when considering any differential model on graphs, it is not enough to prescribe a differential equation that describes the behavior of the system in the interior of each edge. The equation must be complemented with suitable matching conditions at the vertices, specifying how the interaction among edges behaves at the junctions. In the case of nonlinear Schrödinger equations, there is a wide class of vertex conditions that can be considered. In the present paper, we couple (1-1) with a specific choice of boundary conditions. Precisely, given a (not necessarily finite) set $Z \subseteq \mathbb{V} \setminus \mathbb{V}_\infty$ of degree-1 vertices, we are interested in solutions to the problem

$$\begin{cases} u'' + |u|^{p-2} u = \lambda u & \text{on every edge of } \mathcal{G}, \\ u \text{ is continuous} & \text{on } \mathcal{G}, \\ \sum_{e \succ \mathrm{v}} u'_e(\mathrm{v}) = 0 & \text{for every } \mathrm{v} \in \mathbb{V} \setminus (Z \cup \mathbb{V}_\infty), \\ u(\mathrm{v}) = 0 & \text{for every } \mathrm{v} \in Z, \end{cases} \tag{1-3}$$

where $u'_e(\mathrm{v})$ is the outgoing derivative along the edge e incident at the vertex v and $e \succ \mathrm{v}$ means that the sum is extended to all such edges. The boundary condition for $\mathrm{v} \notin Z$ (together with the continuity of u) is the homogeneous Kirchhoff condition, by far the most used in the literature. It is a natural analogue of the Neumann boundary condition for metric graphs (see, e.g., [Berkolaiko and Kuchment 2013, Section 1.4]). The boundary condition for $\mathrm{v} \in Z$ is the homogeneous Dirichlet condition, which by contrast has been discussed only in a few papers (see, for instance, [Esteban 2022]). Here we choose to include mixed conditions to highlight their role in the existence (or nonexistence) of various types of solutions to (1-3). The requirement that all nodes of Z have degree 1 prevents the graph from being disconnected by the Dirichlet conditions, but more general frameworks can easily be treated building on the results of this paper.

Coupling the operator $-\mathrm{d}^2/\mathrm{d}x^2$ with our boundary conditions guarantees its self-adjointness. This is a natural requirement in the analysis of quantum mechanical problems (see, e.g., [Adami et al. 2020] for an overview of boundary conditions ensuring self-adjointness on metric graphs and [Berkolaiko and Kuchment 2013, Section 1.4] for a thorough discussion).

Solutions to (1-3) can be found by a variational approach that has been employed very frequently to deal with this kind of problem or with its variants. In our setting, the appropriate function space to set problem (1-3) is

$$H^1_Z(\mathcal{G}) := \{u \in H^1(\mathcal{G}) \mid u(\mathrm{v}) = 0 \text{ for every } \mathrm{v} \in Z\}.$$

Standard arguments show that the $H^1(\mathcal{G})$ solutions of problem (1-3) are exactly the critical points of the *action* functional $J_\lambda : H^1_Z(\mathcal{G}) \to \mathbb{R}$ defined by

$$J_\lambda(u) := \tfrac{1}{2}\|u'\|^2_{L^2(\mathcal{G})} + \tfrac{1}{2}\lambda \|u\|^2_{L^2(\mathcal{G})} - \frac{1}{p}\|u\|^p_{L^p(\mathcal{G})}, \tag{1-4}$$

that is of class C^2 on $H^1_Z(\mathcal{G})$. Hereafter the parameter λ satisfies as usual $\lambda > -\omega_Z(\mathcal{G})$, where

$$\omega_Z(\mathcal{G}) := \inf_{v\in H^1_Z(\mathcal{G})\setminus\{0\}} \frac{\|v'\|^2_{L^2(\mathcal{G})}}{\|v\|^2_{L^2(\mathcal{G})}}$$

denotes the bottom of the spectrum of the Laplacian on $\mathcal{G}$ associated to the boundary conditions in (1-3). This assumption is standard when working with this problem and is justified by the fact that, under it, the quadratic part in (1-4) provides a norm on $H^1(\mathcal{G})$ equivalent to the usual H^1-norm.

When looking at solutions to (1-3) from the variational perspective, one has to take into account that the functional J_λ is not bounded from below on $H^1_Z(\mathcal{G})$. A standard way to recover the notion of minimality is to introduce the Nehari manifold associated to J_λ, defined by

$$\begin{aligned}\mathcal{N}_{\lambda,Z}(\mathcal{G}) &:= \{u \in H^1_Z(\mathcal{G}) \mid u \neq 0,\ J'_\lambda(u)u = 0\}\\ &= \{u \in H^1_Z(\mathcal{G}) \mid u \neq 0,\ \|u'\|^2_{L^2(\mathcal{G})} + \lambda\|u\|^2_{L^2(\mathcal{G})} = \|u\|^p_{L^p(\mathcal{G})}\}.\end{aligned}$$

Clearly, $\mathcal{N}_{\lambda,Z}(\mathcal{G})$ contains all solutions to (1-3). It is a C^1-manifold diffeomorphic to the unit sphere of $H^1_Z(\mathcal{G})$ and is a natural constraint for J_λ, in the sense that constrained critical points of J_λ are in fact true critical points. Other approaches are possible (for instance, one could constrain J_λ on the unit sphere of $L^p(\mathcal{G})$), but the Nehari approach has the advantage that it works also in cases where the nonlinearity is not homogeneous, thus providing a framework suitable to be generalized to a wider class of nonlinear terms.

Definition 1.1. We say that a function $u \in \mathcal{N}_{\lambda,Z}(\mathcal{G})$ is a *ground state* for problem (1-3) if

$$J_\lambda(u) = \inf_{v\in\mathcal{N}_{\lambda,Z}(\mathcal{G})} J_\lambda(v).$$

Since we want to discuss both one-signed and sign changing solutions, we will also consider *nodal ground states*, roughly the analogue of ground states among sign changing functions. To define rigorously this notion, we let

$$u^+ := \max(u, 0), \qquad u^- := \min(u, 0)$$

and define the *nodal Nehari set* as

$$\mathcal{M}_{\lambda,Z}(\mathcal{G}) := \{u \in H^1_Z(\mathcal{G}) \mid u^\pm \in \mathcal{N}_{\lambda,Z}(\mathcal{G})\} = \{u \in H^1_Z(\mathcal{G}) \mid u^\pm \neq 0,\ J'_\lambda(u)u^\pm = 0\}.$$

The nodal Nehari set contains all nodal solutions of (1-3) but, contrary to $\mathcal{N}_{\lambda,Z}(\mathcal{G})$, in general is not a manifold (see, e.g., [Bartsch and Weth 2003; Castro et al. 1997; Szulkin and Weth 2010]) and is not a natural constraint for J_λ, which causes some extra difficulties when proving existence results.

Definition 1.2. We say that a function $u \in \mathcal{M}_{\lambda,Z}(\mathcal{G})$ is a *nodal ground state* for problem (1-3) if

$$J_\lambda(u) = \inf_{v\in\mathcal{M}_{\lambda,Z}(\mathcal{G})} J_\lambda(v).$$

It is well known that, whenever they exist, ground states (resp. nodal ground states) provide constant sign solutions (resp. sign changing solutions) of (1-1) of minimal action. Actually, to look for one-signed solutions of nonlinear Schrödinger equations as minimizers of suitable functionals is a standard strategy, that has been widely exploited on graphs in the mass constrained setting, where ground states are defined as minimizers of the energy functional $u \mapsto \frac{1}{2}\|u'\|^2_{L^2(\mathcal{G})} - \frac{1}{p}\|u\|^p_{L^p(\mathcal{G})}$ restricted to an L^2-sphere (see, e.g., [Adami et al. 2014a; 2015; 2016; 2019; 2022; Berkolaiko et al. 2021; Boni and Carlone 2023; Besse et al. 2022a; 2022b; Boni and Dovetta 2021; 2022; Dovetta and Tentarelli 2022; Kairzhan et al. 2021; 2022; Pierotti and Soave 2022; Pierotti et al. 2021; Tentarelli 2016]). In particular, these works have shown that the existence of ground states for the prescribed-mass problem on noncompact graphs is a rather unlikely event. Obstructions to existence are provided mostly by the topology of the graph, and sometimes also by its metrical properties. Conversely, the action approach has not received much attention so far (some results in this direction can be found, e.g., in [Adami et al. 2014b; De Coster et al. 2023; Kurata and Shibata 2020; Pankov 2018]). Let us stress that, though clearly critical points of the action on Nehari sets are also critical points of the energy on a suitable L^2-sphere and vice versa, the general relation between the action and the energy approach is not fully understood. First investigations in this direction started only recently in [Dovetta et al. 2023; Jeanjean and Lu 2022] for NLS equations posed on domains of $\mathbb{R}^N$, but many of the results obtained therein extend with no difference to metric graphs. Specifically, if on the one hand those analyses proved that mass constrained ground states of the energy are always also ground states of the action, on the other hand they showed that the converse is in general not true. Hence, there may well exist action ground states that are not energy ground states among functions with the same mass, and the actual occurrence of this phenomenon on metric graphs has been proved, e.g., in [Agostinho et al. 2024, Theorem 1.4; Dovetta 2024, Proposition 2.4]. This somehow further motivates the independent study of the action ground state problem even in a context, as that of graphs, in which a well-developed theory of energy ground states is already available. In addition, to the best of our knowledge, nodal ground states, and more generally sign changing solutions, on general metric graphs have never been investigated up to now, neither for the action nor for the energy problem. In the nodal setting, actually, the asymmetry between the action and the energy point of views is more pronounced, as it is not even clear how to define a general variational framework to deal with sign changing solutions with prescribed mass (that is, no analogue of the nodal Nehari set is known for the energy).

The main concern of the present paper is thus to begin a systematic study of action ground states and nodal ground states for (1-3), characterizing the dependence of the problem on topological and metrical properties of the graph. On one side, as it is reasonable to expect, with purely Kirchhoff vertex conditions (i.e., $Z = \varnothing$), we will find that sometimes the same topological conditions that rule out mass constrained ground states do prevent existence of action ground states too (this is the case for graphs with half-lines, as in Theorem 1.6 below), and analogous conditions for nodal ground states will be identified. On the other side, we will also show that there are graphs (periodic ones and trees) for which action ground states exist for every admissible value of λ, whereas existence of mass constrained ground states depends on the value of the mass.

To begin the discussion of our results, we observe that if $\mathcal{G}$ is compact, the existence of a ground state and of a nodal ground state can be proved via standard compactness arguments. Indeed, the compactness of the domain guarantees compactness for Sobolev embeddings $H^1(\mathcal{G}) \hookrightarrow L^p(\mathcal{G})$, which is all that is needed to obtain strong convergence of minimizing sequences for the above variational problems (see, e.g., [Dovetta 2018, Proposition 3.1] for further details on such compactness results in the context of mass constrained critical points of the energy).

On the contrary, if $\mathcal{G}$ is noncompact, since as we said above the existence of ground states is unlikely, it is not surprising that the analogous eventuality for nodal ground states is even more so. As for ground states, we are going to derive sufficient conditions for both existence and nonexistence of nodal ground states involving topological features, metrical ones and combinations of the two.

Our analysis is based on a rather abstract procedure, typical of problems with lack of compactness, consisting in locating thresholds on the levels of J_λ, involving the so-called level at infinity

$$J_\lambda^\infty(\mathcal{G}; Z) := \inf\bigl\{\liminf_n J_\lambda(u_n) \mid (u_n)_n \subseteq \mathcal{N}_{\lambda,Z}(\mathcal{G}),\ \lim_n u_n = 0 \text{ weakly in } H^1_Z(\mathcal{G})\bigr\}.$$

Theorem 1.3. *Let $\mathcal{G} \in \boldsymbol{G}$ be a noncompact graph and $\lambda > -\omega_Z(\mathcal{G})$.*

(i) *If*

$$\inf_{v\in\mathcal{N}_{\lambda,Z}(\mathcal{G})} J_\lambda(v) < J_\lambda^\infty(\mathcal{G}; Z), \tag{1-5}$$

then there exists a ground state of J_λ in $\mathcal{N}_{\lambda,Z}(\mathcal{G})$. Moreover, ground states have constant sign on $\mathcal{G} \setminus Z$.

(ii) *If*

$$\inf_{v\in\mathcal{M}_{\lambda,Z}(\mathcal{G})} J_\lambda(v) < J_\lambda^\infty(\mathcal{G}; Z) + \inf_{v\in\mathcal{N}_{\lambda,Z}(\mathcal{G})} J_\lambda(v), \tag{1-6}$$

then there exists a nodal ground state of J_λ in $\mathcal{M}_{\lambda,Z}(\mathcal{G})$.

Theorem 1.4. *For every noncompact graph $\mathcal{G} \in \boldsymbol{G}$ and $\lambda > -\omega_Z(\mathcal{G})$,*

$$\inf_{v\in\mathcal{M}_{\lambda,Z}(\mathcal{G})} J_\lambda(v) \geq 2 \inf_{v\in\mathcal{N}_{\lambda,Z}(\mathcal{G})} J_\lambda(v). \tag{1-7}$$

If equality holds, then $\mathcal{G}$ admits no nodal ground states of J_λ in $\mathcal{M}_{\lambda,Z}(\mathcal{G})$.

Remark 1.5. Inequality (1-7) also holds when $\mathcal{G}$ is a compact metric graph, and is then strict as nodal ground states always exist in this case.

This abstract strategy, though general, is absolutely insufficient to obtain existence results if one is not able to compute the level $J_\lambda^\infty(\mathcal{G}; Z)$ in concrete cases. Here we will detect specific properties of the graph that permit such computation and make sure that, in certain cases, the ground state level or the nodal ground state level lie below the level at infinity. Since this is where the topology and the metric of the graph become crucial, the analysis of such questions is carried out separately according to the class of graphs under study.

We first discuss the case of graphs with at least one half-line. For every such graph, $\omega_Z(\mathcal{G}) = 0$ and so the following results hold for every $\lambda > 0$.

We identify topological conditions on $\mathcal{G}$ that prevent the existence of ground states and nodal ground states. We describe them here in a concise way, referring to Section 4 for a more detailed discussion. To begin with, recall that the set of *vertices at infinity* of $\mathcal{G}$ is

$$\mathbb{V}_\infty = \{\mathrm{v} \in \mathbb{V} \mid \mathrm{v} \text{ is the vertex of degree 1 of some half-line}\}$$

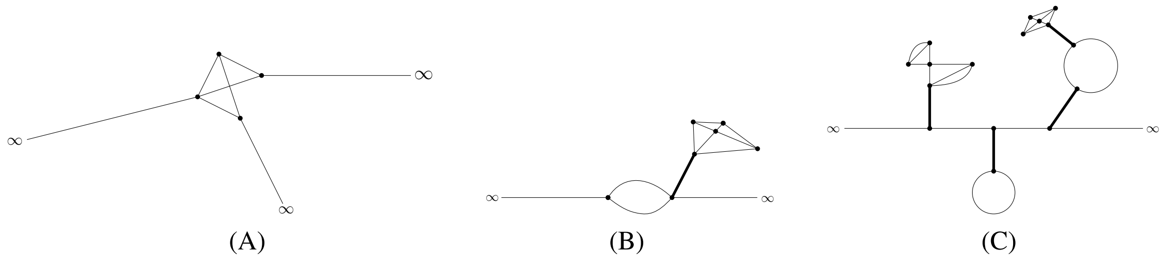


Figure 1. Examples of graphs $\mathcal{G}$ with corresponding set $F(\mathcal{G})$ containing 0 (A), 1 (B), and 4 (C) edges, respectively. Here, Kirchhoff conditions are assumed at every vertex, and edges in $F(\mathcal{G})$ are drawn thicker.

and define the set

$$F(\mathcal{G}) = \{e \in \mathbb{E} \mid \text{at least one connected component of } (\mathbb{V}, \mathbb{E} \setminus \{e\}) \text{ has no vertices in } \mathbb{V}_\infty \cup Z\}.$$

The set $F(\mathcal{G})$ is thus the set of edges of $\mathcal{G}$ (if any) whose removal disconnects $\mathcal{G}$ creating a connected component without vertices in $\mathbb{V}_\infty \cup Z$. Basically, if $F(\mathcal{G})$ is nonempty, there exists at least one "bridging" edge in the graph that, once removed, creates at least one connected component separated from all the half-lines and all the vertices with homogeneous Dirichlet condition (see Figure 1 for a concrete illustration of $F(\mathcal{G})$ on different graph structures). The cardinality of $F(\mathcal{G})$ is a purely topological notion and plays a fundamental role in the nonexistence of ground states and nodal ground states. Roughly, we will see that the presence of bridging edges in $F(\mathcal{G})$ may facilitate existence of such states, especially if the connected components without vertices in $\mathbb{V}_\infty \cup Z$ they isolate have a very simple structure. On the contrary, a low cardinality of $F(\mathcal{G})$ somehow corresponds to a too-intricate graph structure not compatible with existence. This is stated rigorously in the next theorem, where for every $\lambda > 0$ we denote by

$$s_\lambda := \inf_{v \in \mathcal{N}_\lambda(\mathbb{R})} J_\lambda(v)$$

the ground state level of J_λ on $\mathbb{R}$.

Theorem 1.6. *Let $\mathcal{G} \in \mathbf{G}$ be a noncompact graph with at least one half-line and $\lambda > 0$. Then*

$$\inf_{v \in \mathcal{N}_{\lambda,Z}(\mathcal{G})} J_\lambda(v) \le s_\lambda \tag{1-8}$$

and

$$\inf_{v \in \mathcal{M}_{\lambda,Z}(\mathcal{G})} J_\lambda(v) \le s_\lambda + \inf_{v \in \mathcal{N}_{\lambda,Z}(\mathcal{G})} J_\lambda(v). \tag{1-9}$$

Moreover,

(i) *if $\#F(\mathcal{G}) = 0$, then*

$$\inf_{v \in \mathcal{N}_{\lambda,Z}(\mathcal{G})} J_\lambda(v) = s_\lambda \tag{1-10}$$

and it is not achieved, *unless $\mathcal{G}$ is isometric to $\mathbb{R}$ or to a "tower of bubbles" depicted in Figure 2*;

(ii) *if $\#F(\mathcal{G}) \le 1$, then*

$$\inf_{v \in \mathcal{M}_{\lambda,Z}(\mathcal{G})} J_\lambda(v) = s_\lambda + \inf_{v \in \mathcal{N}_{\lambda,Z}(\mathcal{G})} J_\lambda(v) \tag{1-11}$$

and it is never achieved.

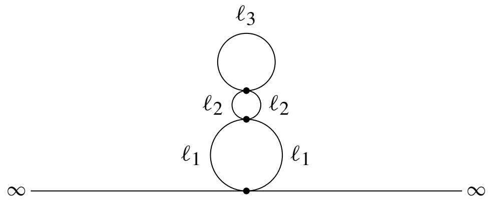


Figure 2. An example of a "tower of bubbles" graph. Each of these graphs, identified in Example 2.4 of [Adami et al. 2015], is built of a real line and a finite sequence of two-by-two tangent circles.

The preceding results are the main examples where a purely topological assumption on the graph rules out the existence of ground states or nodal ground states. The families of graphs fulfilling each of the conditions of Theorem 1.6 are rather large and it is not difficult to exhibit examples of structures with these properties (see Figure 1(A)–(B) and Figure 3). In the case of ground states, the condition $\#F(\mathcal{G}) = 0$ was already shown to prevent existence of mass constrained ground states of the energy in [Adami et al. 2015, Theorem 2.5], where it was named assumption (H). In contrast, the analogous condition for nodal ground states is established here for the first time. We underline that both assumptions on the cardinality of $F(\mathcal{G})$ are sharp for nonexistence. Indeed, in Section 4 we will show that there exist graphs satisfying $\#F(\mathcal{G}) \geq 1$ that admit a ground state, and graphs satisfying $\#F(\mathcal{G}) \geq 2$ that admit a nodal ground state.

These nonexistence results are complemented in Section 4 by a number of sufficient conditions to ensure existence. Relying on techniques developed for energy ground states in [Adami et al. 2015, Section 6; 2016, Section 3], it is easy to construct graphs where existence of action ground states is guaranteed by purely *topological* properties whenever $Z = \varnothing$ (see Theorem 4.8 and Figure 6 below). Notably, this turns out to be impossible as soon as $Z \neq \varnothing$. In this case, a necessary condition of *metrical* nature for the existence of ground states arises: the diameter of the set of all bounded edges of the graph must exceed a threshold depending on λ but not on the graph itself (Theorem 4.9). The same constraint holds true for nodal ground states, where it is not even needed to have a nonempty set Z (Theorem 4.11). In addition to providing purely metrical nonexistence results, these theorems imply that the interplay between topology and metric must be further exploited if one hopes to recover existence. We give examples of this fact by describing two general procedures to construct graphs where existence is granted (Theorems 4.12–4.16). The former relies on the metric only, and shows that one and two sufficiently long edges with vertices of degree 1 not in Z are enough to have ground states and nodal ground states, respectively. The latter basically consists in a suitable gluing of graphs hosting ground states to obtain structures supporting nodal ground states (see, e.g., Figure 7).

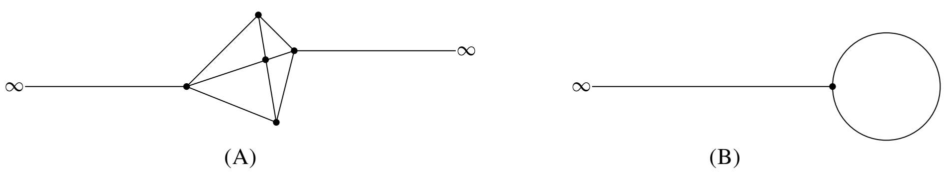


Figure 3. Further examples of graphs with half-lines satisfying $\#F(\mathcal{G}) = 0$ (A) and $\#F(\mathcal{G}) = 1$ (B).

The previous results highlight how the presence of at least one vertex with homogeneous Dirichlet conditions affects the existence of ground states and nodal ground states. Indeed, the fact that vertices in Z play the same role as those at infinity in the definition of $F(\mathcal{G})$ suggests the idea that an edge ending at a vertex with zero Dirichlet conditions behaves as an half-line. This heuristic comparison makes some sense, since H^1 functions tend to zero at infinity along each half-line. However, Theorem 4.9 unravels that the analogy with half-lines is not complete: edges with endpoints in Z are somehow "worse", as they make metrical assumptions necessary to obtain existence. We may be tempted to say that existence of ground states simply requires edges ending in Z to be long enough (and thus sufficiently close to half-lines), but this is not true in general, as ground states can exist even on graphs where all edges with vertices in Z are arbitrarily short (see Remark 4.10 below).

Section 5 of the paper deals with noncompact graphs in the class $\boldsymbol{G}$ with an infinite number of edges, whose length is uniformly bounded from above. Given the huge variety of structures in this class, we confine ourselves to two subclasses of major relevance, that have already been studied extensively in the literature in many contexts (see, e.g., [Adami et al. 2019; Besse et al. 2022a; 2022b; Dovetta and Tentarelli 2022; Dovetta et al. 2020; Gilg et al. 2022; Pankov 2018; Pelinovsky and Schneider 2017] for results related to those we discuss here): periodic graphs and regular trees.

Without entering the details of the definition of periodic graphs (for which we refer to [Berkolaiko and Kuchment 2013, Definition 4.1.1]), let us mention here that we always work assuming that the set Z shares the same type of periodicity as the graph itself. Our main result in this respect completely describes the phenomenology from the point of view of ground states and nodal ground states (results in this direction for ground states on periodic graphs were already given in [Pankov 2018]).

As for graphs with half-lines, if $\mathcal{G}$ is a periodic graph then $\omega_Z(\mathcal{G}) = 0$, so that the next theorem holds again for every $\lambda > 0$.

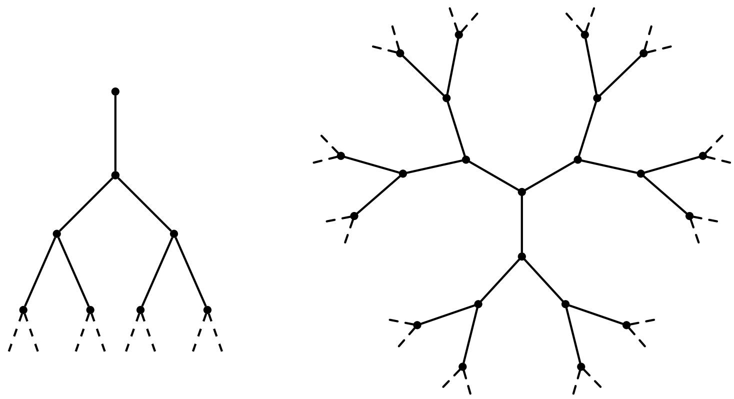
Theorem 1.7. *Let $\mathcal{G} \in \boldsymbol{G}$ be a periodic graph and $\lambda > 0$. Then $\mathcal{G}$ admits a ground state. Furthermore,*

$$\inf_{v \in \mathcal{M}_{\lambda,Z}(\mathcal{G})} J_\lambda(v) = 2 \inf_{v \in \mathcal{N}_{\lambda,Z}(\mathcal{G})} J_\lambda(v)$$

and there are no nodal ground states.

It is interesting to note that the above results are insensitive of the degree of periodicity, i.e., the dimension n of the group $\mathbb{Z}^n$ whose action leaves the graph invariant. This is particularly relevant when put in relation with the available results for prescribed-mass energy ground states (compare, e.g., [Adami et al. 2019, Theorems 1.1–1.2], where $n = 2$, with [Dovetta 2019, Theorem 1.1], where $n = 1$), whose existence has been shown to depend strongly on the value of n.

The last results of Section 5 concern regular trees, i.e., acyclic, noncompact metric graphs with infinitely many bounded edges, all of the same length, and where all the vertices have the same degree, with the possible exception of a unique root vertex of degree 1. If such a vertex with degree 1 is present, we speak of a rooted tree (see Figure 4(A)), otherwise we speak of an unrooted tree (see Figure 4(B)). Regular trees are well-known examples of noncompact graphs satisfying $\omega_Z(\mathcal{G}) > 0$ (see, e.g., [Dovetta et al. 2020]). Hence, in this setting our results involve also negative values of λ.



(A) (B)

Figure 4. Examples of a rooted tree (A) and an unrooted tree (B).

Theorem 1.8. *Let $\mathcal{G}$ be a regular tree and $\lambda > -\omega_Z(\mathcal{G})$. Then*

(i) *if $\mathcal{G}$ is unrooted or if $\mathcal{G}$ is rooted and Z is empty, $\mathcal{G}$ admits a ground state*;

(ii) *if $\mathcal{G}$ is rooted and Z is not empty, there are no ground states on $\mathcal{G}$*;

(iii) *independently of Z, there are no nodal ground states on $\mathcal{G}$.*

As in the case of periodic graphs, the above theorem provides a complete description of the problem for regular trees. As one may expect, the role of the set Z is crucial to discriminate between existence and nonexistence on rooted trees. Moreover, as already seen for periodic graphs, observe that Theorem 1.8(i) establishes the existence of ground states of the action on trees for every admissible value of the parameter λ. It is interesting to compare this result with [Dovetta et al. 2020, Theorem 1.2], where it is shown that existence of mass constrained ground states of the energy on trees does depend on the mass. In particular, when $p \in [4, 6)$, energy ground states do not exist if the mass is smaller than a positive threshold. However, this seeming asymmetry is not sufficient to guarantee that, on trees, the action approach is more general than the energy one. Indeed, [Dovetta et al. 2020] does not provide any information on the values of the parameter λ associated to energy ground states, and nothing is known about the mass of action ground states identified in this paper. Hence, it is not clear whether the ground states of the action given by Theorem 1.8(i) for $\lambda > -\omega_Z(\mathcal{G})$ coincide with the mass constrained ground states of the energy found in [Dovetta et al. 2020, Theorem 1.2].

We observe that the discussion developed here requires no restrictions on the nonlinearity power p, so that all our results apply for every $p > 2$. In particular, the existence statements listed above provide constant sign and sign changing solutions to (1-3) also when $p > 6$, the so-called L^2-supercritical regime, whose analysis is much harder in the context of fixed mass critical points of the energy (first investigations in this direction have been initiated in [Borthwick et al. 2023; Chang et al. 2024]).

To conclude, we study nodal domains (i.e., the connected components of $\mathcal{G} \setminus u^{-1}(0)$) and the nodal set (i.e., the set $u^{-1}(0)$) of nodal ground states u. As one may expect, nodal ground states have exactly two nodal domains (Theorem 6.1). We also show that the nodal set can have an arbitrary number of components and an arbitrary measure. This is in contrast with the case of open domains of $\mathbb{R}^N$, where unique continuation principles forbid nonzero solutions to vanish on nonempty open subsets.

Theorem 1.9. *For every $k, m, n \in \mathbb{N}$ with $m \geq 2$, there exists a graph $\mathcal{G}$ and a nodal ground state u on $\mathcal{G}$ such that $u^{-1}(0)$ is the union of k isolated points, m half-lines and n line segments.*

The remainder of the paper is organized as follows. Section 2 collects some preliminary facts useful for the subsequent analysis, while Section 3 provides the proof of the abstract results contained in Theorems 1.3–1.4. Section 4 analyzes the case of graphs with half-lines, while periodic graphs and trees are dealt with in Section 5. Qualitative properties of nodal ground states are studied in Section 6.

Notation. Throughout, we will drop the dependence of $\mathcal{N}_{\lambda,Z}(\mathcal{G})$, $\mathcal{M}_{\lambda,Z}(\mathcal{G})$, J_λ on λ and $\mathcal{G}$, writing $\mathcal{N}_Z$, $\mathcal{M}_Z$ and J whenever possible, keeping the complete notation only if necessary. Similarly, when the context permits it, we will not explicitly indicate, in norms, the dependence on the domain of integration. Furthermore, when $Z = \varnothing$, we do not put $\varnothing$ as a subscript and simply write $H^1(\mathcal{G})$, $\mathcal{N}$, $\mathcal{M}$, etc.

2. Preliminaries

For the precise notion of metric graphs, we refer to [Berkolaiko and Kuchment 2013]. However, we make precise in the following definition the class of graphs that we consider in this paper.

Definition 2.1. We denote by $\boldsymbol{G}$ the class of metric graphs $\mathcal{G} = (\mathbb{V}, \mathbb{E})$ such that

- $\mathcal{G}$ is connected and has an at most countable number of edges;
- $\deg(\mathrm{v}) < \infty$ for every $\mathrm{v} \in \mathbb{V}$, where $\deg(\mathrm{v})$ denotes the degree of the vertex v, i.e., the number of edges incident at v;
- $\ell := \inf_{e \in \mathbb{E}} \ell_e > 0$, where ℓ_e denotes the length of the edge e.

A graph $\mathcal{G} \in \boldsymbol{G}$ is noncompact as soon as one of the following two eventualities occurs:

(i) $\mathcal{G}$ has at least one unbounded edge (i.e., a half-line),

(ii) the number of edges of $\mathcal{G}$ is infinite.

Remark 2.2. One could add in the definition of $\mathcal{G}$ the assumption that every vertex v satisfies $\deg(\mathrm{v}) \neq 2$. Indeed, vertices v of degree 2 can a priori be eliminated from any metric graph, by melting the two edges incident at v into a single edge. In some cases however (see Remark 3.2) the possibility of using vertices of degree 2 turns out to be quite handy. Adding or removing vertices of degree 2 from a graph changes it combinatorially, but not as a metric space, and in this paper we will identify graphs that differ only by vertices of degree 2.

As anticipated in the Introduction, we couple (1-1) with mixed Kirchhoff and Dirichlet boundary conditions. Given a noncompact graph $\mathcal{G} \in \boldsymbol{G}$, we let $Z \subset \mathbb{V}$ denote a set of vertices of degree 1 (possibly empty or infinite) where we impose homogeneous Dirichlet conditions and we set

$$H^1_Z(\mathcal{G}) := \{u \in H^1(\mathcal{G}) \mid u(\mathrm{v}) = 0 \text{ for every } \mathrm{v} \in Z\}.$$

The Nehari manifold associated to J on $H^1_Z(\mathcal{G})$ is

$$\begin{aligned}\mathcal{N}_Z &:= \{u \in H^1_Z(\mathcal{G}) \mid u \neq 0,\ J'(u)u = 0\}\\ &= \{u \in H^1_Z(\mathcal{G}) \mid u \neq 0,\ \|u'\|_2^2 + \lambda\|u\|_2^2 = \|u\|_p^p\},\end{aligned}$$

while the nodal Nehari set is

$$\mathcal{M}_Z := \{u \in H^1_Z(\mathcal{G}) \mid u^\pm \in \mathcal{N}_Z\} = \{u \in H^1_Z(\mathcal{G}) \mid u^\pm \neq 0,\ J'(u)u^\pm = 0\}.$$

The nodal Nehari set contains all nodal solutions of (1-3), but, generally, it is not a manifold. However, the following fundamental property holds for global minimizers on compact graphs.

Proposition 2.3. *Let $\mathcal{G} \in \boldsymbol{G}$ be compact and $\lambda > -\omega_Z(\mathcal{G})$. If $u \in \mathcal{M}_Z$ satisfies*

$$J(u) = \inf_{v \in \mathcal{M}_Z} J(v),$$

then $J'(u) = 0$.

Proof. The fact that any function realizing the minimum of the action restricted to its nodal Nehari set is in fact a critical point of the action is a very general property, that holds true for a large class of NLS equations including the one we consider in this paper, and is not specific of graphs. A detailed proof can be found, e.g., in [Bartsch et al. 2005, Proposition 3.1] in the case of NLS equations (with more general nonlinearities than the one of this paper) posed on bounded domains of $\mathbb{R}^N$ with homogeneous Dirichlet conditions at the boundary. The proof reported therein uses only abstract tools of critical point theory (in particular, the deformation lemma). For this reason, that argument extends with no modification to compact graphs. □

Obviously $\mathcal{M}_Z \subset \mathcal{N}_Z$ and, for $u \in \mathcal{N}_Z$, the functional J defined in (1-4) takes the simple form

$$J(u) = \kappa\|u\|_p^p = \kappa(\|u'\|_2^2 + \lambda\|u\|_2^2), \quad \kappa := \tfrac{1}{2} - \frac{1}{p}, \tag{2-1}$$

from which we see that J is positive on $\mathcal{N}_Z$. Actually much more can be said, as stated in the next proposition, which rephrases in the present setting an analogous result of [De Coster et al. 2023, Proposition 2.3].

Proposition 2.4. *For every $\lambda > -\omega_Z(\mathcal{G})$ and $p > 2$, there exists a constant $C > 0$ depending only on λ and p such that, for all noncompact $\mathcal{G} \in \boldsymbol{G}$,*

$$\inf_{u \in \mathcal{N}_Z} \|u\|_p \geq C > 0.$$

Moreover, if $(u_n)_n \subset \mathcal{N}_Z$ satisfies $\sup_n J(u_n) < \infty$, then $(u_n)_n$ is bounded in $H^1(\mathcal{G})$ and

$$\inf_n \|u_n\|_2 > 0, \quad \inf_n \|u_n\|_\infty > 0.$$

As is well known, there is a natural continuous projection $\pi_\lambda : H^1_Z(\mathcal{G}) \setminus \{0\} \to \mathcal{N}_Z$, defined by

$$\pi_\lambda(u) = n_\lambda(u)u, \quad n_\lambda(u) = \left(\frac{\|u'\|_2^2 + \lambda\|u\|_2^2}{\|u\|_p^p}\right)^{\frac{1}{p-2}}, \tag{2-2}$$

so that $u \in \mathcal{N}_Z$ if and only if $n_\lambda(u) = 1$. If $u \in H^1_Z(\mathcal{G})$ satisfies $u^\pm \neq 0$, then $\pi_\lambda(u^+) + \pi_\lambda(u^-) \in \mathcal{M}_Z$.

Remark 2.5. For every metric graph $\mathcal{G}$ and every set Z of degree-1 vertices, the map

$$t \mapsto \inf_{v \in \mathcal{N}_{t,Z}(\mathcal{G})} J_t(v)$$

is increasing and continuous on $(-\omega_Z(\mathcal{G}), +\infty)$. This property of the action ground state level is actually general and does not depend on the fact that we are considering the problem on graphs. For this reason, we redirect the interested reader, e.g., to [Dovetta et al. 2023, Lemma 2.4] for a detailed proof (in the context of open subsets of $\mathbb{R}^N$).

3. Proof of the abstract results

In this section we prove the abstract results stated in Theorems 1.3–1.4. The strategy for the proof of the existence results is to construct special minimizing sequences for J on $\mathcal{N}_Z$ or $\mathcal{M}_Z$, to avoid problems caused by the noncompactness of the graphs.

Remark 3.1. In this and in the next sections we will freely use the following fact: if $u \not\equiv 0$ solves problem (1-3) and $u \geq 0$ on $\mathcal{G}$, then $u > 0$ on $\mathcal{G}$, except of course at vertices in Z. For the convenience of the reader we sketch a proof (full details can be found in [Adami et al. 2015]). If the claim were false, there would exist an edge e of the graph on which u is not identically zero but on which there exists $x_0 \in \mathcal{G} \setminus Z$ such that $u(x_0) = 0$. If x_0 belongs to the interior of e, u' vanishes at that point, by regularity. Otherwise, x_0 is a vertex $\mathrm{v} \notin Z$, so that the derivatives $u'_e(\mathrm{v})$ are nonnegative for every $e \succ \mathrm{v}$, thus they all vanish by the Kirchhoff condition. By uniqueness in the Cauchy problem, we deduce that u vanishes identically on the edge e, a contradiction.

Remark 3.2. The proof of the next results relies on the following approximation procedure. Given a noncompact graph $\mathcal{G} \in \boldsymbol{G}$, we construct an increasing sequence $(\mathcal{K}_n)_n \subseteq \mathcal{G}$ of connected compact graphs such that $\bigcup_{n\geq 1} \mathcal{K}_n = \mathcal{G}$, and a sequence $(\chi_n)_n \subseteq H^1(\mathcal{G})$ of cut-off functions such that

$$0 \leq \chi_n \leq 1, \quad \|\chi_n'\|_\infty \leq \frac{1}{\ell}, \quad \chi_{n|\mathcal{K}_{n-1}} = 1, \quad \operatorname{supp} \chi_n \subseteq \mathcal{K}_n,$$

with ℓ as in Definition 2.1.

To describe the graphs $\mathcal{K}_n$ we begin by performing a preliminary operation on $\mathcal{G}$ as follows. On each half-line of $\mathcal{G}$ (if any) we insert vertices of degree 2 at the points of coordinates $k\ell$, $k = 1, 2, \dots$. Every half-line can now be viewed as a sequence of consecutive edges (each of length ℓ). With some abuse of notation, we still call $\mathcal{G} = (\mathbb{V}, \mathbb{E})$ the new graph obtained in this way (see Remark 2.2). Let now $\mathrm{v}_0 \in \mathcal{G}$ be a fixed vertex. For every $n \geq 1$, let $\mathbb{V}_n$ be the set of vertices of $\mathbb{V}$ that can be reached from v_0 traveling on at most n edges. As each node of $\mathcal{G}$ has finite degree, the sets $\mathbb{V}_n$ are finite and, since $\mathcal{G}$ is connected, for each vertex $\mathrm{v} \in \mathcal{G}$ (different from v_0) there exists $n_0(\mathrm{v}) \geq 1$ such that v belongs to $\mathbb{V}_n$ for every $n \geq n_0(\mathrm{v})$. Then we define the graph $\mathcal{K}_n$ as $(\mathbb{V}_n, \mathbb{E}_n)$, where $\mathbb{E}_n$ is the set of edges of $\mathbb{E}$ whose vertices belong to $\mathbb{V}_n$. Clearly, each $\mathcal{K}_n$ is connected and compact, and $\bigcup_{n\geq 1} \mathcal{K}_n = \mathcal{G}$. Finally, we define χ_n to be equal to 1 on $\mathcal{K}_{n-1}$, to 0 on $\mathcal{G} \setminus \mathcal{K}_n$ and affine on every edge of $\mathcal{K}_n \setminus \mathcal{K}_{n-1}$. All the required properties trivially hold (the bound on χ_n' follows from the fact that all edges of $\mathcal{G}$ have length at least ℓ).

Finally, given $u \in H^1_Z(\mathcal{G})$, it is straightforward to check that $\chi_n u \to u$ in $H^1(\mathcal{G})$ as $n \to \infty$.

Exploiting Remark 3.2, we now construct suitable minimizing sequences for J on $\mathcal{N}_Z$ and $\mathcal{M}_Z$.

Proposition 3.3. *Let $\mathcal{G} \in \mathbf{G}$ be noncompact and $\lambda > -\omega_Z(\mathcal{G})$. There exists a minimizing sequence $(u_n)_n \subseteq \mathcal{N}_Z$ for J and $u \in H^1_Z(\mathcal{G})$ such that*

$$u_n \rightharpoonup u \quad \text{weakly in } H^1(\mathcal{G}), \qquad u \geq 0, \qquad J'(u) = 0.$$

Proof. Keeping in mind the notation of Remark 3.2, let $(\mathcal{K}_n)_n$ be the sequence of compact graphs approximating $\mathcal{G}$ and let $\partial\mathcal{K}_n = \mathbb{V}_n \setminus \mathbb{V}_{n-1}$. Define the Hilbert space $H_n := H^1_{Z\cup\partial\mathcal{K}_n}(\mathcal{K}_n)$ and the Nehari manifold associated to J on H_n, namely

$$\mathcal{N}_n := \{u \in H_n \mid u \neq 0,\ J'(u)u = 0\}.$$

If $u \in H_n$, it vanishes on $\partial\mathcal{K}_n$ and, after extending it by 0, it can be viewed as a function in $H^1_Z(\mathcal{G})$, that we still denote by u. Therefore, $\mathcal{N}_n \subseteq \mathcal{N}_Z$ for every $n \geq 1$. Let $u_n \in \mathcal{N}_n$ be a ground state for J restricted to H_n, that is,

$$J(u_n) = \inf_{v\in\mathcal{N}_n} J(v).$$

The existence of u_n is standard by the compactness of the embedding of $H^1(\mathcal{K}_n)$ into $L^p(\mathcal{K}_n)$ observing that, by construction, $\omega_{Z\cup\partial\mathcal{K}_n}(\mathcal{K}_n) \geq \omega_Z(\mathcal{G})$. Also, as $u \in \mathcal{N}_n$ if and only if $|u| \in \mathcal{N}_n$ and $J(u) = J(|u|)$, we can assume that $u_n \geq 0$ on $\mathcal{G}$.

We claim that $(u_n)_n$ is a minimizing sequence for J on $\mathcal{N}_Z$. First, since $\mathcal{K}_{n-1} \subset \mathcal{K}_n$ for every n, the sequence $(J(u_n))_n$ is nonincreasing.

Given any $\varepsilon > 0$, let $\bar{u} \in \mathcal{N}_Z$ be such that $J(\bar{u}) \leq \inf_{v\in\mathcal{N}_Z} J(v) + \varepsilon/2$. Let $(\chi_n)_n$ be the sequence of cut-off functions of Remark 3.2. For every n, the function $\tilde{u}_n := \pi_\lambda(\chi_n\bar{u})$ is in $\mathcal{N}_Z$ and $\operatorname{supp}\tilde{u}_n \subseteq \mathcal{K}_n$, which means, in particular, that $\tilde{u}_n$ (restricted to $\mathcal{K}_n$) is in $\mathcal{N}_n$. Moreover, by Remark 3.2 and the continuity of π_λ, as soon as n is large enough we have

$$J(\tilde{u}_n) \leq \inf_{v\in\mathcal{N}_Z} J(v) + \varepsilon.$$

Therefore, for all n large,

$$J(u_n) = \inf_{v\in\mathcal{N}_n} J(v) \leq J(\tilde{u}_n) \leq \inf_{v\in\mathcal{N}_Z} J(v) + \varepsilon.$$

Thus $(u_n)_n$ is a minimizing sequence for J on $\mathcal{N}_Z$, and the claim is proved. Since $(u_n)_n$ is bounded in $H^1_Z(\mathcal{G})$ (like all minimizing sequences), up to a subsequence it converges weakly to some $u \in H^1_Z(\mathcal{G})$ that also satisfies $u \geq 0$. Since u_n minimizes J over $\mathcal{N}_n$, it follows that $J'(u_n)\phi = 0$ for every $\phi \in H_n$. As $u \mapsto J'(u)\phi$ is weakly continuous on $H^1_Z(\mathcal{G})$, letting $n \to \infty$ shows that $J'(u)\phi = 0$ for every $\phi \in H_n$ and every n, and thus, by density, that $J'(u) = 0$. □

Proposition 3.4. *Let $\mathcal{G} \in \mathbf{G}$ be noncompact and $\lambda > -\omega_Z(\mathcal{G})$. There exists a minimizing sequence $(u_n)_n \subseteq \mathcal{M}_Z$ for J and $u \in H^1_Z(\mathcal{G})$ such that*

$$u_n \rightharpoonup u \quad \text{weakly in } H^1(\mathcal{G}) \qquad \text{and} \qquad J'(u) = 0.$$

Proof. The proof is very similar to the one of Proposition 3.3, to which we refer for the notation. Let

$$\mathcal{M}_n := \{v \in H_n \mid v^{\pm} \in \mathcal{N}_n\}$$

and, for each n, let $u_n \in \mathcal{M}_n$ be a nodal ground state for J restricted to H_n, that is,

$$J(u_n) = \inf_{v \in \mathcal{M}_n} J(v).$$

The existence of u_n follows plainly by the compactness of the embedding of $H^1(\mathcal{K}_n)$ into $L^p(\mathcal{K}_n)$ as, for example, in [Szulkin and Weth 2010, Theorem 18] observing again that $\omega_{Z \cup \partial\mathcal{K}_n}(\mathcal{K}_n) \geq \omega_Z(\mathcal{G})$.

We claim that $(u_n)_n$ is a minimizing sequence for J on $\mathcal{M}_Z$. As above, $(J(u_n))_n$ is nonincreasing. If $u \in \mathcal{M}_Z$, we have $(\chi_n u)^{\pm} = \chi_n u^{\pm}$, and both functions are nonzero if n is large enough. By the continuity of π_λ and Remark 3.2, as $n \to \infty$,

$$\pi_\lambda(\chi_n u^+) + \pi_\lambda(\chi_n u^-) \to \pi_\lambda(u^+) + \pi_\lambda(u^-) = u \quad \text{in } H^1_Z(\mathcal{G}).$$

Now, given any $\varepsilon > 0$, let $\bar{u} \in \mathcal{M}_Z$ satisfy $J(\bar{u}) \leq \inf_{\mathcal{M}_Z} J + \varepsilon/2$. Define $\tilde{u}_n := \pi_\lambda(\chi_n \bar{u}^+) + \pi_\lambda(\chi_n \bar{u}^-)$, so $\tilde{u}_n \in \mathcal{M}_Z$, $\operatorname{supp} \tilde{u}_n \subseteq \mathcal{K}_n$, whence $\tilde{u}_n \in \mathcal{M}_n$. Then, for every n large enough,

$$J(u_n) = \inf_{v \in \mathcal{M}_n} J(v) \leq J(\tilde{u}_n) \leq \inf_{v \in \mathcal{M}_Z} J(v) + \varepsilon,$$

showing that $(u_n)_n$ is a minimizing sequence for J on $\mathcal{M}_Z$. Since, by Proposition 2.3, $J'(u_n)\phi = 0$ for every $\phi \in H_n$, we conclude exactly as in the proof of Proposition 3.3. □

We are now in position to prove Theorems 1.3–1.4.

Proof of Theorem 1.3. Let us prove the two statements separately.

Proof of (i). Let $(u_n)_n \subseteq \mathcal{N}_Z$ be the minimizing sequence for J on $\mathcal{N}_Z$ constructed in Proposition 3.3 and let $u \geq 0$ be its weak limit. We first show that $u \not\equiv 0$. Indeed, if this were the case, then $u_n \rightharpoonup 0$ in $H^1_Z(\mathcal{G})$, so that

$$\inf_{v \in \mathcal{N}_Z} J(v) = \liminf_{n \to \infty} J(u_n) \geq J^\infty(\mathcal{G}; Z),$$

which is ruled out by assumption (1-5). Now as $u \not\equiv 0$ and $J'(u) = 0$, u is a nontrivial solution of (1-3). In particular, $u \in \mathcal{N}_Z$ and then, by (2-1) and weak lower semicontinuity,

$$J(u) = \kappa \|u\|_p^p \leq \liminf_{n \to \infty} \kappa \|u_n\|_p^p = \liminf_{n \to \infty} J(u_n) = \inf_{v \in \mathcal{N}_Z} J(v),$$

showing that u is a ground state. As such, u is positive on $\mathcal{G} \setminus Z$ by Remark 3.1. □

Proof of (ii). Consider the minimizing sequence $(u_n)_n$ given by Proposition 3.4 and its weak limit $u \in H^1_Z(\mathcal{G})$ satisfying $J'(u) = 0$. We first show that $u^{\pm} \not\equiv 0$. For every n,

$$J(u_n) = J(u_n^+) + J(u_n^-) \geq J(u_n^+) + \inf_{v \in \mathcal{N}_Z} J(v).$$

If, for instance, $u^+ \equiv 0$, then $u_n^+ \rightharpoonup 0$ in $H^1_Z(\mathcal{G})$, so that

$$\inf_{v \in \mathcal{M}_Z} J(v) = \liminf_{n \to \infty} J(u_n) \geq \liminf_{n \to \infty} J(u_n^+) + \inf_{v \in \mathcal{N}_Z} J(v) \geq J^\infty(\mathcal{G}; Z) + \inf_{v \in \mathcal{N}_Z} J(v),$$

by definition of $J^\infty(\mathcal{G};\,Z)$, which contradicts (1-6). In the same way one proves that $u^- \not\equiv 0$. As $J'(u)=0$, it follows that u is a nonzero sign changing solution of (1-3), and hence $u \in \mathcal{M}_Z$. Then by weak lower semicontinuity, we conclude that

$$J(u) = \kappa\|u\|_p^p \le \kappa \liminf_{n\to\infty} \|u_n\|_p^p = \liminf_{n\to\infty} J(u_n) = \inf_{v\in\mathcal{M}_Z} J(v),$$

namely that u is the required minimizer, i.e., a nodal ground state of (1-3). □

Proof of Theorem 1.4. Let $u \in \mathcal{M}_Z$. Since $u^\pm \in \mathcal{N}_Z$,

$$J(u) = J(u^+) + J(u^-) \ge 2 \inf_{v\in\mathcal{N}_Z} J(v),$$

which is (1-7).

Now assume that $u \in \mathcal{M}_Z$ satisfies

$$J(u) = \inf_{v\in\mathcal{M}_Z} J(v) = 2 \inf_{v\in\mathcal{N}_Z} J(v).$$

Then $J(u^+)=J(u^-)=\inf_{v\in\mathcal{N}_Z} J(v)$, and therefore $u^\pm$ are both ground states of J. As such, by Remark 3.1, they cannot vanish in $\mathcal{G}\setminus Z$, which is a contradiction since $u^\pm \not\equiv 0$. □

4. Graphs with at least one half-line

In this section we discuss ground states and nodal ground states for noncompact graphs with at least one half-line. These graphs may have infinitely many edges. When a finite number of edges is required, it is explicitly mentioned in the statement of the result. Since for such kind of graphs the bottom of the spectrum of $-\mathrm{d}^2/\mathrm{d}x^2$ on $H^1_Z(\mathcal{G})$ always satisfies

$$\omega_Z(\mathcal{G}) = 0,$$

all the results of this section will hold for every $\lambda \in (0, +\infty)$.

The prototype cases in this context are given by the real line and the half-line, about which everything is known (see, e.g., [Cazenave 2003; Le Coz 2009]). Since the ground states on $\mathbb{R}$ play a very important role in what follows, we recall briefly their main features. On the real line the only nontrivial L^2 solutions to (1-1) are called *solitons* and are unique up to translations and sign. Denoting by ϕ_λ the unique positive and even soliton, for every $\lambda > 0$,

$$s_\lambda := J_\lambda(\phi_\lambda) = \inf_{v\in\mathcal{N}_\lambda(\mathbb{R})} J_\lambda(v),$$

namely the solitons are the ground states on $\mathbb{R}$ (see, e.g., [Le Coz 2009, Proposition 3.12]). Similarly, on the half-line (with $Z=\varnothing$) there is a unique nontrivial L^2 solution (up to sign) to (1-1), given by the so-called *half-soliton* ψ_λ, i.e., the restriction of ϕ_λ to $\mathbb{R}^+$. It is the ground state, and

$$J_\lambda(\psi_\lambda) = \inf_{v\in\mathcal{N}_\lambda(\mathbb{R}^+)} J_\lambda(v) = \tfrac{1}{2} s_\lambda. \tag{4-1}$$

If $Z = \{0\}$ (the vertex of the half-line) there are no nontrivial L^2 solutions to (1-1), as any nontrivial solution of $u'' + |u|^{p-2}u = \lambda u$ on $\mathbb{R}^+$ that vanishes at the origin corresponds to a periodic orbit in the phase plane associated to the equation and thus is not in $L^2(\mathbb{R}^+)$.

For a general graph with half-lines, a first marker of the importance of the level s_λ is given by the following straightforward property.

Proposition 4.1. *Let $\mathcal{G} \in \boldsymbol{G}$ contain at least one half-line and $\lambda > 0$. Then*

$$\tfrac{1}{2} s_\lambda \le \inf_{v \in \mathcal{N}_Z} J(v) \le s_\lambda. \tag{4-2}$$

Proof. The inequalities can be easily proved, using rearrangement techniques, arguing exactly as in the proof of [Adami et al. 2015, Theorem 2.2]. □

In the search for ground states, it is crucial to understand whether one can reverse the second inequality in (4-2) (see, e.g., the discussion in [Adami et al. 2015; 2016] in the context of energy ground states of prescribed mass). In [Adami et al. 2015, Theorems 2.3–2.5] the authors individuated a topological condition on $\mathcal{G}$ under which this can actually be done. To state it we recall that $\mathbb{V}_\infty$ denotes the set of *vertices at infinity* of $\mathcal{G}$. Every vertex at infinity is a vertex of the graph $\mathcal{G}$, but is *not* a point of the metric space $\mathcal{G}$. The assumption introduced in [Adami et al. 2015] is:

$$\text{for every } e \in \mathbb{E}, \text{ every connected component of the graph } (\mathbb{V}, \mathbb{E} \setminus \{e\}) \text{ contains at least one vertex } \mathrm{v} \in \mathbb{V}_\infty. \tag{H}$$

In [Adami et al. 2015, Theorem 2.3] the authors proved that, if $\mathcal{G}$ satisfies assumption (H), then for every $u \in H^1(\mathcal{G})$ we have $\#u^{-1}(t) \ge 2$ for almost every $t \in (0, \|u\|_\infty)$. The main consequence of this (originally proved in [Adami et al. 2015, Theorem 2.5] for the problem of prescribed-mass ground states) is described in the following result.

Theorem 4.2 [De Coster et al. 2023, Theorem 2.6]. *If $\mathcal{G} \in \boldsymbol{G}$ satisfies assumption* (H) *and* $\lambda > 0$, *then*

$$\inf_{v \in \mathcal{N}} J(v) = s_\lambda$$

and it is never achieved, *unless $\mathcal{G}$ is isometric to $\mathbb{R}$ or to a "tower of bubbles" shown in Figure 2.*

In this paper the setting is different from that of [Adami et al. 2015; De Coster et al. 2023] for at least two reasons: first, the boundary conditions are more general and the presence of the set Z must be taken into account; second, we are also interested in nodal ground states. For these reasons it is convenient to reformulate and generalize assumption (H) in a form that is more suited to handle the questions under study. As in the Introduction, consider the set

$$F(\mathcal{G}) = \{e \in \mathbb{E} \mid \text{at least one connected component of } (\mathbb{V}, \mathbb{E} \setminus \{e\}) \text{ has no vertices in } \mathbb{V}_\infty \cup Z\}$$

and the assumptions

$$\#F(\mathcal{G}) = 0, \tag{H0}$$

$$\#F(\mathcal{G}) \le 1. \tag{H1}$$

Note that (H0) and (H1) are, respectively, the assumptions in (i) and (ii) in Theorem 1.6. From now on, with some abuse of notation, we denote the graph $(\mathbb{V}, \mathbb{E} \setminus \{e\})$ simply by $\mathcal{G} \setminus e$.

To investigate the relations between assumptions (H0) and (H), it is convenient to define a new graph $\widetilde{\mathcal{G}}$ in the following way. If $Z = \varnothing$, we set $\widetilde{\mathcal{G}} = \mathcal{G}$. Otherwise, we replace every (finite) edge e ending at a vertex of Z by a half-line, still called e. We obtain in this way a new graph $\widetilde{\mathcal{G}} = (\widetilde{\mathbb{V}}, \widetilde{\mathbb{E}})$ that has the same number of vertices and edges as $\mathcal{G}$. The only difference is that edges of $\mathcal{G}$ terminating at vertices of Z are replaced, in $\widetilde{\mathcal{G}}$, by half-lines terminating at vertices in $\widetilde{\mathbb{V}}_\infty$.

Then it is easily seen that

$$\mathcal{G} \text{ satisfies (H0)} \iff \widetilde{\mathcal{G}} \text{ satisfies (H)}. \tag{4-3}$$

Indeed, to say that $\mathcal{G}$ satisfies (H0) means that there are no edges in $\mathbb{E}$ whose removal generates a connected component without vertices in $\mathbb{V}_\infty \cup Z$, namely that for every $e \in \mathbb{E}$, every connected component of $\mathcal{G} \setminus e$ has a vertex in $\mathbb{V}_\infty \cup Z$. But this, read on $\widetilde{\mathcal{G}}$, means that every connected component of $\widetilde{\mathcal{G}} \setminus e$ has a vertex in $\widetilde{\mathbb{V}}_\infty$, which is (H) for $\widetilde{\mathcal{G}}$.

Furthermore, to say that $\#F(\mathcal{G}) = 1$, namely that $F(\mathcal{G}) = \{e\}$ for exactly one edge e, means that the graph $\mathcal{G} \setminus e$ decomposes as

$$\mathcal{G} \setminus e = \mathcal{G}_K \cup \mathcal{G}', \tag{4-4}$$

where $\mathcal{G}_K$ is connected and has no vertices in $\mathbb{V}_\infty \cup Z$, while $\mathcal{G}'$ is connected and contains *all* the vertices of $\mathbb{V}_\infty \cup Z$. Also, there are no edges other than e that permit a decomposition like (4-4). As $\mathcal{G}$ has at least one half-line, the unique $e \in F(\mathcal{G})$ can never have a vertex in Z. However, e can be a half-line. In this case, though, $\mathcal{G} \setminus e = \mathcal{G}_K \cup \{\mathrm{v}_\infty\}$, where v_∞ is the vertex at infinity of the half-line e. Thus in this case the graph $\mathcal{G}$ is made of a set of bounded edges without vertices in Z and a *single* half-line attached to it.

The next result plays a key role in the proof of some of the subsequent results. Roughly, it states that any graph satisfying $\#F(\mathcal{G}) = 1$ can be turned into a graph satisfying (H0) by attaching to it a suitable half-line.

Lemma 4.3. *Let $\mathcal{G} \in \mathbf{G}$ be a graph with at least one half-line satisfying $\#F(\mathcal{G}) = 1$. Let e be such that $F(\mathcal{G}) = \{e\}$ and $\mathcal{G}_K$ be the connected component of $\mathcal{G} \setminus e$ as in* (4-4). *Choose a vertex v in $\mathcal{G}_K$ and define a new graph $\widetilde{\mathcal{G}}_\mathrm{v}$ by*[1] *$\widetilde{\mathcal{G}}_\mathrm{v} = \mathcal{G} \cup h$, where h is a half-line attached at v. Then $\widetilde{\mathcal{G}}_\mathrm{v}$ satisfies* (H0).

Proof. Let v_∞ be the vertex at infinity of h and assume by contradiction that $\#F(\widetilde{\mathcal{G}}_\mathrm{v}) \geq 1$, namely that there exists $\tilde{e} \in F(\widetilde{\mathcal{G}}_\mathrm{v})$. We claim that $\tilde{e} \neq h$. Indeed, removing h from $\widetilde{\mathcal{G}}_\mathrm{v}$ would leave v_∞ isolated, splitting $\widetilde{\mathcal{G}}_\mathrm{v} \setminus h$ into the two connected components $\mathcal{G}$ and $\{\mathrm{v}_\infty\}$. Since both of them contain vertices in $\widetilde{\mathbb{V}}_\infty$, this violates the definition of $\tilde{e}$. Similarly, it cannot be $\tilde{e} = e$: removing e from $\widetilde{\mathcal{G}}_\mathrm{v}$, and recalling that h is attached to $\mathcal{G}_K$, would decompose $\widetilde{\mathcal{G}}_\mathrm{v}$ into connected components as $(\mathcal{G}_K \cup h) \cup \mathcal{G}'$, violating again the definition of $\tilde{e}$ as before. We are left with the case where $\tilde{e}$ is different from both h and e. In this case we have the decomposition

$$\widetilde{\mathcal{G}}_\mathrm{v} \setminus \tilde{e} =: \widetilde{\mathcal{G}}_K \cup \widetilde{\mathcal{G}}',$$

[1] Shorthand for $(\mathbb{V} \cup \{\mathrm{v}_\infty\}, \mathbb{E} \cup \{h\})$, where v_∞ is the vertex at infinity of h.

with obvious meaning of the symbols. By construction, the half-line h is attached to $\widetilde{\mathcal{G}}'$. Removing h *and* v_∞ from $\widetilde{\mathcal{G}}'$ does not disconnect it and, since $\widetilde{\mathcal{G}}'$ contains at least another vertex in $\mathbb{V}_\infty \cup Z$, we see that $\widetilde{\mathcal{G}}' \setminus (\{\mathrm{v}_\infty\}, \{h\})$ is not empty. Therefore $\widetilde{\mathcal{G}}_K$ and $\widetilde{\mathcal{G}}' \setminus (\{\mathrm{v}_\infty\}, \{h\})$ are both nonempty, connected, disjoint and their union is $\mathcal{G} \setminus \tilde{e}$, namely $\tilde{e} \in F(\mathcal{G})$. Since we also have $e \in F(\mathcal{G})$, this shows that $\#F(\mathcal{G}) \geq 2$, violating the assumption. □

We can now prove that the assumptions (H0) and (H1) are sufficient to rule out the existence of ground states and nodal ground states respectively, as stated in Theorem 1.6.

Proof of Theorem 1.6. We split the proof into two parts.

Part 1: *proof of* (1-8) *and* (1-10). Of course it is sufficient to work with nonnegative functions, which we do without further warnings. Since $\mathcal{G}$ contains at least one half-line, Proposition 4.1 guarantees that $\inf_{v \in \mathcal{N}_Z} J(v) \leq s_\lambda$. To prove the reverse inequality under assumption (H0), let $\widetilde{\mathcal{G}}$ be the graph defined after the statement of assumptions (H0)–(H1).

Since, as metric spaces, $\mathcal{G} \subseteq \widetilde{\mathcal{G}}$, every function $u \in H^1_Z(\mathcal{G})$ extended by 0 on $\widetilde{\mathcal{G}} \setminus \mathcal{G}$ can be seen as a function $\tilde{u} \in H^1(\widetilde{\mathcal{G}})$. Plainly,

$$\|\tilde{u}\|_{L^q(\widetilde{\mathcal{G}})} = \|u\|_{L^q(\mathcal{G})} \quad \text{for every } q \in [1, +\infty], \qquad \|\tilde{u}'\|_{L^2(\widetilde{\mathcal{G}})} = \|u'\|_{L^2(\mathcal{G})}.$$

This implies that $\tilde{u} \in \mathcal{N}(\widetilde{\mathcal{G}})$ and since $\widetilde{\mathcal{G}}$ satisfies (H) (because $\mathcal{G}$ satisfies (H0); see (4-3)),

$$J(u) = \kappa \|u\|^p_{L^p(\mathcal{G})} = \kappa \|\tilde{u}\|^p_{L^p(\widetilde{\mathcal{G}})} = J(\tilde{u}) \geq \inf_{v \in \mathcal{N}(\widetilde{\mathcal{G}})} J(v) = s_\lambda$$

by Theorem 4.2. As this holds for every (nonnegative) $u \in \mathcal{N}_Z$, (1-10) is proved.

Assume now that for some nonnegative $u \in \mathcal{N}_Z$ we have $J(u) = s_\lambda$. Considering, as above, the function $\tilde{u} \in \mathcal{N}(\widetilde{\mathcal{G}})$, we see that $J(\tilde{u}) = J(u) = s_\lambda$, namely that $\tilde{u}$ is a ground state for J on $\mathcal{N}(\widetilde{\mathcal{G}})$. As such, $\tilde{u}(x) > 0$ for every $x \in \widetilde{\mathcal{G}}$, which shows that $Z = \varnothing$, namely that $\widetilde{\mathcal{G}} = \mathcal{G}$. We then conclude by Theorem 4.2.

Part 2: *proof of* (1-9) *and* (1-11). We first prove (1-9). By density, for every $\varepsilon > 0$ there exists a nonnegative $u_1 \in \mathcal{N}_Z(\mathcal{G})$ with compact support such that

$$J(u_1) \leq \inf_{v \in \mathcal{N}_Z(\mathcal{G})} J(v) + \varepsilon.$$

Similarly, there exists a nonnegative $u_2 \in \mathcal{N}(\mathbb{R})$ with compact support such that $J(u_2) \leq s_\lambda + \varepsilon$. By taking a translation of u_2 (if necessary), we can make sure that its support, identified with an interval on some half-line of $\mathcal{G}$, does not intersect the support of u_1. We then define $w \in H^1(\mathcal{G})$ by

$$w(x) = \begin{cases} u_1(x) & \text{if } x \in \mathcal{G} \setminus \operatorname{supp}(u_2), \\ -u_2(x) & \text{if } x \in \operatorname{supp}(u_2). \end{cases}$$

Obviously, $w \in \mathcal{M}_Z$ and

$$J(w) = J(u_1) + J(u_2) \leq s_\lambda + \inf_{v \in \mathcal{N}_Z} J(v) + 2\varepsilon.$$

Since ε is arbitrary, we conclude.

We now prove the reverse inequality in (1-11) under assumption (H1). If $\#F(\mathcal{G})=0$, then $\mathcal{G}$ satisfies (H0) and Theorem 1.6(i) shows that $\inf_{v\in\mathcal{N}_Z} J(v)=s_\lambda$, so that the inequality to be proved is $\inf_{v\in\mathcal{M}_Z} J(v)\geq 2s_\lambda$. Given any $u\in\mathcal{M}_Z$, applying Theorem 1.6(i) to u^+ and u^- immediately yields

$$J(u)=J(u^+)+J(u^-)>2s_\lambda,$$

the inequality being strict since both u^+ and u^- vanish somewhere on $\mathcal{G}$. This ensures that nodal ground states do not exist in this case.

Suppose now that $\#F(\mathcal{G})=1$. Let e be the unique element of $F(\mathcal{G})$ and consider the decomposition (4-4):

$$\mathcal{G}\setminus e=\mathcal{G}_K\cup\mathcal{G}'.$$

Given a vertex v of $\mathcal{G}_K$, for every $u\in\mathcal{M}_Z$, at least one among u^+ and u^-, say u^+, vanishes at v. Let $\widetilde{\mathcal{G}}_{\mathrm{v}}$ be the graph constructed in Lemma 4.3, obtained by attaching to v a half-line h. Since u^+ vanishes at v, it can be extended to a function $\tilde{u}^+$ simply by defining it to be 0 on h. Clearly, $\tilde{u}^+\in\mathcal{N}_Z(\widetilde{\mathcal{G}}_{\mathrm{v}})$ and, since $\widetilde{\mathcal{G}}_{\mathrm{v}}$ satisfies (H0) by Lemma 4.3, we obtain $J(\tilde{u}^+)\geq s_\lambda$. Then

$$J(u)=J(u^+)+J(u^-)=J(\tilde{u}^+)+J(u^-)\geq s_\lambda+\inf_{v\in\mathcal{N}_Z} J(v),$$

concluding the proof of (1-11).

It remains to show that the infimum is not achieved when $\#F(\mathcal{G})=1$. To this end, it suffices to observe that the inequality used above, $J(\tilde{u}^+)\geq s_\lambda$, is in fact strict. Indeed if $J(\tilde{u}^+)=s_\lambda=\inf_{v\in\mathcal{N}(\widetilde{\mathcal{G}})} J(v)$, then $\tilde{u}^+$ is a ground state on $\widetilde{\mathcal{G}}$, and hence it cannot vanish anywhere, contrary to the fact that $\tilde{u}^+\equiv 0$ on h. □

Remark 4.4. The assumptions of Theorem 1.6 are sharp. Indeed, Theorem 4.8 below shows that there exist graphs $\mathcal{G}$ satisfying $\#F(\mathcal{G})\geq 1$ that admit ground states, while in Theorem 4.16 and Remark 4.18 we exhibit graphs $\mathcal{G}$ satisfying $\#F(\mathcal{G})\geq 2$ that admit nodal ground states.

Theorem 1.6 shows that nonexistence of ground states or nodal ground states can be determined by purely topological properties of the graph. The situation for existence is, on the contrary, more involved.

In some cases, existence results for ground states based solely on the topology of the graph can be easily obtained when $Z=\varnothing$, as, for example, if $\mathcal{G}$ has a finite number of edges. In this respect, there is not much to say since the techniques developed in [Adami et al. 2016, Section 3] for the problem of prescribed-mass minimizers of the energy work in the present setting as well, as we now briefly show.

For the reader's convenience, let us first recall with the next lemma a standard relation between the action of a function and the number of preimages of each value it attains. These properties are stated in [De Coster et al. 2023, Propositions 2.2 and 2.8] and are consequences of standard rearrangement techniques on graphs. For this reason, we omit the proof of the lemma.

Lemma 4.5. *Let $\mathcal{G}$ be a noncompact metric graph. Given $\lambda>0$ and an integer $K\geq 1$, let $u\in\mathcal{N}_{\lambda,Z}$ satisfy $u\geq 0$ on $\mathcal{G}$ and $\#u^{-1}(t)\geq K$ for almost every $t\in(0,\max_{\mathcal{G}} u)$. Then $J_\lambda(u)\geq K\frac{1}{2}s_\lambda$. Furthermore, if equality holds then*

- *$\#u^{-1}(t)=K$ for almost every $t\in(0,\max_{\mathcal{G}} u)$;*
- *the support of u has infinite measure;*
- *$u^{-1}(t)$ has zero measure for all $t\in(0,\max_{\mathcal{G}} u)$.*

Since we use Theorem 1.3 in what follows, we prove the following characterization of $J^\infty(\mathcal{G}; Z)$.

Proposition 4.6. *Let $\mathcal{G} \in \mathbf{G}$ be a noncompact graph with a finite number of edges and $\lambda > 0$. Then*

$$J_\lambda^\infty(\mathcal{G}; Z) = s_\lambda. \tag{4-5}$$

Proof. By density, for every $\varepsilon > 0$ there exists $u = u_\varepsilon \in \mathcal{N}(\mathbb{R})$ with compact support such that $J(u) \le s_\lambda + \varepsilon$. For every n large enough, the function $u_n(x) = u(x-n)$ is supported in $\mathbb{R}^+$ and, as such, it can be seen as an element of $\mathcal{N}_Z$ by placing its support on a half-line of $\mathcal{G}$ and then extending it by 0 outside its support. Clearly $u_n \rightharpoonup 0$ in $H^1(\mathcal{G})$ and

$$\liminf_n J(u_n) \le s_\lambda + \varepsilon.$$

Since ε is arbitrary, the "$\le$" part is proved. For the reverse inequality, let $(u_n)_n \subset \mathcal{N}_Z$ be a sequence converging weakly to 0 in $H^1(\mathcal{G})$ with $J_\lambda(u_n) \to J_\lambda^\infty(\mathcal{G}; Z)$. We can assume $u_n \ge 0$ for every n since otherwise we replace it by $|u_n|$ that is still in $\mathcal{N}_Z$. By weak convergence, we also see that $u_n \to 0$ in $L^\infty_{\mathrm{loc}}(\mathcal{G})$. Hence, if ε_n denotes the maximum of u_n on the set of all bounded edges of $\mathcal{G}$, clearly $\varepsilon_n \to 0$. Therefore, letting $v_n := (u_n - \varepsilon_n)^+$, we see from Proposition 2.4 that $v_n \not\equiv 0$ for every n large enough. Since $\mathcal{G}$ contains at least one half-line, by construction $\# v_n^{-1}(t) \ge 2$ for every $t \in (0, \max v_n)$ and every n, since v_n vanishes on the set of all bounded edges, and the same holds for $\pi_\lambda(v_n)$. So $J(\pi_\lambda(v_n)) \ge s_\lambda$ by Lemma 4.5. Furthermore, as $n \to \infty$,

$$n_\lambda(v_n)^{p-2} = \frac{\|v_n'\|_2^2 + \lambda \|v_n\|_2^2}{\|v_n\|_p^p} \le \frac{\|u_n'\|_2^2 + \lambda \|u_n\|_2^2}{\|u_n\|_p^p + o(1)} = 1 + o(1), \tag{4-6}$$

entailing

$$s_\lambda \le J(\pi_\lambda(v_n)) = J\big(n_\lambda(v_n) v_n\big) = \kappa n_\lambda(v_n)^p \|v_n\|_p^p \le \kappa(1+o(1))\|u_n\|_p^p = J(u_n) + o(1),$$

from which we obtain $\liminf_n J(u_n) \ge s_\lambda$. Since this holds for every sequence converging weakly to 0, the proof is complete. □

Remark 4.7. The assumption that the graph has a finite number of edges in Proposition 4.6 cannot be removed. This can be seen considering, for instance, the following example. On a real line we insert, for each integer $k \ge 1$, a node v_k at the point of coordinate k and a terminal edge L_k of length k, by identifying v_k with an endpoint of L_k (Figure 5). By density, for every $\varepsilon > 0$ there exist $k \ge 1$ and $u_k \in \mathcal{N}(\mathbb{R}^+)$ with compact support in $[0, k]$ such that $J(u_k) \le \frac{1}{2} s_\lambda + \varepsilon$. Since u_k can be considered as a function on the edge L_k, we obtain a sequence $(u_k)_k \in \mathcal{N}(\mathcal{G})$ that converges weakly to 0 and such that $\liminf_k J_\lambda(u_k) \le \frac{1}{2} s_\lambda + \varepsilon$. This proves that $J_\lambda^\infty(\mathcal{G}) \le \frac{1}{2} s_\lambda$. By Proposition 4.1, we obtain in fact $J_\lambda^\infty(\mathcal{G}) = \frac{1}{2} s_\lambda$.

Having established (4-5), Theorem 1.3 yields existence of a ground state on a noncompact graph with a finite number of edges as soon as one can prove that $\inf_{v \in \mathcal{N}_Z} J(v) < s_\lambda$. This condition is analogous to the one appearing in the fixed mass case. As we anticipated above, such an inequality can be shown to hold for a number of graphs with $Z = \varnothing$ exploiting only topological properties, by the use of the "graph surgery" techniques developed in [Adami et al. 2016, Section 3].

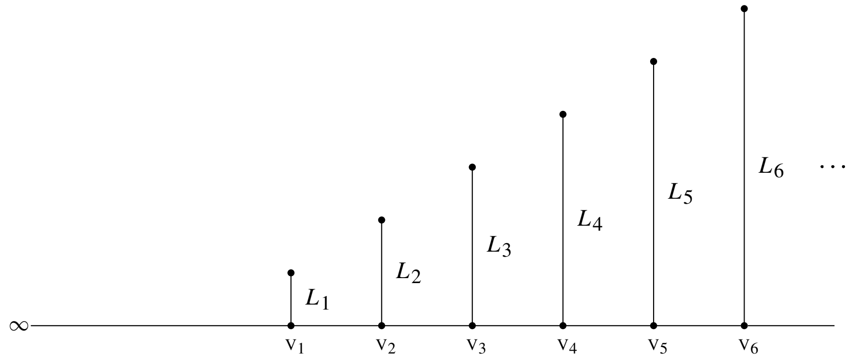


Figure 5. The graph $\mathcal{G}$ described in Remark 4.7.

Theorem 4.8. *For every $\lambda > 0$, every graph $\mathcal{G}$ depicted in Figure 6, for every length of its edges, satisfies*

$$\inf_{v\in\mathcal{N}} J(v) < s_\lambda$$

and therefore admits a ground state.

Proof. The inequality can be proved starting with a soliton on $\mathbb{R}$, via rearrangement techniques, exactly as in the final part of Section 3 in [Adami et al. 2016]. The basic idea is that, on each of these graphs, one can construct explicit functions built from pieces of the positive even soliton ϕ_λ on $\mathbb{R}$ and pieces of its monotone rearrangement on $\mathbb{R}^+$, then projected on the Nehari manifold. For instance, on the tadpole such a function coincides on the loop of the graph (of total length L) with the restriction of the soliton to the interval $[-L/2, L/2]$, and on the half-line with the monotone rearrangement on $\mathbb{R}^+$ of the restriction of the soliton to $\mathbb{R}\setminus[-L/2, L/2]$. The construction on the other graphs in Figure 6 is analogous. Since rearrangements always lower the normalizing factor n_λ defined in (2-2), it is then easy to check that these functions realize action levels strictly smaller than that of the soliton s_λ. Existence of a ground state follows then from Theorem 1.3. □

When Z is not empty, the existence of a ground state is harder to obtain and further conditions of metrical nature have to be imposed. Indeed, the next theorem shows that, if a graph hosts a ground state,

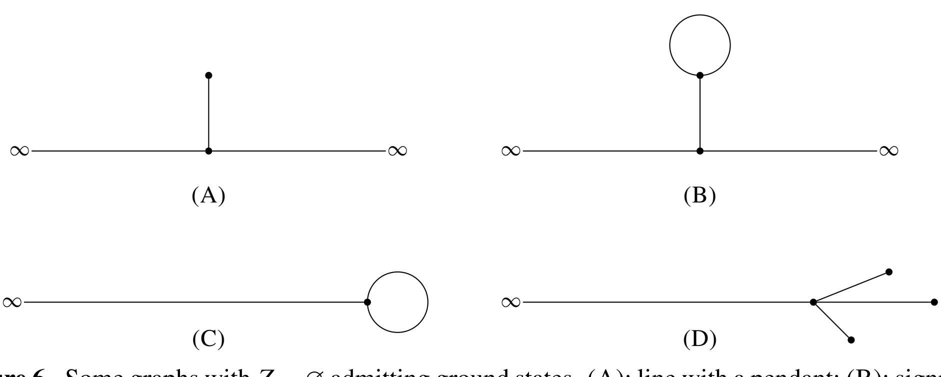


Figure 6. Some graphs with $Z = \varnothing$ admitting ground states. (A): line with a pendant; (B): signpost; (C): tadpole; (D): 3-fork.

the diameter of the set $\mathcal{B}$ of all bounded edges cannot be arbitrarily small. Recall that diam($\mathcal{B}$) is given by the supremum of lengths of the shortest paths between any two points of $\mathcal{B}$.

Theorem 4.9. *There exists a constant $C > 0$ depending only on $\lambda > 0$ and p such that, for every $\mathcal{G} \in \mathbf{G}$ with at least one half-line and every $Z \neq \varnothing$ such that $\inf_{v \in \mathcal{N}_Z} J(v)$ is achieved, we have*

$$\operatorname{diam}(\mathcal{B}) \geq C,$$

where, as above, $\mathcal{B}$ is the set of all bounded edges of $\mathcal{G}$.

Proof. Let $u \in \mathcal{N}_Z$ satisfy $J(u) = \inf_{v \in \mathcal{N}_Z} J(v)$. As usual we can assume that $u \geq 0$. Let us show that u attains its L^∞-norm in $\mathcal{B}$. Suppose by contradiction that u instead attains its maximum at a point y on a half-line h. Then $\#u^{-1}(t) \geq 2$ for every $0 < t < \max u$. Indeed, t is attained at least once on h and once on a path γ joining y to a point in Z. Thus Lemma 4.5 and Proposition 4.1 imply that $J(u) \geq s_\lambda = \inf_{v \in \mathcal{N}_Z} J(v)$. Let us show that the inequality must be strict, which gives the desired contradiction. If this were not the case, Lemma 4.5 would imply that $\#u^{-1}(t) = 2$ for almost every $t \in (0, \max u)$. Since u already has two preimages on $h \cup \gamma$, this means that u must be constant on $\mathcal{G} \setminus (h \cup \gamma)$. This contradicts the last assertion of Lemma 4.5 unless $\mathcal{G} = h \cup \gamma$, that is $\mathcal{G}$ is a half-line and homogeneous Dirichlet conditions are imposed at its origin. But this is impossible, because, as we already recalled, on the half-line with zero Dirichlet boundary conditions there is no nonzero solution.

Let then $\bar{x} \in \mathcal{B}$ be such that $\|u\|_\infty = u(\bar{x})$. By the Cauchy–Schwarz inequality, (2-1) and Proposition 4.1, letting z be any vertex in Z, we have

$$\|u\|_\infty = |u(\bar{x})| = |u(\bar{x}) - u(z)| \leq \sqrt{\operatorname{diam}(\mathcal{B})}\,\|u'\|_{L^2(\mathcal{G})} \leq \sqrt{\operatorname{diam}(\mathcal{B})}\sqrt{\frac{s_\lambda}{\kappa}}$$

which, coupled with Proposition 2.4, yields

$$C \leq \|u\|_p^p \leq \|u\|_\infty^{p-2}\|u\|_2^2 \leq \frac{1}{\lambda}\operatorname{diam}(\mathcal{B})^{\frac{p}{2}-1}\left(\frac{s_\lambda}{\kappa}\right)^{\frac{p}{2}}$$

for a suitable constant $C > 0$ depending on λ and p only. □

Remark 4.10. Comparing Theorems 4.8 and 4.9 highlights the effect of the set Z on the existence of ground states. One may wonder whether Theorem 4.9 can be improved to obtain a universal lower bound involving only the total length of the edges with a vertex in Z, rather than the whole set $\mathcal{B}$. However, this cannot be done in general: it is easy to exhibit graphs where ground states do exist and the length of the edges with vertices in Z is arbitrarily small. To see this, let $\mathcal{G}$ be any given graph with $Z = \varnothing$ and such that $\inf_{v \in \mathcal{N}(\mathcal{G})} J(v) < s_\lambda$ (e.g., any of the graphs in Figure 6). Exploiting, for instance, the approximation procedure described in Remark 3.2, one can construct a function $u \in \mathcal{N}(\mathcal{G})$ so that $J(u) < s_\lambda$ and the support of u is contained in a suitable neighborhood of $\mathcal{B}$. In particular, there exists $M > 0$ such that the restriction of u to each half-line of $\mathcal{G}$ satisfies $u \equiv 0$ on $[M, +\infty)$. For every $\ell > 0$, let then $\mathcal{G}_\ell$ be the graph obtained by attaching a single edge of length ℓ at the point $x = M$ of one of the half-lines of $\mathcal{G}$, and assume that the vertex of degree 1 of this edge is the only vertex in Z. Clearly, one can think of u as a function in $\mathcal{N}_Z(\mathcal{G}_\ell)$ for every ℓ, so that $\inf_{v\in\mathcal{N}_Z(\mathcal{G}_\ell)} J(v) \le J(u) < s_\lambda$, thus implying existence of ground states in $\mathcal{N}_Z(\mathcal{G}_\ell)$ by Theorem 1.3 and Proposition 4.6.

In the case of nodal ground states, it is not even needed to have $Z \neq \varnothing$ to recover the analogue of Theorem 4.9.

Theorem 4.11. *There exists a constant $C > 0$ depending only on $\lambda > 0$ and p such that, for every $\mathcal{G} \in \boldsymbol{G}$ with at least one half-line and every Z such that $\inf_{v\in\mathcal{M}_Z} J(v)$ is achieved, we have*

$$\operatorname{diam}(\mathcal{B}) \ge C,$$

where, as above, $\mathcal{B}$ is the set of all bounded edges of $\mathcal{G}$.

Proof. Let u be a nodal ground state. Observe that if u^+ attains its L^∞-norm on a half-line, as in Theorem 4.9, we prove that $J_\lambda(u^+) > s_\lambda$. Hence $J_\lambda(u) = J_\lambda(u^+) + J_\lambda(u^-) > s_\lambda + \inf_{v\in\mathcal{N}_Z(\mathcal{G})} J_\lambda(v)$ which contradicts (1-9). The same is valid for u^-. Hence both u^+ and u^- attain their L^∞-norm on $\mathcal{B}$ only. Thus u changes sign in $\mathcal{B}$ and as such, has a zero in $\mathcal{B}$. We then conclude as in Theorem 4.9 working on u^+. □

In view of Theorems 1.6, 4.9 and 4.11, it is clear that a suitable combination of topological and metrical features is needed to guarantee existence of ground states with $Z \neq \varnothing$ and nodal ground states. Towards this direction, we conclude the discussion of this section with two general procedures to construct graphs where ground states and nodal ground states do exist. The first one is genuinely of metrical nature, in that it is completely independent of the topology of the graph. The second one mixes topological and metrical properties.

In the next statement, by *pendant* we mean a finite-length terminal edge whose vertex of degree 1 is not in Z.

Theorem 4.12. *There exists a constant $C > 0$ depending only on $\lambda > 0$ and p such that, for every noncompact graph $\mathcal{G} \in \boldsymbol{G}$ with a finite number of edges,*

(i) *if $\mathcal{G}$ has a pendant of length $a \ge C$, then $\inf_{v\in\mathcal{N}_Z} J(v)$ is achieved*;

(ii) *if $\mathcal{G}$ has two pendants of lengths $a_1, a_2 \ge C$, then $\inf_{v\in\mathcal{M}_Z} J(v)$ is achieved.*

Remark 4.13. The assumption that $\mathcal{G}$ has a finite number of edges cannot be removed. This can be easily seen as follows. For point (1) it is enough to consider the graph $\mathcal{G}$ in Remark 4.7, for which $\inf_{v\in\mathcal{N}_\lambda(\mathcal{G})} J(v) = \frac{1}{2}s_\lambda$. Therefore, if u were a (positive) ground state, by Lemma 4.5, almost every $t \in (0, \max u)$ would be attained only once on $\mathcal{G}$, which is incompatible with the presence of vertices of degree 3. For point (2) one can simply consider any periodic graph, since such graphs admit no nodal ground state by Theorem 1.7.

Remark 4.14. In Theorem 4.12, C is the same for ground states and for nodal ground states and depends on the presence of the pendants but not on the rest of the graph. This will be of great help in Section 6.

Proof of Theorem 4.12. Let $\psi_\lambda \in H^1(\mathbb{R}^+)$ be the positive half-soliton satisfying, by (4-1), $J(\psi_\lambda) = \frac{1}{2}s_\lambda$. By density, there exists a function $u_1 \in \mathcal{N}(\mathbb{R}^+)$ supported in some interval $[0, C]$ such that

$$J(u_1) < \tfrac{3}{4}s_\lambda$$

(for example, one may take $(\psi_\lambda - \delta)^+$ with δ small and then project it on $\mathcal{N}_\lambda(\mathbb{R}^+)$).

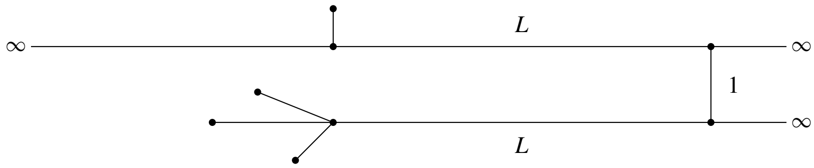


Figure 7. Example of a graph $\mathcal{G}_L$ as in Theorem 4.16, constructed starting with two graphs in Figure 6. If the vertical edge on the right is sufficiently far from the pendants of the graph, nodal ground states exist.

(1) Let $\mathcal{G}_a$ be a graph with at least one pendant of length a. If a is larger than C, we may consider $[0, C]$ as contained in the pendant, identifying $x = 0$ with its vertex of degree 1. Extending u_1 by 0 on the remaining part of $\mathcal{G}_a$, we obtain a function $\tilde{u}_1 \in \mathcal{N}_Z(\mathcal{G}_a)$ such that

$$J(\tilde{u}_1) = J(u_1) < \tfrac{3}{4}s_\lambda.$$

The existence of a ground state follows from Proposition 4.6 and Theorem 1.3.

(2) We denote by $\mathcal{G}_{a_1,a_2}$ a graph with two pendants e_1, e_2 of lengths a_1, a_2 and we show that if $a_1 \geq C$ and $a_2 \geq C$, then

$$\inf_{v\in\mathcal{M}_Z(\mathcal{G}_{a_1,a_2})} J(v) < J^\infty(\mathcal{G}_{a_1,a_2}; Z) + \inf_{v\in\mathcal{N}_Z(\mathcal{G}_{a_1,a_2})} J(v), \tag{4-7}$$

which, via Theorem 1.3, establishes the existence of a nodal ground state. By Propositions 4.1–4.6, for every a_1, a_2,

$$J^\infty(\mathcal{G}_{a_1,a_2}; Z) = s_\lambda, \qquad \inf_{v\in\mathcal{N}_Z(\mathcal{G}_{a_1,a_2})} J(v) \geq \tfrac{1}{2}s_\lambda,$$

so that

$$J^\infty(\mathcal{G}_{a_1,a_2}; Z) + \inf_{v\in\mathcal{N}_Z(\mathcal{G}_{a_1,a_2})} J(v) \geq \tfrac{3}{2}s_\lambda.$$

Now, using the same u_1 as in (1), we define

$$\tilde{u}_1(x) = \begin{cases} u_1(x) & \text{if } x \in [0, a_1] \subset e_1, \\ -u_1(x) & \text{if } x \in [0, a_2] \subset e_2, \\ 0 & \text{elsewhere on } \mathcal{G}_{a_1,a_2}. \end{cases}$$

Clearly $\tilde{u}_1 \in \mathcal{M}_Z(\mathcal{G}_{a_1,a_2})$ and

$$J(\tilde{u}_1) = 2J(u_1) < \tfrac{3}{2}s_\lambda.$$

This proves (4-7). □

We now discuss the second procedure to find nodal ground states. The idea is to take two graphs admitting ground states and connect them by the addition of a faraway edge. So, let $\mathcal{G}^1$, $\mathcal{G}^2$ be any two noncompact graphs with a finite number of edges for which $\inf_{v\in\mathcal{N}_{Z^i}(\mathcal{G}^i)} J(v) < s_\lambda$. Given $L > 0$, we glue together $\mathcal{G}^1$ and $\mathcal{G}^2$ by taking a new edge of length 1, attaching its first endpoint to the point $x = L$ on a half-line h^1 of $\mathcal{G}^1$ and its second endpoint to the point $x = L$ on a half-line h^2 of $\mathcal{G}^2$. We call $\mathcal{G}_L$ the resulting graph (see Figure 7) and we let the set Z_L of vertices of degree 1 in $\mathcal{G}_L$ with homogeneous Dirichlet conditions be given by the union of the corresponding sets of vertices in $\mathcal{G}^1$ and $\mathcal{G}^2$.

Lemma 4.15. *Let $\lambda > 0$ and $\mathcal{G}^1$, $\mathcal{G}^2$, $\mathcal{G}_L$ be the graphs described above. Then*

$$\lim_{L\to\infty} \inf_{v\in\mathcal{N}_{Z_L}(\mathcal{G}_L)} J(v) = \min\Big(\inf_{v\in\mathcal{N}_{Z^1}(\mathcal{G}^1)} J(v), \inf_{v\in\mathcal{N}_{Z^2}(\mathcal{G}^2)} J(v)\Big).$$

Proof. Without loss of generality, assume that

$$c_1 := \inf_{v\in\mathcal{N}_{Z^1}(\mathcal{G}^1)} J(v) \le \inf_{v\in\mathcal{N}_{Z^2}(\mathcal{G}^2)} J(v) =: c_2. \tag{4-8}$$

For every $\varepsilon > 0$ there exists a function $u_\varepsilon \in \mathcal{N}_{Z^1}(\mathcal{G}^1)$ with compact support such that $J(u_\varepsilon) \le c_1 + \varepsilon$. For every L large enough, we can view u_ε as a function in $\mathcal{N}_{Z_L}(\mathcal{G}_L)$, after extending it to zero on $\mathcal{G}_L$ outside its support. Therefore

$$\limsup_{L\to\infty} \inf_{v\in\mathcal{N}_{Z_L}(\mathcal{G}_L)} J(v) \le \limsup_{L\to\infty} J(u_\varepsilon) = J(u_\varepsilon) \le c_1 + \varepsilon$$

and since ε is arbitrary we deduce that

$$\limsup_{L\to\infty} \inf_{v\in\mathcal{N}_{Z_L}(\mathcal{G}_L)} J(v) \le c_1. \tag{4-9}$$

We now prove a complementary inequality. For every L, let $u_L \in \mathcal{N}_{Z_L}(\mathcal{G}_L)$ satisfy

$$J(u_L) \le \inf_{v\in\mathcal{N}_{Z_L}(\mathcal{G}_L)} J(v) + \frac{1}{L} \tag{4-10}$$

and notice that by (2-1), (4-9) and (4-10), u_L is bounded independently of L. Let

$$u_L(x_L) = \min_{h^1\cap[0,L]} u_L(x), \quad u_L(y_L) = \min_{h^2\cap[0,L]} u_L(x)$$

and set

$$\delta_L = \max(u_L(x_L), u_L(y_L)).$$

Since u_L is uniformly bounded in $L^2(\mathcal{G}_L)$, $\delta_L \to 0$ as $L \to \infty$.

Consider the function $(u_L - \delta_L)^+ \in H^1_{Z_L}(\mathcal{G}_L)$, which does not vanish identically, for all L large, by Proposition 2.4. Exactly as in (4-6), $n_\lambda((u_L - \delta_L)^+) \le 1 + o(1)$ as $L \to \infty$.

Set $v_L = \pi_\lambda((u_L - \delta_L)^+)$. Now $v_L \in \mathcal{N}_{Z_L}(\mathcal{G}_L)$, it vanishes at x_L, y_L and

$$J(v_L) = \kappa n_\lambda((u_L - \delta_L)^+)^p \|(u_L - \delta_L)^+\|_p^p \le \kappa(1 + o(1))\|u_L\|_p^p = J(u_L) + o(1) \tag{4-11}$$

as $L \to \infty$.

We now cut $\mathcal{G}_L$ at x_L and y_L, splitting it into three parts $\overline{\mathcal{G}}^1 \subseteq \mathcal{G}^1$, $\overline{\mathcal{G}}^2 \subseteq \mathcal{G}^2$ and $\mathcal{G}^3 = \mathcal{G}_L \setminus (\overline{\mathcal{G}}^1 \cup \overline{\mathcal{G}}^2)$. We call v_i $(i = 1, 2)$ the two vertices of $\mathcal{G}^3$ created on h^i (see Figure 8).

We can use v_L to construct a function $v_L^1 \in H^1_{Z^1}(\mathcal{G}^1)$ by setting

$$v_L^1(x) = \begin{cases} v_L(x) & \text{if } x \in \overline{\mathcal{G}}^1, \\ 0 & \text{elsewhere on } \mathcal{G}^1 \end{cases}$$

and in the same way we construct a function $v_L^2 \in H^1_{Z^2}(\mathcal{G}^2)$. Finally, we call v_L^3 the restriction of v_L to $\mathcal{G}^3$. Setting $Z^3 = \{\mathrm{v}_1, \mathrm{v}_2\}$, by construction we have $v_L^3 \in H^1_{Z^3}(\mathcal{G}^3)$.

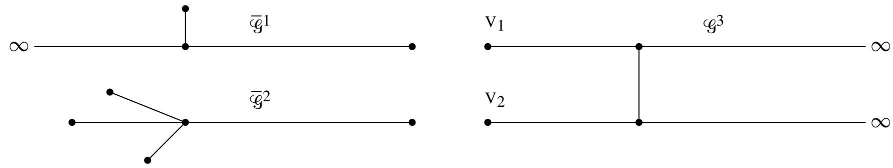


Figure 8. The graph $\mathcal{G}_L$ of Figure 7 splits into the three graphs $\overline{\mathcal{G}}^1$, $\overline{\mathcal{G}}^2$ and $\mathcal{G}^3$.

If $v_L^i \neq 0$, then there exists $\theta_i \in \mathbb{R}$ so that $v_L^i \in \mathcal{N}_{\theta_i, Z^i}(\mathcal{G}^i)$. Taking $\theta_i = 0$ if $v_L^i = 0$ and recalling that $v_L \in \mathcal{N}_{Z_L}(\mathcal{G}_L)$, we obtain

$$\lambda = \frac{\|v_L^1\|_2^2}{\|v_L\|_2^2}\theta_1 + \frac{\|v_L^2\|_2^2}{\|v_L\|_2^2}\theta_2 + \frac{\|v_L^3\|_2^2}{\|v_L\|_2^2}\theta_3. \tag{4-12}$$

Furthermore,

$$J(v_L) = \kappa(\|v_L^1\|_p^p + \|v_L^2\|_p^p + \|v_L^3\|_p^p) \geq \kappa \max\{\|v_L^1\|_p^p, \|v_L^2\|_p^p, \|v_L^3\|_p^p\}.$$

Since, by (4-12), λ is a convex combination of the θ_i's, at least one of the three will satisfy $\theta_i \geq \lambda$.

If $\theta_1 \geq \lambda$, by Remark 2.5, we have $\kappa\|v_L^1\|_p^p \geq c_1$. If $\theta_2 \geq \lambda$, by (4-8), we have $\kappa\|v_L^2\|_p^p \geq c_2 \geq c_1$. If $\theta_3 \geq \lambda$, we have $\kappa\|v_L^3\|_p^p \geq \inf_{\mathcal{N}_{\lambda,Z^3}(\mathcal{G}_3)} J \geq s_\lambda \geq c_1$ since $\mathcal{G}^3$ satisfies (H0) and by the assumptions on $\mathcal{G}^1$. In each case we deduce, via (4-11), that

$$J(u_L) \geq J(v_L) + o(1) \geq c_1 + o(1)$$

as $L \to \infty$, so that by (4-10),

$$\liminf_L \inf_{v \in \mathcal{N}_{Z_L}(\mathcal{G}_L)} J(v) \geq \liminf_L \left(J(u_L) - \frac{1}{L} \right) \geq c_1.$$

In view of (4-9), this ends the proof. □

Theorem 4.16. *Let* $\lambda > 0$ *and* $\mathcal{G}^1$, $\mathcal{G}^2$ *and* $\mathcal{G}_L$ *be the graphs considered above. If L is large enough, then there exist nodal ground states on* $\mathcal{G}_L$.

Proof. Without loss of generality, we assume that

$$\min\Big(\inf_{v \in \mathcal{N}_{Z^1}(\mathcal{G}^1)} J(v), \inf_{v \in \mathcal{N}_{Z^2}(\mathcal{G}^2)} J(v) \Big) = \inf_{v \in \mathcal{N}_{Z^1}(\mathcal{G}^1)} J(v).$$

Let $\varepsilon := \frac{1}{3}\big(s_\lambda - \inf_{v \in \mathcal{N}_{Z^2}(\mathcal{G}^2)} J(v)\big)$. By Lemma 4.15, we choose L so large that

$$\inf_{v \in \mathcal{N}_{Z_L}(\mathcal{G}_L)} J(v) \geq \inf_{v \in \mathcal{N}_{Z^1}(\mathcal{G}^1)} J(v) - \varepsilon \tag{4-13}$$

and that there exist nonnegative $u^i \in \mathcal{N}_{Z^i}(\mathcal{G}^i)$, with compact support satisfying

$$J(u^i) \leq \inf_{v \in \mathcal{N}_{Z^i}(\mathcal{G}^i)} J(v) + \varepsilon.$$

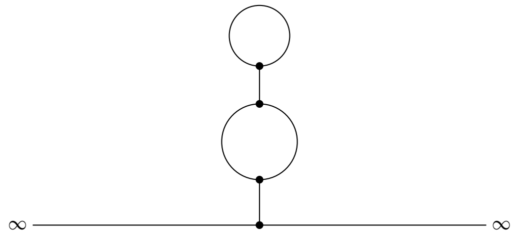


Figure 9. A graph with $\#F(\mathcal{G}) = 2$ where nodal ground states never exist, independently of the length of the edges.

In particular, there is $M > 0$ such that the restriction of u^i to each half-line of $\mathcal{G}^i$ vanishes on $[M, +\infty)$. Hence, for every $L \geq M$, we define $w : \mathcal{G}_L \to \mathbb{R}$ as

$$w(x) := \begin{cases} u^1(x) & \text{if } x \in \mathcal{G}^1, \\ -u^2(x) & \text{if } x \in \mathcal{G}^2, \\ 0 & \text{elsewhere on } \mathcal{G}_L, \end{cases}$$

where with a slight abuse of notation we still denote by $\mathcal{G}^1$, $\mathcal{G}^2$ the corresponding subgraphs of $\mathcal{G}_L$. Clearly, $w \in \mathcal{M}_{Z_L}(\mathcal{G}_L)$ and, by (4-13) and the choice of ε, we have

$$\inf_{v \in \mathcal{M}_{Z_L}(\mathcal{G}_L)} J(v) \leq J(w) = J(u^1) + J(u^2) \leq \inf_{v \in \mathcal{N}_{Z^1}(\mathcal{G}^1)} J(v) + \inf_{v \in \mathcal{N}_{Z^2}(\mathcal{G}^2)} J(v) + 2\varepsilon < \inf_{v \in \mathcal{N}_{Z_L}(\mathcal{G}_L)} J(v) + s_\lambda,$$

in turn implying existence of nodal ground states by Theorem 1.3 and Proposition 4.6. □

Remark 4.17. Concrete examples of graphs fulfilling the hypotheses of Theorem 4.16 can be produced starting, for instance, from any of the graphs in Figure 6 (see, e.g., Figure 7). Since $\inf_{v \in \mathcal{N}_Z(\mathcal{G})} J(v) < s_\lambda$ implies $\#F(\mathcal{G}) \geq 1$, by construction we have $\#F(\mathcal{G}_L) \geq 2$.

Remark 4.18. Theorems 1.6(ii) and 4.11 show that, if (H1) holds, or if the set of all bounded edges of $\mathcal{G}$ is too small, nodal ground states never exist, whereas Theorem 4.16 proves that there exist graphs with $\#F(\mathcal{G}) \geq 2$ and a sufficiently large compact core where nodal ground states do exist. However, even though the former provides sufficient conditions for nonexistence, the latter are not sufficient conditions for existence. It is in fact not difficult to produce examples of graphs with $\#F(\mathcal{G}) = 2$, and compact core of arbitrary size, where nodal ground states do not exist. For instance, consider the graph in Figure 9. If u is a nodal ground state on this graph, we know that either u is identically equal to zero on the two half-lines or it has constant sign on them. Assume thus that $u \geq 0$ on the half–lines. Then, since u^+ is not identically zero, u^+ vanishes on the set $\mathcal{B}$ of the bounded edges of $\mathcal{G}$ at least at a point different from the vertex of the half-lines. We then have that u^+ has always at least two preimages for every $t \in (0, \max u^+)$ by Theorem 6.1 and hence $J(u^+) \geq s_\lambda$ by Lemma 4.5. In view of Remark 3.1, as $u^- \in \mathcal{N}_Z(\mathcal{G})$ vanishes somewhere on the graph, we have also that $J(u^-) > \inf_{v \in \mathcal{N}_Z(\mathcal{G})} J(v)$. This implies that

$$J(u) = J(u^-) + J(u^+) > \inf_{v \in \mathcal{N}_Z(\mathcal{G})} J(v) + s_\lambda,$$

which contradicts (1-9).

5. Graphs with infinitely many bounded edges

In this section we extend our discussion about ground states and nodal ground states to graphs with infinitely many edges whose length is uniformly bounded. In particular, we focus on two subclasses of such graphs that have already been considered in the literature: periodic graphs and regular trees.

5.1. ***Periodic graphs.*** Throughout this section, when we speak of a periodic metric graph we mean a graph fulfilling [Berkolaiko and Kuchment 2013, Definition 4.1.1]. We avoid reporting the full details of the definition here. For our purposes, it is enough to recall that, if $\mathcal{G}$ is a periodic graph, then there exists a number $n \in \mathbb{N}$ and a compact subset $W \subset \mathcal{G}$, called a *fundamental domain* of $\mathcal{G}$, such that

$$\mathcal{G} = \bigcup_{k \in \mathbb{Z}^n} W_k,$$

where W_k is a copy of W for every $k \in \mathbb{Z}^n$, and $W_i \cap W_j$ contains at most finitely many points for every $i \neq j$. In this case, we say that $\mathcal{G}$ is a $\mathbb{Z}^n$-periodic graph.

Since we are concerned with problems involving homogeneous Dirichlet conditions on a subset Z of the vertices of $\mathcal{G}$, we specify that when $\mathcal{G}$ is a $\mathbb{Z}^n$-periodic graph, we only consider here $\mathbb{Z}^n$-periodic subsets Z (that is, $Z \cap W_k$ is a copy of $Z \cap W$ for every $k \in \mathbb{Z}^n$).

Proof of Theorem 1.7. We address independently the case of ground states and nodal ground states.

Part 1: *existence of ground states.* Let $(u_n)_n \subset \mathcal{N}_Z$ be such that $\lim_n J(u_n) = \inf_{v \in \mathcal{N}_Z} J(v)$. Exploiting the periodicity of $\mathcal{G}$ and Z, we can assume with no loss of generality that u_n attains its L^∞-norm on W_0, for every n. Since $(u_n)_n$ is bounded in $H^1(\mathcal{G})$, up to subsequences $u_n \rightharpoonup u$ in $H^1(\mathcal{G})$ and $u_n \to u$ in $L^\infty_{\text{loc}}(\mathcal{G})$ as $n \to \infty$. Furthermore, $u \not\equiv 0$ on $\mathcal{G}$ because, if this were not the case, by the strong convergence of (u_n) to u in $L^\infty(W_0)$ we would have $\|u_n\|_{L^\infty(\mathcal{G})} = \|u_n\|_{L^\infty(W_0)} \to 0$ as $n \to \infty$, contradicting Proposition 2.4.

If $u_n \to u$ in $L^2(\mathcal{G})$, then by standard Gagliardo–Nirenberg inequalities $u_n \to u$ in $L^p(\mathcal{G})$ and, by weak lower semicontinuity, $n_\lambda(u) \leq 1$, so that

$$\inf_{v \in \mathcal{N}_Z} J(v) \leq J(\pi_\lambda(u)) = \kappa n_\lambda(u)^p \|u\|_p^p \leq \lim_n \kappa \|u_n\|_p^p = \inf_{v \in \mathcal{N}_Z} J(v),$$

i.e., $\pi_\lambda(u)$ is a ground state.

Let us thus show that u_n converges to u strongly in $L^2(\mathcal{G})$. Assume by contradiction that

$$\liminf_n \|u_n - u\|_2^2 > 0.$$

Let $\theta \in \mathbb{R}$ and $(\lambda_n)_n \subset \mathbb{R}$ be such that $u \in \mathcal{N}_{\theta,Z}$, $u_n - u \in \mathcal{N}_{\lambda_n,Z}$ for every n. By the weak convergence of $(u_n)_n$ to u in $H^1(\mathcal{G})$, Brézis–Lieb lemma [1983] and the fact that $u_n \in \mathcal{N}_{\lambda,Z}$, we have

$$\begin{aligned} \lambda_n &= \frac{\|u_n - u\|_p^p - \|u_n' - u'\|_2^2}{\|u_n - u\|_2^2} = \frac{\|u_n\|_p^p - \|u_n'\|_2^2 - \|u\|_p^p + \|u'\|_2^2 + o(1)}{\|u_n - u\|_2^2} \\ &= \frac{\lambda \|u_n\|_2^2 - \theta \|u\|_2^2 + o(1)}{\|u_n - u\|_2^2} = \lambda + \frac{(\lambda - \theta)\|u\|_2^2 + o(1)}{\|u_n - u\|_2^2} = \lambda + \frac{\|u\|_2^2}{\|u_n - u\|_2^2}(\lambda - \theta) + o(1) \end{aligned} \qquad (5\text{-}1)$$

as $n \to \infty$. Applying again Brézis–Lieb lemma, we obtain

$$\inf_{v \in \mathcal{N}_{\lambda,Z}} J_\lambda(v) = \lim_n \kappa \|u_n\|_p^p = \lim_n \kappa \|u_n - u\|_p^p + \kappa \|u\|_p^p. \tag{5-2}$$

Keeping in mind that $\lambda > 0$, we distinguish three cases. If $\theta > \lambda$, then, by Remark 2.5,

$$\lim_n \kappa \|u_n - u\|_p^p + \kappa \|u\|_p^p \geq \kappa \|u\|_p^p \geq \inf_{v \in \mathcal{N}_{\theta,Z}} J_\theta(v) > \inf_{v \in \mathcal{N}_{\lambda,Z}} J_\lambda(v).$$

If $\theta = \lambda$, we see from (5-1) that $\lambda_n \to \lambda$ as $n \to \infty$. Therefore, using again Remark 2.5,

$$\lim_n \kappa \|u_n - u\|_p^p + \kappa \|u\|_p^p \geq \liminf_n \inf_{v \in \mathcal{N}_{\lambda_n,Z}} J_{\lambda_n}(v) + \inf_{v \in \mathcal{N}_{\theta,Z}} J_\theta(v) = 2 \inf_{v \in \mathcal{N}_{\lambda,Z}} J_\lambda(v).$$

If $\theta < \lambda$, we have $\liminf_n \lambda_n > \lambda$ and, similarly,

$$\lim_n \kappa \|u_n - u\|_p^p + \kappa \|u\|_p^p \geq \liminf_n \inf_{v \in \mathcal{N}_{\lambda_n,Z}} J_{\lambda_n}(v) > \inf_{v \in \mathcal{N}_{\lambda,Z}} J_\lambda(v).$$

In all three cases, (5-2) yields a contradiction.

Part 2: *nonexistence of nodal ground states.* By Theorem 1.4, it is enough to show that

$$\inf_{v \in \mathcal{M}_Z} J(v) \leq 2 \inf_{v \in \mathcal{N}_Z} J(v).$$

To this end, given $\varepsilon > 0$, let $u \in \mathcal{N}_Z$ be such that $J(u) \leq \inf_{v \in \mathcal{N}_Z} J(v) + \varepsilon$. With no loss of generality, we can take such u to be nonnegative, compactly supported on $\mathcal{G}$ and attaining its L^∞-norm on W_0 (it is, for instance, enough to apply Remark 3.2 to a suitable ground state of J in $\mathcal{N}_Z$, that exists by the first part of the proof). Hence, there exists $M > 0$ such that $\operatorname{supp}(u) \subset \bigcup_{|k| \leq M} W_k$. Let then $\bar{u} \in \mathcal{N}_Z$ be a translation of u on $\mathcal{G}$ such that $\operatorname{supp}(\bar{u}) \subset \bigcup_{|k|>M} W_k$ and define $w : \mathcal{G} \to \mathbb{R}$ as

$$w(x) := \begin{cases} u(x) & \text{if } x \in \operatorname{supp}(u), \\ -\bar{u}(x) & \text{if } x \in \operatorname{supp}(\bar{u}), \\ 0 & \text{elsewhere on } \mathcal{G}. \end{cases}$$

By construction, $w \in \mathcal{M}_Z$ and $J(w) = J(u) + J(\bar{u}) \leq 2 \inf_{v \in \mathcal{N}_Z} J(v) + 2\varepsilon$. Given the arbitrariness of $\varepsilon > 0$, we conclude. □

Remark 5.1. Observe that $J^\infty(\mathcal{G}; Z) = \inf_{v \in \mathcal{N}_Z} J(v)$ for every periodic graph $\mathcal{G}$ and every set Z with the same periodicity. This is the reason why it is not possible to rely directly on the abstract result of Theorem 1.3 to prove Theorem 1.7.

5.2. *Regular trees.* Recall that a regular tree is an acyclic, noncompact metric graph with edges all of the same length and vertices all of the same degree $d \geq 3$ (unrooted tree), with the possible exception of a single vertex of degree 1 (rooted tree). If $\mathcal{G}$ is an unrooted tree, then necessarily $Z = \varnothing$ since every vertex has degree at least 3, whereas if $\mathcal{G}$ is a rooted tree either $Z = \varnothing$ or it coincides with the root of $\mathcal{G}$ (i.e., the unique vertex of degree 1).

We divide the proof of Theorem 1.8 into two parts, proving first statements (i)–(ii) on ground states and then statement (iii) on nodal ground states.

Proof of Theorem 1.8. We split the proof in several steps.

Step 1: *ground states when $\mathcal{G}$ is an unrooted tree.* Let $(u_n)_n \subset \mathcal{N}$ be such that $\lim_n J(u_n) = \inf_{v\in\mathcal{N}} J(v)$. Exploiting the symmetry of $\mathcal{G}$, it is not restrictive to assume that u_n attains its L^∞-norm in the same fixed edge of $\mathcal{G}$, for every n. Indeed, the problem is invariant under any isometry of $\mathcal{G}$ and the isometry group of the tree $\mathcal{G}$ acts transitively on the edges of $\mathcal{G}$. Hence, arguing as in the proof of Theorem 1.7 shows that the weak limit in $H^1(\mathcal{G})$ of $(u_n)_n$ provides a desired ground state for J in $\mathcal{N}$.

Step 2: *ground states when $\mathcal{G}$ is a rooted tree and $Z = \varnothing$.* Let r be the root of $\mathcal{G}$, $d \geq 3$ be the degree of each vertex of $\mathcal{G}$ different from the root, and $\overline{\mathcal{G}}$ be the unrooted tree obtained by gluing together d copies of $\mathcal{G}$ at their roots. We first prove that

$$J^\infty(\mathcal{G}) = \inf_{v\in\mathcal{N}_{\{r\}}(\mathcal{G})} J(v) = \inf_{v\in\mathcal{N}(\overline{\mathcal{G}})} J(v). \tag{5-3}$$

To this aim, given any function $u \in \mathcal{N}_{\{r\}}(\mathcal{G})$, we construct a sequence $(u_n)_n \subset \mathcal{N}_{\{r\}}(\mathcal{G})$ converging weakly to 0 in $H^1(\mathcal{G})$ by translating u along $\mathcal{G}$ and extending it by 0 on the remaining part of the graph. This proves that $J^\infty(\mathcal{G}) \leq \inf_{v\in\mathcal{N}_{\{r\}}(\mathcal{G})} J(v)$. Next, let $(u_n)_n \subset \mathcal{N}(\mathcal{G})$ be a sequence converging weakly to 0 in $H^1(\mathcal{G})$ and such that $J(u_n) \to J^\infty(\mathcal{G})$. Since $u_n(r) \to 0$ by $L^\infty_{\text{loc}}(\mathcal{G})$ convergence, we can assume without loss of generality that each u_n satisfies $u_n(r) = 0$, namely that $u_n \in \mathcal{N}_{\{r\}}(\mathcal{G})$. This shows that $J^\infty(\mathcal{G}) \geq \inf_{v\in\mathcal{N}_{\{r\}}(\mathcal{G})} J(v)$, and the first equality is proved.

To prove the second equality, notice that any $u \in \mathcal{N}_{\{r\}}(\mathcal{G})$ can be seen as an element of $\mathcal{N}(\overline{\mathcal{G}})$, after extending it by 0 on $\overline{\mathcal{G}} \setminus \mathcal{G}$. On the other hand, any $u \in \mathcal{N}(\overline{\mathcal{G}})$ with compact support can be considered (when translated in such a way that $r \notin \operatorname{supp}(u)$) as an element of $\mathcal{N}_{\{r\}}(\mathcal{G})$. By density this is enough to conclude the proof of (5-3).

By (5-3) and Theorem 1.3, in order to prove the existence of a ground state, it is sufficient to show that

$$\inf_{v\in\mathcal{N}(\mathcal{G})} J(v) < \inf_{v\in\mathcal{N}(\overline{\mathcal{G}})} J(v). \tag{5-4}$$

To this end, let $u \in \mathcal{N}(\overline{\mathcal{G}})$ be a positive ground state of J in $\mathcal{N}(\overline{\mathcal{G}})$, whose existence is guaranteed by the previous step. Take a vertex v of $\overline{\mathcal{G}}$ and split the graph at v into d disjoint rooted trees $\mathcal{G}_i$, $i = 1, \dots, d$. For every i, let $u_i > 0$ be the restriction of u to $\mathcal{G}_i$ and $\lambda_i \in \mathbb{R}$ be such that $u_i \in \mathcal{N}_{\lambda_i}(\mathcal{G}_i)$. Since $u \in \mathcal{N}(\overline{\mathcal{G}})$ and $u > 0$ on $\overline{\mathcal{G}}$, we have

$$\lambda = \sum_{i=1}^{d} \frac{\|u_i\|^2_{L^2(\mathcal{G}_i)}}{\|u\|^2_{L^2(\overline{\mathcal{G}})}} \lambda_i,$$

so that

$$\lambda \leq \bigl(\max_{1\leq i\leq d} \lambda_i\bigr) \sum_{i=1}^{d} \frac{\|u_i\|^2_{L^2(\mathcal{G}_i)}}{\|u\|^2_{L^2(\overline{\mathcal{G}})}} = \max_{1\leq i\leq d} \lambda_i.$$

Hence, there exists $j \in \{1, \dots, d\}$ such that $n_\lambda(u_j) \leq 1$. Since each $\mathcal{G}_i$ is a copy of $\mathcal{G}$, we then have

$$\inf_{v\in\mathcal{N}(\mathcal{G})} J(v) \leq J(\pi_\lambda(u_j)) = \kappa n_\lambda(u_j)^p \|u_j\|^p_{L^p(\mathcal{G}_j)} < \kappa \sum_{i=1}^{d} \|u_i\|^p_{L^p(\mathcal{G}_i)} = \kappa \|u\|^p_{L^p(\overline{\mathcal{G}})} = \inf_{v\in\mathcal{N}(\overline{\mathcal{G}})} J(v),$$

that is (5-4).

Step 3: *ground states when $\mathcal{G}$ is a rooted tree and $Z \neq \varnothing$.* Since Z coincides with the root of $\mathcal{G}$, as in the first part of Step 2 we have

$$\inf_{v\in\mathcal{N}_Z(\mathcal{G})} J(v) = \inf_{v\in\mathcal{N}(\overline{\mathcal{G}})} J(v),$$

where $\overline{\mathcal{G}}$ is the unrooted tree corresponding to $\mathcal{G}$ as above. That the problem on $\mathcal{G}$ has no ground state follows by the fact that, if u were a ground state in $\mathcal{N}_Z(\mathcal{G})$, it would be also a ground state in $\mathcal{N}(\overline{\mathcal{G}})$, as any function on $\mathcal{G}$ vanishing at the root can be regarded as a function on $\overline{\mathcal{G}}$ as well after extending it by 0. Since this is impossible because ground states never vanish on $\overline{\mathcal{G}}$, we conclude.

Step 4: *nodal ground states when $\mathcal{G}$ is an unrooted tree or $\mathcal{G}$ is a rooted tree and $Z \neq \varnothing$.* If $\mathcal{G}$ is an unrooted tree, exploiting again its symmetry, it is easy to adapt the argument developed in the proof of Theorem 1.7 to show again that

$$\inf_{v\in\mathcal{M}(\mathcal{G})} J(v) = 2 \inf_{v\in\mathcal{N}(\mathcal{G})} J(v),$$

and likewise, if $\mathcal{G}$ is a rooted tree with $Z \neq \varnothing$, that

$$\inf_{v\in\mathcal{M}_Z(\mathcal{G})} J(v) = 2 \inf_{v\in\mathcal{N}_Z(\mathcal{G})} J(v).$$

This implies that nodal ground states do not exist by Theorem 1.4.

Step 5: *nodal ground states when $\mathcal{G}$ is a rooted tree and $Z = \varnothing$.* Since, given any $u \in \mathcal{M}$, at least one between u^+ and u^- vanishes at the root r, it follows that

$$\inf_{v\in\mathcal{M}(\mathcal{G})} J(v) = \inf_{v\in\mathcal{N}(\mathcal{G})} J(v) + \inf_{v\in\mathcal{N}_{\{r\}}(\mathcal{G})} J(v).$$

Arguing as in the proof of Theorem 1.4, this immediately implies that nodal ground states do not exist. □

6. Qualitative properties of nodal ground states

The first result of this section concerns the *nodal domains* (i.e., the connected components of $\mathcal{G} \setminus u^{-1}(0)$) of any minimizer u in $\mathcal{M}_{\lambda,Z}(\mathcal{G})$.

Theorem 6.1. *Let $\mathcal{G} \in \boldsymbol{G}$ and $\lambda > -\omega_Z(\mathcal{G})$. Let $u \in \mathcal{M}_Z$ be a nodal ground state. Then u has exactly two nodal domains.*

Proof. Assume for contradiction that there are at least three nodal domains. Up to a change of sign, we can make sure that on at least two of them u is positive, and we call $\mathcal{G}_1$ one of the two. Since u solves (1-1), multiplying by u and integrating on $\mathcal{G}_1$ we have

$$\int_{\mathcal{G}_1} (|u'|^2 + \lambda|u|^2 - |u|^p)\,\mathrm{d}x = uu'_{|\partial\mathcal{G}_1} + \int_{\mathcal{G}_1} (-u'' + \lambda u - |u|^{p-2}u)u\,\mathrm{d}x = 0, \tag{6-1}$$

because on $\partial\mathcal{G}_1$ either $u = 0$ or $u' = 0$ (this happens at vertices of degree 1 not in Z).

Now we define $v \in H^1_Z(\mathcal{G})$ by

$$v(x) := \begin{cases} u(x) & \text{if } x \in \mathcal{G} \setminus \mathcal{G}_1, \\ 0 & \text{if } x \in \mathcal{G}_1, \end{cases}$$

and we observe that $v^- = u^- \in \mathcal{N}_Z$ and that v^+ (not identically zero by construction) satisfies

$$\int_{\mathcal{G}}(|(v^+)'|^2+\lambda|v^+|^2-|v^+|^p)\,\mathrm{d}x = \int_{\mathcal{G}}(|(u^+)'|^2+\lambda|u^+|^2-|u^+|^p)\,\mathrm{d}x - \int_{\mathcal{G}_1}(|u'|^2+\lambda|u|^2-|u|^p)\,\mathrm{d}x = 0$$

by (6-1) and because $u^+ \in \mathcal{N}_Z$. Therefore $v \in \mathcal{M}_Z$ and

$$J(v) = \kappa\|v\|^p_{L^p(\mathcal{G})} = \kappa\|u\|^p_{L^p(\mathcal{G})} - \kappa\|u\|^p_{L^p(\mathcal{G}_1)} < \kappa\|u\|^p_{L^p(\mathcal{G})} = J(u),$$

violating the minimality of u. □

To conclude we are left to prove Theorem 1.9. To this end, we will actually prove three independent statements, the full proof of Theorem 1.9 then following by their combination. Each of these statements exhibits a graph supporting a nodal ground state with nodal set respectively given by

(1) k isolated points;

(2) $m \geq 2$ half-lines all attached to the same vertex;

(3) n line segments all attached to the same vertex.

These three constructions, though mutually independent, can all be carried out on the same kind of graph, that we now describe. Given $N \in \mathbb{N}$ and $L > 0$, let v_1, v_2 be two vertices joined by N edges $e_1, \ldots, e_N$, each of length L. Attach to v_1 a pendant and a half-line and do the same to v_2. In this way we obtain the graph $\mathcal{G}_{N,L}$ depicted in Figure 10. Throughout, we fix $\lambda > 0$ and the length of the two pendants so that nodal ground states in $\mathcal{M}_\lambda(\mathcal{G}_{N,L})$ exist (independently of any other feature of the graph), which is possible by Theorem 4.12.

Proof of (1). Here we show that, for a suitable choice of L, the graph $\mathcal{G}_{k,L}$ admits a nodal ground state u such that $u^{-1}(0)$ consists of k isolated points.

Proposition 6.2. *For every $k \in \mathbb{N}$ there exists $\bar{L} > 0$, depending on λ and k, such that, for every $L \geq \bar{L}$, every nodal ground state u on $\mathcal{G}_{k,L}$ has a nodal set of the form $u^{-1}(0) = \{x_1, \ldots, x_k\}$, where x_i belongs to the interior of the edge e_i.*

To prove this proposition we consider also the graph $\overline{\mathcal{G}}_{k+1}$ made of $k+1$ half-lines and a pendant all attached at the same vertex. The length of the pendant of $\overline{\mathcal{G}}_{k+1}$ coincides with that of the two pendants of $\mathcal{G}_{k,L}$. Hence, by Theorem 4.12, ground states exist in $\mathcal{N}_\lambda(\overline{\mathcal{G}}_{k+1})$.

Lemma 6.3. *For every $k \in \mathbb{N}$,*

$$\lim_{L\to\infty} \inf_{v\in\mathcal{N}_\lambda(\mathcal{G}_{k,L})} J(v) = \inf_{v\in\mathcal{N}_\lambda(\overline{\mathcal{G}}_{k+1})} J(v).$$

Proof. The argument is similar to that in the proof of Lemma 4.15. Using suitable compactly supported functions in $\mathcal{N}_\lambda(\overline{\mathcal{G}}_{k+1})$, one immediately checks that

$$\limsup_{L\to\infty} \inf_{v\in\mathcal{N}_\lambda(\mathcal{G}_{k,L})} J(v) \leq \inf_{v\in\mathcal{N}_\lambda(\overline{\mathcal{G}}_{k+1})} J(v).$$

To show that

$$\liminf_{L\to\infty} \inf_{v\in\mathcal{N}_\lambda(\mathcal{G}_{k,L})} J(v) \geq \inf_{v\in\mathcal{N}_\lambda(\overline{\mathcal{G}}_{k+1})} J(v), \tag{6-2}$$

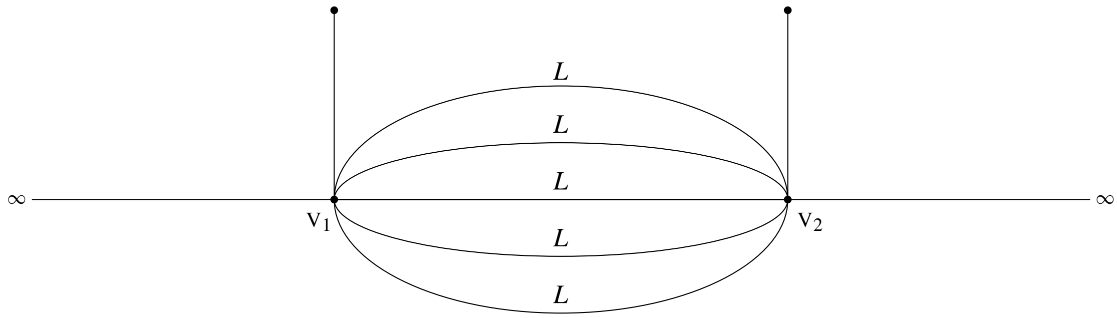


Figure 10. The graph $\mathcal{G}_{N,L}$ with $N = 5$.

it is enough to note that, if $u_L \in \mathcal{N}_\lambda(\mathcal{G}_{k,L})$ satisfies

$$J(u_L) \le \inf_{v \in \mathcal{N}_\lambda(\mathcal{G}_{k,L})} J(v) + \frac{1}{L},$$

then

$$\max_{1 \le i \le k} \min_{x \in e_i} |u_L(x)| \to 0 \quad \text{as } L \to \infty.$$

This allows one to obtain (6-2) working exactly as in the proof of Lemma 4.15. □

Lemma 6.4. *If* $L \to \infty$, *then*

$$\limsup_{L \to \infty} \inf_{v \in \mathcal{M}_\lambda(\mathcal{G}_{k,L})} J(v) \le 2 \inf_{v \in \mathcal{N}_\lambda(\overline{\mathcal{G}}_{k+1})} J(v).$$

Proof. The proof follows the same lines as the one of Theorem 4.16. □

Proof of Proposition 6.2. Let u be a nodal ground state in $\mathcal{M}_\lambda(\mathcal{G}_{k,L})$.

Step 1: *for L long enough, either $u \equiv 0$ on the pendants or it has no zero on their closure.* Assume by contradiction that $u \not\equiv 0$ on a pendant p, but $u(x_0) = 0$ for some x_0 on p. With no loss of generality, let $u > 0$ at the vertex of degree 1 of p. Outside p, $u < 0$ thanks to Theorem 6.1. Denoting as usual by $|p|$ the length of p, since u is a solution to (1-1), we have $u^+ \in \mathcal{N}_\lambda(0, |p|)$ with $u^+(|p|) = 0$, so that

$$J(u^+) \ge \inf_{\substack{v \in \mathcal{N}_\lambda(0,|p|) \\ v(|p|)=0}} J(v) > \inf_{v \in \mathcal{N}_\lambda(\overline{\mathcal{G}}_{k+1})} J(v).$$

This is because the pendant of $\overline{\mathcal{G}}_{k+1}$ can be identified with the interval $[0, |p|]$, but u^+ is not a ground state in $\mathcal{N}_\lambda(\overline{\mathcal{G}}_{k+1})$ as ground states never vanish.

Letting then

$$\delta := \inf_{\substack{v \in \mathcal{N}_\lambda(0,|p|) \\ v(|p|)=0}} J(v) - \inf_{v \in \mathcal{N}_\lambda(\overline{\mathcal{G}}_{k+1})} J(v) > 0$$

and recalling that $u^- \in \mathcal{N}_\lambda(\mathcal{G}_{k,L})$, it follows that

$$\inf_{v \in \mathcal{M}_\lambda(\mathcal{G}_{k,L})} J(v) = J(u) = J(u^-) + J(u^+) \ge \inf_{v \in \mathcal{N}_\lambda(\mathcal{G}_{k,L})} J(v) + \inf_{v \in \mathcal{N}_\lambda(\overline{\mathcal{G}}_{k+1})} J(v) + \delta,$$

contradicting Lemmas 6.3–6.4 for L large enough.

Step 2: $u(\mathrm{v}_1)u(\mathrm{v}_2) < 0$. Assume that this is not the case. Since u solves (1-1), on any of the two half-lines either $u \equiv 0$ or it never vanishes. Combining with Step 1, this implies that there exist $i \in \{1, \dots, k\}$ and $\bar{x}_1, \bar{x}_2 \in e_i \cup \{\mathrm{v}_1, \mathrm{v}_2\}$ with $u(\bar{x}_1) = u(\bar{x}_2) = 0$ and, for all $x \in (\bar{x}_1, \bar{x}_2)$, $u \neq 0$. Without loss of generality, let $u > 0$ on $(\bar{x}_1, \bar{x}_2)$. By Theorem 6.1, we know that $u < 0$ on the remaining part of the graph and $u^- \in \mathcal{N}_\lambda(\mathcal{G}_{k,L})$, while we can think of u^+ as a function in $\mathcal{N}_\lambda(\mathbb{R})$ with compact support. Hence we have

$$\inf_{v \in \mathcal{M}_\lambda(\mathcal{G}_{k,L})} J(v) = J(u^+) + J(u^-) > s_\lambda + \inf_{v \in \mathcal{N}_\lambda(\mathcal{G}_{k,L})} J(v),$$

which contradicts Theorem 1.6.

Step 3: *conclusion.* The previous steps ensure that $u^{-1}(0) \subset \bigcup_{i=1}^N e_i$ and that it is a finite union of points by uniqueness of the solution of the Cauchy problem for (1-1). The uniqueness of the zero of u on each e_i follows then by Theorem 6.1. □

Proof of (2). Here we prove the following result.

Proposition 6.5. *Let $m \geq 2$. There exists a graph $\overline{\mathcal{G}}$ that admits a nodal ground state u such that $u^{-1}(0)$ is the union of $m \geq 2$ half-lines attached at the same vertex.*

The graph $\overline{\mathcal{G}}$ is obtained from the graph $\mathcal{G}_{1,L}$ by attaching m half-lines at a suitable point. Before proving Proposition 6.5 we establish the following lemma.

Lemma 6.6. *Let $\mathcal{G}$ be a noncompact graph with a finite number of edges. Let $\widetilde{\mathcal{G}}$ be a graph obtained from $\mathcal{G}$ by attaching $m \geq 2$ half-lines $h_1, \dots, h_m$ at one of its points p. If there exists a nodal ground state in $\mathcal{M}_\lambda(\widetilde{\mathcal{G}})$, then*

$$\inf_{v \in \mathcal{M}_\lambda(\widetilde{\mathcal{G}})} J(v) \geq \inf_{v \in \mathcal{M}_\lambda(\mathcal{G})} J(v). \tag{6-3}$$

Proof. Let $\tilde{u}$ be a nodal ground state on $\widetilde{\mathcal{G}}$ and assume without loss of generality that $\tilde{u}(\mathrm{p}) \geq 0$. Denote by u the restriction of $\tilde{u}$ on $\mathcal{G}$ and by ϕ_i the restriction of $\tilde{u}$ to the half-line h_i for $i = 1, \dots, m$.

If $\tilde{u}(\mathrm{p}) = 0$, since $\tilde{u}$ solves (1-1), each ϕ_i vanishes identically. Hence, $u \in \mathcal{M}_\lambda(\mathcal{G})$, $J(\tilde{u}) = J(u)$ and (6-3) follows.

If $\tilde{u}(\mathrm{p}) > 0$, each ϕ_i coincides with a portion of the same soliton ϕ_λ. With a slight abuse of notation we denote by $\phi_i'(\mathrm{p})$ the outgoing derivative of ϕ_i at p along h_i. Note that $\phi_i'(\mathrm{p}) < 0$ for every i. Indeed, if on the contrary we had, for instance, $\phi_1'(\mathrm{p}) \geq 0$, then the restriction of $\tilde{u}$ to the union of the h_i's would contain at least one full soliton ϕ_λ, so that $\|\tilde{u}\|^p_{L^p(\bigcup_i h_i)} \geq \|\phi_\lambda\|^p_p$. This would lead to

$$\inf_{v \in \mathcal{M}_\lambda(\widetilde{\mathcal{G}})} J(v) = J(\tilde{u}) = \kappa(\|\tilde{u}^+\|^p_p + \|\tilde{u}^-\|^p_p) > \kappa\|\phi_\lambda\|^p_p + \inf_{v \in \mathcal{N}_\lambda(\widetilde{\mathcal{G}})} J(v) = s_\lambda + \inf_{v \in \mathcal{N}_\lambda(\widetilde{\mathcal{G}})} J(v),$$

which contradicts (1-9).

As, for all $i \in \{1, \dots, m\}$, ϕ_i is a solution to (1-1), we have in particular $\phi_i \in \mathcal{N}_{\theta_i}(h_i)$ with

$$\theta_i = \frac{\int_{h_i} \phi_i^p \,\mathrm{d}x - \int_{h_i} (\phi_i')^2 \,\mathrm{d}x}{\int_{h_i} \phi_i^2 \,\mathrm{d}x} = \frac{\int_{h_i} \phi_i^p \,\mathrm{d}x + \phi_i(\mathrm{p})\phi_i'(\mathrm{p}) + \int_{h_i} \phi_i''\phi_i \,\mathrm{d}x}{\int_{h_i} \phi_i^2 \,\mathrm{d}x} = \frac{\lambda \int_{h_i} \phi_i^2 \,\mathrm{d}x + \phi_i(\mathrm{p})\phi_i'(\mathrm{p})}{\int_{h_i} \phi_i^2 \,\mathrm{d}x} < \lambda$$

since ϕ_i is a portion of ϕ_λ and $\phi_i'(\mathrm{p}) < 0$. Letting then μ be the number such that $u^+ \in \mathcal{N}_\mu(\mathcal{G})$,

$$\lambda = \sum_{i=1}^{m} \frac{\|\phi_i\|^2_{L^2(h_i)}}{\|\tilde{u}^+\|^2_{L^2(\widetilde{\mathcal{G}})}}\theta_i + \frac{\|u^+\|^2_{L^2(\mathcal{G})}}{\|\tilde{u}^+\|^2_{L^2(\widetilde{\mathcal{G}})}}\mu,$$

which, combined with the preceding inequality, yields $\mu > \lambda$.

Since, analogously to Remark 2.5, for a given λ, the map

$$\mu \mapsto \inf_{v\in\mathcal{M}_{\mu,\lambda}(\mathcal{G})} \tfrac{1}{2}\|v'\|^2_{L^2(\mathcal{G})} + \tfrac{1}{2}\mu\|v^+\|^2_{L^2(\mathcal{G})} + \tfrac{1}{2}\lambda\|v^-\|^2_{L^2(\mathcal{G})} - \frac{1}{p}\|v\|^p_{L^p(\mathcal{G})},$$

where $\mathcal{M}_{\mu,\lambda}(\mathcal{G}) := \{v \in H^1(\mathcal{G}) \mid v^+ \in \mathcal{N}_\mu(\mathcal{G}) \text{ and } v^- \in \mathcal{N}_\lambda(\mathcal{G})\}$, is increasing, we have

$$\inf_{v\in\mathcal{M}_\lambda(\widetilde{\mathcal{G}})} J(v) = J(\tilde{u}) = \kappa(\|\tilde{u}^+\|^p_p + \|\tilde{u}^-\|^p_p) \geq \kappa(\|u^+\|^p_p + \|u^-\|^p_p) \geq \inf_{v\in\mathcal{M}_{\mu,\lambda}(\mathcal{G})} J(v) > \inf_{v\in\mathcal{M}_\lambda(\mathcal{G})} J(v). \qquad \square$$

Proof of Proposition 6.5. Consider the graph $\mathcal{G}_{1,L}$ with $L \geq \bar{L}$ given by Proposition 6.2. On this graph, by Theorem 4.12 and Proposition 6.2, we have a nodal ground state u with $u^{-1}(0) = \{x_0\}$. Let now $\overline{\mathcal{G}}$ be the graph obtained from $\mathcal{G}_{1,L}$ by attaching m half-lines at the point x_0 and let $\bar{u} \in \mathcal{M}_\lambda(\overline{\mathcal{G}})$ be the function obtained extending u by 0 on each of the additional half-lines.

By Theorem 4.12, nodal ground states exist on $\overline{\mathcal{G}}$ and, by Lemma 6.6,

$$\inf_{v\in\mathcal{M}_\lambda(\mathcal{G}_{1,L})} J(v) = J(u) = J(\bar{u}) \geq \inf_{v\in\mathcal{M}_\lambda(\overline{\mathcal{G}})} J(v) \geq \inf_{v\in\mathcal{M}_\lambda(\mathcal{G}_{1,L})} J(v).$$

This proves that $\bar{u}$ is a nodal ground state on $\overline{\mathcal{G}}$ and hence the existence of a nodal ground state whose nodal set is given by m half-lines attached at the same point. $\square$

Proof of (3). Here we prove the following statement.

Proposition 6.7. *Let $n \in \mathbb{N}$. There exist a graph $\overline{\mathcal{G}}$, a subset $Z \subseteq \mathbb{V} \setminus \mathbb{V}_\infty$ of its vertices of degree* 1 *and a nodal ground state $u \in \mathcal{M}_{\lambda,Z}(\overline{\mathcal{G}})$ such that $u^{-1}(0)$ consists of n line segments attached at the same point, each of length smaller than or equal to $\frac{\kappa}{2s_\lambda}\left(\frac{p\lambda}{2}\right)^{2/(p-2)}$.*

Similarly to construction (2), the graph $\overline{\mathcal{G}}$ will be obtained from $\mathcal{G}_{1,L}$ by attaching n line segments at one of its points. To do this we need the next lemma.

Lemma 6.8. *Let $\mathcal{G}$ be a noncompact graph with a finite number of edges. Let $\widetilde{\mathcal{G}}$ be a graph obtained from $\mathcal{G}$ by attaching n line segments $s_1, \dots, s_n$ at one of its points p. Assume that each line segment has a length smaller than or equal to a number $S > 0$ and ends at a vertex with Dirichlet boundary condition. Suppose also that $\tilde{u}$ and S are such that $\tilde{u}$ is a nodal ground state on $\widetilde{\mathcal{G}}$ and that $S \leq \frac{\kappa}{J(\tilde{u})}\left(\frac{p\lambda}{2}\right)^{2/(p-2)}$. Then*

$$\inf_{v\in\mathcal{M}_{\lambda,Z}(\widetilde{\mathcal{G}})} J(v) \geq \inf_{v\in\mathcal{M}_{\lambda,Z}(\mathcal{G})} J(v).$$

Proof. We proceed in the same way as in the proof of Lemma 6.6. With no loss of generality, let $\tilde{u}(\mathrm{p}) \geq 0$. Denote by u the restriction of $\tilde{u}$ to $\mathcal{G}$ and by u_i the restriction of u to s_i for every i. Moreover, let $u_i'(\mathrm{p})$ be the outward derivative of u_i at p along s_i. As $\tilde{u}$ is a nodal ground state, $u_i(\mathrm{p})u_i'(\mathrm{p}) \leq 0$. Indeed, if this were not the case, we would have $u_i'(\mathrm{p}) > 0$ and, since u_i satisfies the Dirichlet condition at the end of s_i,

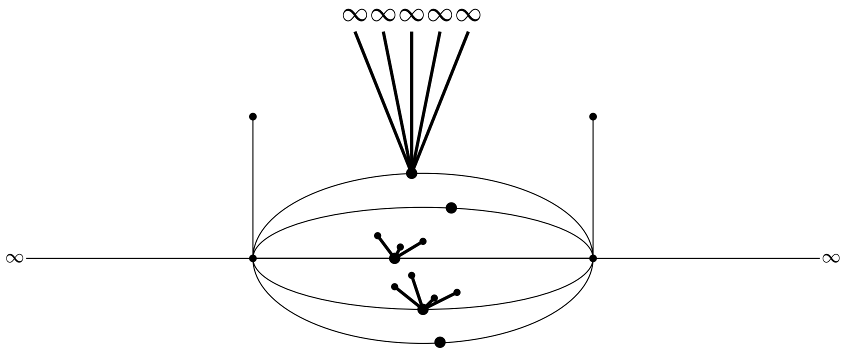


Figure 11. Example of a graph as in Theorem 1.9 hosting a nodal ground state whose nodal set (thick on the picture) is made of two isolated points, two groups of three and four line segments respectively, and a group of five half-lines.

by a phase plane analysis we would have $u_i(x_0) := \max u_i \geq \max \phi_\lambda = \left(\frac{1}{2}p\lambda\right)^{1/(p-2)}$. Considering the first zero $x_1 \in s_i$ of u_i, it would then follow that

$$\left(\frac{p\lambda}{2}\right)^{1/(p-2)} \leq u_i(x_0) - u_i(x_1) = \int_{x_1}^{x_0} u_i'(s)\,ds \leq \sqrt{x_0 - x_1}\,\|\tilde{u}'\|_2 < \sqrt{\frac{SJ(\tilde{u})}{\kappa}},$$

which contradicts the choice of S. The rest of the proof follows as in that of Lemma 6.6. □

Proof of Proposition 6.7. The proof is the same as the one of Proposition 6.5, using Lemma 6.8 instead of Lemma 6.6 and observing that, by Theorem 4.12, $J(\tilde{u}) \leq 2s_\lambda$. □

Remark 6.9. Graphs fulfilling Theorem 1.9 can be obtained combining ad libitum the constructions (1), (2), (3). The general result is a graph as the one depicted in Figure 11.

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CONTROLLABILITY OF PARABOLIC EQUATIONS WITH INVERSE SQUARE INFINITE POTENTIAL WELLS VIA GLOBAL CARLEMAN ESTIMATES

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We consider heat operators on a convex domain Ω, with a critically singular potential that diverges as the inverse square of the distance to the boundary of Ω. We establish a general boundary controllability result for such operators in all dimensions, in particular providing the first such result in more than one spatial dimension. The key step in the proof is a new global Carleman estimate with a carefully chosen weight that captures the appropriate boundary conditions, the global geometry of the domain Ω, and the H^1-energy for this problem. The estimate is derived by combining two intermediate Carleman inequalities with distinct and carefully constructed weights involving nonsmooth powers of the boundary distance.

1. Introduction

We consider, on a bounded domain in $\mathbb{R}^n$, the heat operator with a potential that diverges as the inverse square of the distance to the boundary hypersurface. More precisely, our setting will be the following:

Setting. Throughout the paper, we let Γ denote a closed, connected, and convex C^4-hypersurface in $\mathbb{R}^n$ ($n \geqslant 1$), and we let Ω denote the interior domain that is bounded by Γ. In addition, we let $d_\Gamma : \Omega \to \mathbb{R}$ denote the distance to Γ.

We will consider the following equation on Ω and over a time interval:

$$-\partial_t v + \left(\Delta + \frac{\sigma}{d_\Gamma^2}\right) v + Y \cdot \nabla v + W v = 0. \tag{1-1}$$

Here, $\sigma \in \mathbb{R}$ is a parameter measuring the strength of the singular potential, while Y and W represent first and zero-order coefficients that are less singular at Γ.

Our main objective in this paper is to derive boundary null controllability for the above equation. Given any initial state $v(0)$ and $T > 0$, the question is whether one can pick some control f on the boundary $(0, T) \times \Gamma$ so that the evolution through (1-1) — together with the boundary control — drives the solution to the target state $v(T) = 0$ at time T. While results have been established in one spatial dimension using moment methods (see [Biccari 2019]), here we provide, to our best knowledge, the first such result for general domains in arbitrary dimensions.

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To show the above property, we derive sharp Carleman estimates for the operator in (1-1). Indeed, genuinely new estimates are needed, since the singular potential scales as the Laplacian near the hypersurface Γ, hence one cannot treat (1-1) as a perturbation of the standard heat equation. Moreover, these estimates will enable us to obtain robust boundary observability and controllability results, in that we both treat any spatial dimension and deal with a large class of lower-order coefficients. Note the inclusion of Y and W in (1-1) is very natural in our context, as d_Γ itself fails to be regular and well-behaved away from Γ.

1.1. ***Boundary asymptotics.*** Let us start by describing the role of the strength parameter σ in the boundary asymptotics of solutions to (1-1). We let $\sigma < \frac{1}{4}$, and we consider the Cauchy problem associated to (1-1), with initial data $v(0) = v_0$. Moreover, it will often be convenient to write $\sigma := \kappa(1-\kappa)$, with $\kappa := \kappa(\sigma) < \frac{1}{2}$.

According to the classical Frobenius theory for ODEs, the inverse-square singularity of the potential at $d_\Gamma = 0$ implies the characteristic exponents of this equation are precisely κ and $1-\kappa$. Therefore, if κ is not a half-integer (which ensures that logarithmic branches will not appear), solutions to the equation are expected to behave either like d_Γ^κ or $d_\Gamma^{1-\kappa}$ close to Γ and correspond to the Dirichlet and Neumann branches, respectively. As a result, the boundary data for our problem must be formulated with these d_Γ-weights taken into account.

Now, as such quantities will naturally appear throughout the article, we set the following notation for future convenience:

Definition 1.1. Given a strength parameter $\sigma \in \left(-\infty, \frac{1}{4}\right)$:

- We let $\kappa := \kappa(\sigma) \in \mathbb{R}$ be the unique parameter satisfying

$$\sigma := \kappa(1-\kappa), \quad \kappa < \tfrac{1}{2}. \tag{1-2}$$

- We define the associated Dirichlet and Neumann trace operators:

$$\mathcal{D}_\sigma \phi := d_\Gamma^{-\kappa} \phi|_{d_\Gamma \searrow 0}, \quad \mathcal{N}_\sigma \phi := d_\Gamma^{2\kappa} \nabla d_\Gamma \cdot \nabla(d_\Gamma^{-\kappa} \phi)|_{d_\Gamma \searrow 0}. \tag{1-3}$$

- In addition, we introduce the following notation:

$$\Delta_\sigma := \Delta + \frac{\sigma}{d_\Gamma^2}. \tag{1-4}$$

Remark 1.2. We stress that throughout the paper, κ will always implicitly depend on σ via the relation (1-2). Note that there is a one-to-one correspondence between the values of $\sigma \in \left(-\infty, \frac{1}{4}\right)$ and $\kappa \in \left(-\infty, \frac{1}{2}\right)$. In particular:

$$\begin{aligned} \sigma \nearrow \tfrac{1}{4} \quad &\leftrightarrow \quad \kappa \nearrow \tfrac{1}{2}, \\ \sigma = 0 \quad &\leftrightarrow \quad \kappa = 0, \\ \sigma = -\tfrac{3}{4} \quad &\leftrightarrow \quad \kappa = -\tfrac{1}{2}. \end{aligned}$$

In addition, all the associated quantities in (1-1) and Definition 1.1 reduce to the standard ones in the absence of the singular potential, i.e., when $\sigma = 0$.

Later in this paper, we will show that the Dirichlet and Neumann traces in (1-3) indeed lead to viable well-posedness theories for (1-1), at least for a subset of values σ; see Sections 3 and 4. As a result, (1-3) provides natural notions of boundary data for our upcoming main boundary control results.

The specific range of σ for which we will develop well-posedness results is discussed further below. For the moment, we note $\sigma = \frac{1}{4}$ can be viewed as a critical threshold, as (1-1) is expected to be ill-posed for $\sigma > \frac{1}{4}$; see [Baras and Goldstein 1984; Biccari 2019; Vazquez and Zuazua 2000]. (Moreover, Biccari [2019] showed — in one spatial dimension — that the cost of boundary control blows up in the limit $\sigma \nearrow \frac{1}{4}$.) We also highlight $\sigma = -\frac{3}{4}$ as another natural threshold, since the Dirichlet branch fails to lie in L^2 once $\sigma \leqslant -\frac{3}{4}$.

Remark 1.3. Analogues of the adapted boundary data (1-3) have been considered before in the literature in different contexts for other singular operators; see, e.g., [Mazzeo and Melrose 1987; Warnick 2013]. The boundary conditions (1-3) were also used in [Enciso et al. 2021] toward Carleman and observability estimates for the wave equation analogue of (1-1).

1.2. *Motivation.* Parabolic problems involving inverse square potentials have been intensively studied in the past decades; see [Baras and Goldstein 1984; García Azorero and Peral Alonso 1998], for instance, as well as references within for some early results. Since the literature in this area is far too extensive to describe in full, we restrict our focus here to null controllability and Carleman estimates to keep the present discussion concise.

First, in one spatial dimension, in which we can set $\Omega := (0, 1)$ without loss of generality, there are ample results treating the singular heat operator

$$-\partial_t + \partial_x^2 + \frac{\sigma}{x^2}. \tag{1-5}$$

For instance, interior null controllability results for (1-5) — with the control supported away from $x = 0$ — were established in [Cannarsa et al. 2005; 2008; 2020; Martinez and Vancostenoble 2006]. Also, various boundary null controllability results for (1-5) have been proven, both at $x = 1$ (away from the singularity) [Cannarsa et al. 2020] and at $x = 0$ (at the singularity) [Biccari 2019; Cannarsa et al. 2017; Gueye 2014].

Remark 1.4. Many of the above results treated the degenerate parabolic operator

$$-\partial_t + \partial_x (x^\alpha \partial_x \cdot), \quad \alpha \in (0, 2). \tag{1-6}$$

However, this can be transformed to (1-5) through an appropriate change of variables, at least for a subset of parameters σ; see [Biccari 2019, Appendix A] for details.

Of particular relevance is the recent result of Biccari [2019], which established boundary null controllability at $x = 0$ for (1-5), with $\sigma < \frac{1}{4}$. As Biccari [2019] applied the moment method, which relied strongly upon an eigenfunction decomposition of $\partial_x^2 + \sigma x^{-2}$, the results do not readily extend to higher dimensions, nor to parabolic equations with general lower-order terms as in (1-1). Partly for this reason, the author listed several open questions of interest; see [Biccari 2019, Section 8].

A key motivation of the present work is to address a number of these points:

(1) We use *Carleman estimates* to prove our controllability result. Such techniques have the advantage of being more robust, in that they allow one to treat lower-order terms and to more easily extend to nonlinear problems.

(2) We treat the case where the potential diverges on all of Γ. As mentioned in [Biccari 2019], even in one spatial dimension, the case of a potential singular at both $x = 0$ and $x = 1$ cannot be treated via the moment method.

(3) We obtain boundary null controllability in *all spatial dimensions*, under the assumption Γ is convex. To our knowledge, this is the first such boundary control result in higher dimensions; see the discussions below.

In particular, [Biccari 2019] highlighted the problem of developing Carleman estimates adapted to the weighted boundary data (1-3) as being especially challenging.

Next, turning to higher dimensions (with general $\Omega \subseteq \mathbb{R}^n$), [Cannarsa et al. 2009; Ervedoza 2008; Vancostenoble and Zuazua 2008] established interior controllability results for the singular heat operator,

$$-\partial_t + \Delta + \frac{\sigma}{|x - x_0|^2}, \quad x_0 \in \Omega, \tag{1-7}$$

i.e., a singular potential that diverges as an inverse square of the distance to a single interior point. The above results were then extended in [Cazacu 2014] to the case $x_0 \in \Gamma$, in which the potential instead diverges at a single boundary point.

The case of higher dimensional settings (1-1), where the potential becomes singular on all of Γ, is known to be particularly difficult. Incidentally, these arise naturally when considering parabolic equations on conformally compact Riemannian manifolds; see, e.g., [Vázquez 2015]. Along this direction, Biccari and Zuazua [2016] first proved interior null controllability for the operator $-\partial_t + \Delta_\sigma$ using Carleman estimates.

Biccari and Zuazua [2016] stress that one cannot employ their results to derive boundary controllability or boundary observability properties. The key reason is that their Carleman estimates do not capture an appropriate notion of the Neumann data at the boundary, (1-3) in particular. Moreover, the Carleman estimate in [Biccari and Zuazua 2016] only captures the full L^2-norm, and not the (unweighted) H^1-norm; as we shall see, the full H^1-norm will be a critical part of our setup.

1.3. ***Boundary controllability and observability.*** In this subsection, we state the main results of this paper. However, before doing so, we first give a precise description of the lower-order coefficients Y and W in (1-1):

Definition 1.5. We let $\mathcal{Z}$ denote the collection of all pairs (Y, W), where:

- $Y : \Omega \to \mathbb{R}^n$ is a C^1-vector field, and $W : \Omega \to \mathbb{R}$ is an L^∞-function.
- Y extends to a C^3-vector field on a neighborhood of Γ.
- $d_\Gamma W$ extends to a C^2-function on a neighborhood of Γ.

While the exact form of Definition 1.5 is technical in nature, at an informal level, our results will require Y and W to have sufficient regularity at Γ. On the other hand, since d_Γ fails to be regular away from Γ, it will also be useful for Y and W to be less regular away from Γ; see Remark 3.2. Though the conditions in Definition 1.5 are not optimal, we adopt these particular assumptions in their current form, since they allow for a simpler presentation.

The main result of this paper is the boundary null controllability for the singular parabolic equation (1-1). More precisely, we consider the following Cauchy problem:

Problem (C). *Given initial data v_0 on Ω, as well as Dirichlet boundary data f on $(0, T) \times \Gamma$, solve the initial-boundary value problem for v,*

$$\begin{aligned} -\partial_t v + \Delta_\sigma v + Y \cdot \nabla v + W v = 0 \quad & \text{on } (0, T) \times \Omega, \\ v(0) = v_0 \quad & \text{on } \Omega, \\ \mathcal{D}_\sigma v = f \quad & \text{on } (0, T) \times \Gamma, \end{aligned} \tag{1-8}$$

where $\sigma \in \left(-\frac{3}{4}, 0\right)$, and where the lower-order coefficients satisfy $(Y, W) \in \mathcal{Z}$.

The following statement, which is a simplification of the more precise Theorem 4.6 in the main text, represents our main boundary control result:

Theorem 1.6. *Let $\Omega \subseteq \mathbb{R}^n$ be a bounded domain, with a convex, connected, C^4-boundary Γ, and fix $\sigma \in \left(-\frac{3}{4}, 0\right)$. Then, Problem (C) is boundary null controllable in any positive time — for any initial data $v_0 \in L^2(\Omega)$ and any $T > 0$, there exists Dirichlet boundary data $f \in L^2((0, T) \times \Gamma)$ such that the corresponding solution v to (1-8), with the above v_0 and f, satisfies $v(T) \equiv 0$.*

Theorem 1.6 is, to our best knowledge, the first boundary controllability result for $(-\partial_t + \Delta_\sigma)v = 0$ in spatial dimensions higher than 1, and for equation (1-1) — containing also general lower-order terms — in any dimension.

To prove Theorem 1.6, we employ (the variational formulation of) the celebrated Hilbert uniqueness method (HUM); see [Lions 1988; Micu and Zuazua 2005]. As is standard, the main step is to obtain key estimates — most crucially an appropriate *observability inequality* — for the dual problem. Thus, in the context of observability, we will consider the following Cauchy problem for the backwards singular heat equation:

Problem (O). *Given final data u_T on Ω, solve the following problem for u,*

$$\begin{aligned} \partial_t u + \Delta_\sigma u + X \cdot \nabla u + V u = 0 \quad & \text{on } (0, T) \times \Omega, \\ u(T) = u_T \quad & \text{on } \Omega, \\ u = 0 \quad & \text{on } (0, T) \times \Gamma, \end{aligned} \tag{1-9}$$

where $\sigma \in \left(-\frac{3}{4}, 0\right)$, and where the lower-order coefficients satisfy $(X, V) \in \mathcal{Z}$.

Remark 1.7. Since $\sigma < 0$, the boundary condition in (1-9) implies $\mathcal{D}_\sigma u = 0$. While one could develop an equivalent theory using instead the condition $\mathcal{D}_\sigma u = 0$, here we remain with $u = 0$ to be consistent with the existing literature, e.g., [Biccari 2019; Biccari and Zuazua 2016].

A first consideration in the proof of Theorem 1.6 is finding an appropriate choice of spaces for the controllability Problem (C), as well as the corresponding spaces for the observability Problem (O). To apply the HUM, one requires estimates for an appropriately defined Neumann trace in Problem (O):

- The Neumann trace should be bounded by the final data u_T.
- The Neumann trace should satisfy a boundary observability estimate; that is, it should be bounded from below by $u(0)$.

We will show that the above indeed holds when u_T lies in the usual energy space.

In particular, in Section 3, we briefly summarize the well-posedness theory for Problem (O) with final data $u_T \in H_0^1(\Omega)$ — that is, the analogue of strict solutions in [Biccari 2019; Biccari and Zuazua 2016]. We then show (in Proposition 3.14) that if $\sigma \in \left(-\frac{3}{4}, \frac{1}{4}\right)$, then the quantity $\mathcal{N}_\sigma u$ from (1-3) is indeed well-defined and bounded in L^2 by the H^1-norm of u_T. Furthermore, if $\sigma < 0$ as well, then we prove (in Theorem 3.17) observability by bounding $\mathcal{N}_\sigma u$ in L^2 from below by the H^1-norm of $u(0)$. The above two estimates can be roughly summarized by the following theorem:

Theorem 1.8. *Let $\Omega \subseteq \mathbb{R}^n$ be a bounded domain, with a convex, connected, C^4-boundary Γ, and fix $\sigma \in \left(-\frac{3}{4}, 0\right)$. Moreover, let u be a solution to Problem* (O), *with final data $u_T \in H_0^1(\Omega)$. Then, the Neumann data $\mathcal{N}_\sigma u$ on Γ is finite, and*

$$\int_\Omega |\nabla u(0)|^2 \lesssim \int_{(0,T)\times\Gamma} (\mathcal{N}_\sigma u)^2 \lesssim \int_\Omega |\nabla u_T|^2.$$

Using the estimates of Theorem 1.8, the boundary null controllability of Theorem 1.6 then follows by adapting standard duality arguments. In Section 4, we develop the dual theory of weak (or transposition) (H^{-1}-)solutions for Problem (C), now in the presence of the singular potential. We then show (in Theorem 4.6) that in this setting, one can construct the desired null boundary controls in L^2.

We stress that the well-posedness theories for Problems (C) and (O) are far from direct due to the singular potential, and are further complicated by the lower-order terms. Thus, for completeness, we develop both theories in Sections 3 and 4.

The key ingredient to establishing the crucial Theorem 1.8 is a new global Carleman estimate, proved in this paper, that captures both the boundary data (1-3) and the H^1-energy of the solutions. This is discussed in the following subsection.

1.4. *Global Carleman inequality.* Carleman estimates have found many applications in PDEs, such as in unique continuation [Aronszajn 1957; Calderón 1958; Carleman 1939; Dos Santos Ferreira 2005; Escauriaza and Fernández 2003; Hörmander 1985; Tataru 1995], control theory [Duyckaerts et al. 2008; Fursikov and Imanuvilov 1996; Laurent and Léautaud 2019; López et al. 2000; Tataru 1992; 1994], inverse problems [Belishev and Kurylev 1992; Bukhgeim and Klibanov 1981; Klibanov 1992], and embedded eigenvalues in the continuous spectrum of Schrödinger operators.

We next motivate and state the new global Carleman estimate for the singular parabolic operator $\pm\partial_t + \Delta_\sigma$. The premier issue is that of capturing the Neumann boundary data from (1-3), which now involves powers of d_Γ that blow up at Γ. This is achieved through a specially constructed Carleman weight that is designed to generate precisely the correct power of d_Γ at Γ.

In the Carleman estimate of [Biccari and Zuazua 2016] (which yielded interior observability for solutions of $(\partial_t + \Delta_\sigma)u = 0$), the authors employed a weight having, near Γ, the form

$$f_0(t,x) := \frac{1}{t^3(T-t)^3}\left[C - d_\Gamma(x)^2\psi(x) - \left(\frac{d_\Gamma(x)}{d_0}\right)^s e^{s\psi(x)}\right], \tag{1-10}$$

with s a large enough real number, C and d_0 constants, and $\psi \in C^4(\bar{\Omega})$ a function of d_Γ so that f_0 is sufficiently smooth near and at Γ. For our case, we must replace s by a smaller power depending on κ, so that appropriate singular weights appear upon differentiation. In particular, near Γ, our weight will be of the form

$$F_0(t,x) := \frac{1}{t(T-t)}\left[\frac{1}{1+2\kappa} d_\Gamma(x)^{1+2\kappa} + \beta\right], \tag{1-11}$$

with $\beta > 0$ a suitably chosen constant. A key step will be then to show that the weight (1-11) indeed suffices to capture the Neumann trace from (1-3) on Γ.

Next, observe that in order to prove Theorem 1.8, our Carleman estimate will also need to control the H^1-norm on Ω. In [Biccari and Zuazua 2016], their choice of weight (1-10) yields control of a bulk quantity that is roughly of the form

$$\int_0^T \frac{1}{t^3(T-t)^3} \int_\Omega d_\Gamma^s |\nabla u|^2 \, dx \, dt, \qquad s > 0.$$

Because of the factor $d_\Gamma(x)^s$, which vanishes near Γ, their estimate fails to capture the full H^1-energy of u. (Only the full L^2-norm was needed in [Biccari and Zuazua 2016].)

For our setting, we show that by using the weight (1-11) instead, we can capture the full $\dot{H}^1$-norm, without a weight that degenerates at Γ. Here, we note that our assumption of Γ being convex is crucial, as this ensures that the bulk terms in our Carleman estimate containing $|\nabla u|^2$ are uniformly positive.

Unfortunately, (1-11) does not yet suffice for a global Carleman estimate on all of Ω. This is because while d_Γ is C^4 near Γ (by the regularity of Γ), it can fail to be differentiable elsewhere in Ω due to the presence of caustics. To get around this, we replace d_Γ by a more general *boundary defining function* $y \in C^4(\Omega)$ that coincides with d_Γ in a thin neighborhood of Γ. While this function y remains regular away from Γ, it also retains almost the same convexity properties as d_Γ. See Definition 2.1 for the precise properties of y, and Lemma 2.4 for its construction.

Thus, for our global Carleman weight, we replace d_Γ in (1-11) by y:

$$F(t,x) := \frac{1}{t(T-t)}\left[\frac{1}{1+2\kappa} y(x)^{1+2\kappa} + \beta\right]. \tag{1-12}$$

Since y is "close enough" to d_Γ for our purposes, by using F, we both capture the Neumann trace and bound the global $\dot{H}^1$-norm on all of Ω as desired.

We emphasize that the above still leaves untreated one fundamental issue — while these arguments suffice to control the L^2-norm of ∇u, the same cannot be said for the L^2-norm of u itself. Away from the (unique by construction) critical point x_* of y, our Carleman inequality allows us to control bulk integrals (over $(0,T)\times\Omega$) of u^2 with uniformly positive weights, provided $\sigma\in\left(-\frac{3}{4},0\right)$. However, these weights, which are accompanied by factors of $|\nabla y|^2$, can become nonpositive near x_*.

To overcome this rather serious obstacle, we construct *two* boundary defining functions y_1, y_2 with distinct critical points $x_{1,*}\neq x_{2,*}$; see Lemma 2.4. We then *sum the two Carleman estimates* arising from y_1 and y_2. In particular, the above-mentioned nonpositivity for the y_1-Carleman estimate near $x_{1,*}$ can be overcome by a positive L^2-contribution in the y_2-estimate (since $x_{1,*}$ is away from $x_{2,*}$), which also has an extra factor of the large Carleman parameter λ. Thus, by combining two Carleman estimates, we can absorb all nonpositive terms into positive ones.

Remark 1.9. Similar tricks involving summing two Carleman estimates with different weights were used in [Alexakis and Shao 2015; Jena 2021; Shao 2019], in the context of wave equations.

Combining all the above leads to our Carleman estimate, for which an informal simplified version is stated below; see Theorem 2.9 for the precise statement.

Theorem 1.10 (global Carleman estimate). *Let $\Omega\subseteq\mathbb{R}^n$ be a bounded domain, with a convex, connected, C^4-boundary Γ, and fix $\sigma\in\left(-\frac{3}{4},0\right)$. Then, there are two boundary defining functions y_1, $y_2\in C^4(\Omega)$, such that, for any $T>0$ and $\lambda\gg 1$, and for any sufficiently regular function u satisfying $u=0$ on $(0,T)\times\Gamma$,*

$$C\lambda\int_{(0,T)\times\Gamma}(\mathcal{N}_\sigma u)^2\,dS\,dt+\sum_{j=1,2}\int_{(0,T)\times\Omega}e^{-2\lambda F_j}(\pm\partial_t u+\Delta_\sigma u)^2 \gtrsim \lambda\sum_{j=1,2}\int_{(0,T)\times\Omega}e^{-2\lambda F_j}\big[y_j^{2\kappa}|\nabla u|^2+y_j^{6\kappa-1}(\lambda^2+y_j^{-1-4\kappa})u^2\big], \tag{1-13}$$

where F_j is the Carleman weight (1-12), *but with y replaced by y_j.*

The proof of Theorem 1.10 follows the usual multiplier approach to Carleman estimates for heat equations, using the weights (1-12) for both y_1 and y_2. Aside from the ideas mentioned before, there are two key technical challenges to overcome. The first is showing that the boundary terms capture the Neumann trace; this follows from computations for the boundary terms (Lemma 2.7), along with the detailed understanding of boundary asymptotics gained from Proposition 3.14.

The second, and more difficult, challenge is to ensure all the top-order bulk terms obtained in the computations have good sign. As there are many singular weights involved, we have more dangerous terms to consider than in standard derivations of Carleman estimates. These are treated via extensive computations (see Lemma 2.7) that use, in an essential way, both the geometry of the domain — via convexity of the level hypersurfaces of y — and our assumption that $\sigma\in\left(-\frac{3}{4},0\right)$.

Remark 1.11. In the full statement, Theorem 2.9, of our Carleman estimate, the power $1+2\kappa$ in (1-12) is replaced by a more general parameter $2p$. For purposes of boundary control, one requires $2p=1+2\kappa$ to capture the Neumann trace. However, allowing for more general powers p leads to unique continuation properties for a larger range of σ. We plan to revisit this point in a future paper.

Remark 1.12. Note the estimate in the precise Theorem 2.9 differs from that of Theorem 1.10 in that the Neumann integral in (1-13) is replaced by various boundary limits of integrals over hypersurfaces $\{y_j = \delta\}$, as $\delta \searrow 0$. However, one can show that, in the context of Problem (O), each of these boundary limits will either vanish or be bounded by the desired Neumann integral; for details, see the proof of Theorem 3.17, as well as Section 3.3 for the limit computations. The simpler Neumann integral was written in (1-13) for conceptual clarity.

1.5. ***Further discussion.*** Let us now elaborate on the specific range $\sigma \in \left(-\frac{3}{4}, 0\right)$ that is assumed in all our main results. As mentioned before, this is required in the proof of Theorem 1.10 to ensure positivity of the bulk L^2-terms. However, there are also conceptual reasons for applying this particular restriction.

First, the condition $\sigma > -\frac{3}{4}$ is crucial to the setup of our well-posedness theories. As mentioned before, on the control side (Problem (C)), this is needed for solutions of (1-8) with inhomogeneous Dirichlet data to be L^2-integrable on Ω. Furthermore, on the observability side (Problem (O)), this seems necessary in order to bound the Neumann trace from above by the H^1-energy; see Proposition 3.14. The latter is an essential part of the Hilbert uniqueness method setup we apply here. Thus, we do not expect our results to extend to $\sigma \leqslant -\frac{3}{4}$, at least within the well-posedness and HUM settings adopted in this paper.

Of course, the case $\sigma = 0$ is just the classical heat equation, for which global Carleman estimates are now standard. However, one should note that the proof of Theorem 1.10 does not carry over to this case simply by setting $\sigma = 0$, as it uses in a crucial way the critical singularity of the potential.

On the other hand, it is less clear whether our results can be extended beyond to the range $\sigma \in \left(0, \frac{1}{4}\right)$, though there seem to be some obstacles. For one, note the Carleman estimate (1-13) fails to control the full H^1-energy when $\sigma > 0$ ($\kappa > 0$). Furthermore, in this regime, the boundary condition $u = 0$ in (1-9) does not directly imply $\mathcal{D}_\sigma u = 0$. Therefore, one could expect that our Carleman weight (1-12) and our choice of spaces are not well-adapted to this case $\sigma \in \left(0, \frac{1}{4}\right)$.

Remark 1.13. Also worth mentioning is the result of Gueye [2014], which established boundary controllability of the degenerate parabolic equation (1-6) in one spatial dimension using spectral theoretic methods and a variant of Ingham's inequality. However, this result cannot be directly compared to ours, since [Gueye 2014] uses different spaces in its HUM setup. In particular, [Gueye 2014] showed that the L^2-norm of the Neumann datum controls the fractional $H^{-\kappa}$-norm of the solution, and vice versa. In contrast, we are less optimal with regards to regularity, but we use the smoothing property of parabolic equations to our advantage.

Finally, for wave operators having the same singular potential (i.e., $-\partial_t^2 + \Delta_\sigma$), we recently established in [Enciso et al. 2021] — in the special case $n > 2$ and Ω a unit ball — boundary observability through a similar sharp global Carleman estimate. While the Carleman weight is different from (1-12), due to the equation being hyperbolic, it is built upon the same sharp power of d_Γ yielding both the H^1-energy and the Neumann boundary trace. Interestingly, this observability fails to imply boundary control for wave operators, as the lack of smoothing prevents us from applying the HUM machinery. Using this framework, boundary controllability would necessitate working with fractional Sobolev spaces of optimal regularity, as in [Gueye 2014].

One can also view Theorem 1.10 partly as extending the methods of [Enciso et al. 2021] (which hold only for Ω being a unit ball) to all convex domains. It would be interesting to determine whether the results of [Enciso et al. 2021] also hold for general convex Ω.

1.6. ***Organization of the paper.*** In Section 2, we construct boundary defining functions that coincide with the distance d_Γ near the boundary Γ. These are then used to prove a precise version of our global Carleman estimate, Theorem 1.10. The applications of this Carleman estimate to boundary observability and controllability are then presented in Sections 3 and 4, respectively.

2. The Carleman estimate

In this section, we prove a precise version of Theorem 1.10 — our main Carleman estimate for parabolic operators with inverse square potentials.

In the remainder of the paper, we adopt the setting described in the beginning of the introduction — in particular the domain $\Omega \subseteq \mathbb{R}^n$, its convex boundary Γ, and the distance d_Γ to the boundary. Moreover, since d_Γ is always C^4 in a neighborhood of Γ, we can also adopt the following for convenience:

Setting (regularity of d_Γ). Let $0 < d_0 \ll 1$ be such that d_Γ is C^4 on the domain

$$\{x \in \Omega \mid d_\Gamma(x) < 2d_0\}.$$

2.1. ***Construction of boundary defining functions.*** As described in the introduction, the proof of our Carleman estimate will require, as weights, boundary defining functions that extend d_Γ while essentially preserving concavity and regularity. Here, we detail the construction of such functions.

First, we list the precise conditions needed for our constructions:

Definition 2.1. Given constants $\varepsilon, \varepsilon' > 0$, we call $y \in C^4(\Omega)$ an $(\varepsilon, \varepsilon')$-*boundary defining function* for Ω if and only if the following properties hold:

(a) y is strictly positive on Ω, and $y = d_\Gamma$ on $\{x \in \Omega : d_\Gamma(x) < d_0\}$.

(b) y has a unique critical point $x_* \in \Omega$, with $d_\Gamma(x_*) > 2d_0$.

(c) y satisfies the following gradient bounds:

$$\begin{cases} |\nabla y|^2 = 1, & d_\Gamma(x) \leqslant d_0, \\ |\nabla y|^2 \geqslant \frac{1}{2}, & d_0 < d_\Gamma < 2d_0. \end{cases} \tag{2-1}$$

(d) y satisfies the following concavity properties for each $x \in \Omega$ and $\xi \in \mathbb{R}^n$:

$$\begin{cases} -\xi \cdot \nabla^2 y(x) \cdot \xi \geqslant 0, & d_\Gamma(x) \leqslant d_0, \\ -\xi \cdot \nabla^2 y(x) \cdot \xi \geqslant -\varepsilon' |\xi|^2, & d_0 < d_\Gamma(x) < 2d_0, \\ -\xi \cdot \nabla^2 y(x) \cdot \xi \geqslant \varepsilon |\xi|^2, & d_\Gamma(x) \geqslant 2d_0. \end{cases} \tag{2-2}$$

Remark 2.2. Definition 2.1 implies x_* is a nondegenerate maximum of y, that is, $\nabla y(x_*) = 0$ and $\nabla^2 y(x_*)$ is negative-definite. Furthermore, note that x_* is the only maximum of y, so that ∇y vanishes only at x_*.

Definition 2.3. Given any $\varepsilon, \varepsilon' > 0$, we refer to (y_1, y_2) as an $(\varepsilon, \varepsilon')$-*boundary defining pair* in Ω if and only if the following properties hold:

(i) Both y_1 and y_2 are $(\varepsilon, \varepsilon')$-boundary defining functions.

(ii) The (unique) critical points of y_1 and y_2 are distinct: $x_{1,*} \neq x_{2,*}$.

In the proof of our global Carleman estimates, we will employ a carefully constructed boundary defining pair. As the first step, we show that any convex domain admits such a pair, given sufficiently small parameters:

Lemma 2.4. *There exist $C, C', \varepsilon_0 > 0$ — depending only on Ω, d_0 — such that, for any $0 < \varepsilon < \varepsilon_0$, there exists a $(C\varepsilon, C'\varepsilon)$-boundary defining pair (y_1, y_2) in Ω.*

Proof. We begin by constructing one such boundary defining function y_1. First, note that if $T_p\Gamma$ is the tangent hyperplane to Γ at a point p and $x \in \Omega$, then

$$d_\Gamma(x) = \inf_{p \in \Gamma} \operatorname{dist}(x, T_p\Gamma),$$

by the convexity of Γ. This implies d_Γ is a concave function on Ω; in particular, for any $\xi \in \mathbb{R}^n$, the distributional derivative $-\xi \cdot \nabla^2 d_\Gamma \cdot \xi$ is a nonnegative measure.

Consider now the function

$$d^\varepsilon := \phi^\varepsilon * d_\Gamma, \quad \phi^\varepsilon(x) := \varepsilon^{-n}\phi\left(\frac{x}{\varepsilon}\right) \tag{2-3}$$

for a small parameter $0 < \varepsilon < \varepsilon_0$, where ϕ is a standard positive mollifier:

$$\phi \in C_c^\infty(B_1(0), [0, \infty)), \qquad \int_{\mathbb{R}^n} \phi(x)\,dx = 1.$$

Note d^ε is smooth and concave by the concavity of d_Γ — indeed, for all $\xi \in \mathbb{R}^n$,

$$-\xi \cdot \nabla^2 d^\varepsilon \cdot \xi = \phi^\varepsilon * (-\xi \cdot \nabla d_\Gamma \cdot \xi) \geqslant 0, \tag{2-4}$$

since $\phi \geqslant 0$ and $-\xi \cdot \nabla^2 d_\Gamma \cdot \xi$ is a nonnegative measure on Ω.

We now introduce a new cutoff $\varphi \in C^\infty(\Omega)$ such that

$$\varphi(x) = \begin{cases} 1, & d_\Gamma(x) \leqslant d_0, \\ 0, & d_\Gamma(x) \geqslant 2d_0. \end{cases} \tag{2-5}$$

In terms of these functions, we then set $y_1 \in C^4(\Omega)$ as

$$y_1(x) := d_\Gamma(x) + [1 - \varphi(x)][d^\varepsilon(x) - d_\Gamma(x) - \varepsilon|x|^2], \tag{2-6}$$

with $\varepsilon < \varepsilon_0 \ll d_0$. (Note $1 - \varphi \equiv 0$ near Γ, where d^ε fails to be defined.)

To begin with, in the region $\{d_\Gamma \leqslant d_0\}$, we note that $y_1 = d_\Gamma$, since $\varphi = 1$ there by (2-5). Furthermore, the above implies

$$|\nabla y_1|^2 = 1, \qquad -\xi \cdot \nabla^2 y_1 \cdot \xi \geqslant 0, \quad \xi \in \mathbb{R}^n.$$

In particular, all the conditions in Definition 2.1 are satisfied by y_1 on $\{d_\Gamma \leqslant d_0\}$.

Next, consider the intermediate region $\{d_0 < d_\Gamma < 2d_0\}$. Since d_Γ is C^4 there,

$$\|d^\varepsilon - d_\Gamma\|_{C^4(\{d_0<d_\Gamma<2d_0\})} \leqslant C\varepsilon.$$

Moreover, since $|\nabla d_\Gamma| = 1$ and $|1-\varphi| \leqslant 1$ in this region, the above implies

$$y_1 \geqslant \frac{d_0}{2} - C'\varepsilon > 0, \quad |\nabla y_1|^2 \geqslant 1 - C'\varepsilon^2 > \tfrac{1}{2}, \tag{2-7}$$

for sufficiently small ε_0 (depending on Ω, d_0), as well as

$$-\xi \cdot \nabla^2 y_1 \cdot \xi = -\xi \cdot \nabla^2 d_\Gamma \xi - \xi \cdot \nabla^2\big[(1-\varphi)(d^\varepsilon - d_\Gamma - \varepsilon|x|^2)\big] \cdot \xi \geqslant -C'\varepsilon|\xi|^2 \tag{2-8}$$

for all $\xi \in \mathbb{R}^n$, where $C' > 0$ denotes constants (depending on Ω, d_0) that can change between lines. Thus, y_1 satisfies the conditions of Definition 2.1 on $\{d_0 < d_\Gamma < 2d_0\}$.

Lastly, consider the region $\{d_\Gamma \geqslant 2d_0\}$, on which

$$y_1 = d^\varepsilon - \varepsilon|x|^2.$$

The above, along with (2-3), implies that y_1 is uniformly positive on this region for sufficiently small ε_0, and that y_1 is uniformly concave, since by (2-4),

$$-\xi \cdot \nabla^2 y_1 \cdot \xi = -\xi \cdot \nabla^2 d^\varepsilon \cdot \xi + 2\varepsilon|\xi|^2 \geqslant 2\varepsilon|\xi|^2, \quad \xi \in \mathbb{R}^n.$$

Moreover, since y_1 is a positive function on Ω whose gradient does not vanish on $\{d_\Gamma \leqslant 2d_0\}$ and which is uniformly concave on $\{d_\Gamma \geqslant 2d_0\}$, y_1 must have a unique critical point $x_{1,*} \in \{d_\Gamma > 2d_0\}$, its maximum. Therefore, y_1 satisfies all the conditions of Definition 2.1 on $\{d_0 \geqslant 2d_0\}$.

The above yields that y_1 is a $(C\varepsilon, C'\varepsilon)$-boundary defining function, for appropriate constants C, C' and sufficiently small ε_0. It remains to construct a new function y_2 so that (y_1, y_2) defines a corresponding boundary defining pair.

To this end, note by the Morse lemma, there is a neighborhood $U \subset \{d_\Gamma > 2d_0\}$ around $x_{1,*}$ and local coordinates $z : U \to \mathbb{R}^n$ such that y_1 is a quadratic form on U: $y_1 = z \cdot A \cdot z$, with A a nonsingular $n \times n$ matrix. Furthermore, without loss of generality, one can assume $z(x_{1,*}) = 0$, and U is an open ball $B_{2\eta}(0)$ in z-coordinates, for some small $\eta > 0$. As the critical point $x_{1,*}$ is nondegenerate, $|\nabla y_1| \geqslant c_0 > 0$ on $U \setminus U'$, where $U' = B_\eta(0)$ in z-coordinates.

We then take a cutoff function $\chi \in C^\infty(\Omega)$ satisfying $\chi \equiv 1$ on U' and $\chi \equiv 0$ on $\Omega \setminus U$, and we define the function

$$y_2 := y_1 + \delta\chi b \cdot z, \quad b \in \mathbb{S}^{n-1}, \ \ \delta \ll 1. \tag{2-9}$$

Since y_2 coincides with y_1 on $\Omega \setminus U$, then y_2 satisfies all the conditions of Definition 2.1 (with the same parameters) on both $\{d_\Gamma \leqslant d_0\}$ and $\{d_0 < d_\Gamma < 2d_0\}$.

For the remaining inner region, note we have on U' that

$$\nabla_z y_2 = 2A \cdot z + \delta b,$$

so that y_2 has a critical point at

$$z(x_{2,*}) = -\tfrac{1}{2}\delta A^{-1} b \neq 0,$$

which is unique in U'. Moreover, as the shift $\delta\chi b\cdot z$ is supported in U and

$$\|\delta\chi b\cdot z\|_{C^j}\lesssim\delta\eta^{1-j},\quad j\leqslant 4,\tag{2-10}$$

no new critical points are introduced as long as δ is taken small enough with respect to η; in particular, we can ensure that $|\nabla_z y_2|>0$ in $U\setminus U'$. Similarly, by further shrinking δ if needed, (2-9) and (2-10) also ensure that, on $\{d_\Gamma>2d_0\}$,

$$-\xi\cdot\nabla^2 y_2\cdot\xi\geqslant C\varepsilon|\xi|^2,\quad \xi\in\mathbb{R}^n,$$

possibly with a different value of C. Thus, y_2 satisfies all the conditions of Definition 2.1, hence (y_1, y_2) is our desired boundary defining pair. □

Finally, since d_Γ fails to be regular away from Γ, it will often be useful to replace our singular operator by a smoother variant:

Definition 2.5. Given any $y\in C^4(\Omega)$, we define the y-modified operators

$$\Delta_{\sigma,y}:=\Delta+\sigma y^{-2},\quad \sigma\in\mathbb{R}.\tag{2-11}$$

For convenience, we also adopt the following notation for the y-derivative:

$$D_y v:=\nabla y\cdot\nabla v,\quad v\in C^1(\Omega).\tag{2-12}$$

In particular, when y is a boundary defining function, so that $y=d_\Gamma$ near Γ, the difference $d_\Gamma^{-2}-y^{-2}$ is hence bounded on Ω. Thus, it will suffice to prove Carleman estimates for $\pm\partial_t+\Delta_{\sigma,y}$, which has a C^4 singular potential, rather than $\pm\partial_t+\Delta_\sigma$.

With this notation in hand, we prove a pointwise Hardy-type inequality associated with D_y-derivatives that will useful in proving our Carleman estimates:

Lemma 2.6. *The following holds for any $q\in\mathbb{R}$, $y\in C^4(\Omega)$, and $v\in C^1(\Omega)$:*

$$\begin{aligned}y^{2q}(D_y v)^2\geqslant{}&\tfrac14(1-2q)^2y^{2q-2}|\nabla y|^4v^2+\nabla\cdot\big[\tfrac12(1-2q)y^{2q-1}\nabla y|\nabla y|^2v^2\big]\\&-\tfrac12(1-2q)\big[y^{2q-1}\Delta y|\nabla y|^2v^2+2y^{2q-1}(\nabla y\cdot\nabla^2y\cdot\nabla y)v^2\big].\end{aligned}\tag{2-13}$$

Proof. This is a direct consequence of the inequality

$$\begin{aligned}0&\leqslant(y^qD_yv+by^{q-1}|\nabla y|^2v)^2\\&=y^{2q}(D_yv)^2+b^2y^{2q-2}|\nabla y|^4v^2+2by^{2q-1}|\nabla y|^2vD_yv\\&=y^{2q}(D_yv)^2+b(b-2q+1)y^{2q-2}|\nabla y|^4v^2-2by^{2q-1}(\nabla y\cdot\nabla^2y\cdot\nabla y)v^2\\&\qquad-by^{2q-1}\Delta y|\nabla y|^2v^2+\nabla\cdot(by^{2q-1}\nabla y|\nabla y|^2v^2),\end{aligned}$$

which holds for any constants $q, b\in\mathbb{R}$. Equation (2-13) is then obtained by taking the optimal value of the parameter $b:=\frac12(2q-1)$. □

2.2. ***The global pointwise inequality.*** Our aim here is to prove the following key lemma, which serves as the pointwise Carleman inequality obtained from a single boundary defining function y. In particular, this attains adequate control for our solutions everywhere except near the critical point of y.

Lemma 2.7. *Fix $T > 0$, and let $p, \sigma \in \mathbb{R}$ satisfy*

$$0 < p < \tfrac{1}{2}, \quad p^2 - 2p + \sigma \geqslant -\tfrac{3}{4}. \tag{2-14}$$

Let $\varepsilon, \varepsilon', \delta > 0$ be sufficiently small (depending on T, Ω, d_0, σ, p), let $y \in C^4(\Omega)$ be an $(\varepsilon, \varepsilon')$-boundary defining function, and let x_* denote the critical point of y. Then, there exist $C, C', \lambda_0 > 0$ (depending on T, Ω, d_0, σ, p, ε, ε', δ) such that the following inequality holds on $[0, T] \times \Omega$ for any $\lambda \geqslant \lambda_0$ and any $u \in C^2([0, T] \times \Omega)$:

$$\begin{aligned} e^{-2\lambda F}|(\pm\partial_t + \Delta_{\sigma,y})u|^2 - 4(\partial_t J^t + \nabla\cdot J) \geqslant C\lambda\theta e^{-2\lambda F} y^{-1+2p}|\nabla u|^2 - C'\lambda^2\theta^3 e^{-2\lambda F} y^{-3+4p} \mathbb{1}_{B_\delta(x_*)} u^2 \\ + Ce^{-2\lambda F}(\lambda^3\theta^3 y^{-4+6p} + \lambda\theta y^{-3+2p})\mathbb{1}_{\Omega\setminus B_\delta(x_*)} u^2, \end{aligned} \tag{2-15}$$

where the weight F is given by

$$F(t, x) := \theta(t) f(y(x)), \quad \theta(t) := \frac{1}{t(T-t)}, \quad f(y) := \frac{1}{2p} y^{2p} + \beta, \tag{2-16}$$

with $\beta > 0$ an arbitrary constant, where J^t is a scalar function satisfying

$$|J^t| \leqslant Ce^{-2\lambda F}|\nabla u|^2 + Ce^{-2\lambda F}\lambda^2\theta^2 y^{-2} u^2, \tag{2-17}$$

and where J is a vector field satisfying, sufficiently near Γ,

$$\nabla y \cdot J - e^{-2\lambda F}\partial_t u D_y u \leqslant Ce^{-2\lambda F}\lambda\theta y^{-1+2p}(D_y u)^2 + Ce^{-2\lambda F}\lambda^3\theta^3 y^{-3+2p} u^2. \tag{2-18}$$

Proof. Throughout, we let $C, C' > 0$ denote constants with the same dependencies as in the lemma statement, and such that their values can change from line to line. Furthermore, it suffices to prove (2-15) for just the backward operator $\partial_t + \Delta_{\sigma,y}$, as the estimate for $-\partial_t + \Delta_{\sigma,y}$ then follows via a time reversal $t \mapsto T - t$.

For clarity of exposition, we divide the proof into four steps.

Step 1. The conjugate inequality. First, we prove the key preliminary commutator estimates for the operator $\partial_t + \Delta_{\sigma,y}$. For this, let us set

$$v := e^{-\lambda F} u. \tag{2-19}$$

Furthermore, the following constant will be useful later in the proof:

$$z := \frac{1-2p}{2y(x_*)} > 0. \tag{2-20}$$

Using (2-19) and (2-20), we expand $(\partial_t + \Delta_{\sigma,y})u$ as

$$e^{-\lambda F}(\partial_t + \Delta_{\sigma,y})u = e^{-\lambda F}(\partial_t + \Delta_{\sigma,y})(e^{\lambda F} v) = Sv + \Delta v + \mathcal{A}_0 v, \tag{2-21}$$

where Sv and $\mathcal{A}_0$ are given by

$$Sv := \partial_t v + 2\lambda \nabla F \cdot \nabla v + \lambda(\Delta F - 2z D_y F)v, \quad \mathcal{A}_0 := \lambda \partial_t F + 2\lambda z D_y F + \lambda^2 |\nabla F|^2 + \sigma y^{-2}. \tag{2-22}$$

Multiplying (2-21) by Sv, and noting from Cauchy's inequality that

$$e^{-\lambda F}(\partial_t + \Delta_{\sigma,y})u Sv \leqslant \tfrac{1}{4} e^{-2\lambda F} |(\partial_t + \Delta_{\sigma,y})u|^2 + |Sv|^2,$$

we then conclude

$$\tfrac{1}{4} e^{-2\lambda F} |(\partial_t + \Delta_{\sigma,y})u|^2 \geqslant \Delta v Sv + \mathcal{A}_0 v Sv. \tag{2-23}$$

We now expand the terms on the right-hand side of (2-23). First, we have

$$\Delta v Sv = \Delta v \partial_t v + 2\lambda \Delta v (\nabla F \cdot \nabla v) + \lambda(\Delta F - 2z D_y F) v \Delta v = I_t^\Delta + I_1^\Delta + I_0^\Delta. \tag{2-24}$$

The first term on the right-hand side is straightforward:

$$I_t^\Delta = \nabla \cdot (\nabla v \partial_t v) + \partial_t \big(\tfrac{1}{2} |\nabla^2 v|\big). \tag{2-25}$$

The most involved term is I_1^Δ, requiring multiple applications of the Leibniz rule:

$$\begin{aligned} I_1^\Delta &= \nabla \cdot [2\lambda \nabla v (\nabla F \cdot \nabla v)] - \lambda \nabla F \cdot \nabla (|\nabla v|^2) - 2\lambda (\nabla v \cdot \nabla^2 F \cdot \nabla v) \\ &= \nabla \cdot [2\lambda \nabla v (\nabla F \cdot \nabla v) - \lambda \nabla F |\nabla v|^2] + \lambda \Delta F |\nabla v|^2 - 2\lambda (\nabla v \cdot \nabla^2 F \cdot \nabla v). \end{aligned} \tag{2-26}$$

A similar computation also yields

$$\begin{aligned} I_0^\Delta &= \nabla \cdot [\lambda(\Delta F - 2z D_y F) v \nabla v] - \lambda(\Delta F - 2z D_y F)|\nabla v|^2 - \tfrac{1}{2}\lambda \nabla(\Delta F - 2z D_y F) \cdot \nabla(v^2) \\ &= \nabla \cdot \big[\lambda(\Delta F - 2z D_y F) v \nabla v - \tfrac{1}{2}\lambda \nabla(\Delta F - 2z D_y F) v^2\big] - \lambda(\Delta F - 2z D_y F)|\nabla v|^2 \\ &\qquad + \tfrac{1}{2}\lambda \Delta(\Delta F - 2z D_y F) v^2. \end{aligned} \tag{2-27}$$

Moreover, for the remaining term in (2-23), we expand

$$\begin{aligned} \mathcal{A}_0 v Sv &= \tfrac{1}{2}\mathcal{A}_0 \partial_t (v^2) + \lambda \mathcal{A}_0 \nabla F \cdot \nabla (v^2) + \lambda(\Delta F - 2z D_y F)\mathcal{A}_0 v^2 \\ &= \partial_t \big(\tfrac{1}{2}\mathcal{A}_0 v^2\big) + \nabla \cdot (\lambda \mathcal{A}_0 \nabla F v^2) - \tfrac{1}{2}\partial_t \mathcal{A}_0 v^2 - \lambda \nabla F \cdot \nabla \mathcal{A}_0 v^2 - 2z\lambda D_y F \mathcal{A}_0 v^2. \end{aligned} \tag{2-28}$$

Combining (2-24)–(2-28), the estimate (2-23) then becomes

$$\tfrac{1}{4} e^{-2\lambda F} |(\partial_t + \Delta_{\sigma,y})u|^2 \geqslant \partial_t J_t^0 + \nabla \cdot J^0 + 2z\lambda D_y F |\nabla v|^2 - 2\lambda (\nabla v \cdot \nabla^2 F \cdot \nabla v) + \mathcal{A} v^2, \tag{2-29}$$

where the zero-order coefficient $\mathcal{A}$ is given by

$$\mathcal{A} := -\tfrac{1}{2}\partial_t \mathcal{A}_0 - \lambda \nabla F \cdot \nabla \mathcal{A}_0 - 2z\lambda D_y F \mathcal{A}_0 + \tfrac{1}{2}\lambda \Delta(\Delta F - 2z D_y F), \tag{2-30}$$

and where the scalar J^t and vector field J_0 are given by

$$\begin{aligned} J^t &= \tfrac{1}{2}|\nabla v|^2 + \tfrac{1}{2}\mathcal{A}_0 v^2, \\ J_0 &= \nabla v \partial_t v + 2\lambda \nabla v (\nabla F \cdot \nabla v) - \lambda \nabla F |\nabla v|^2 + \lambda(\Delta F - 2z D_y F) v \nabla v \\ &\qquad - \tfrac{1}{2}\lambda \nabla(\Delta F - 2z D_y F) v^2 + \lambda \mathcal{A}_0 \nabla F v^2. \end{aligned} \tag{2-31}$$

Step 2. First-order terms. We record here the following identities for F:

$$\begin{aligned}\nabla F &= \theta y^{-1+2p}\nabla y,\\ \nabla^2 F &= -(1-2p)\theta y^{-2+2p}(\nabla y\otimes\nabla y)+\theta y^{-1+2p}\nabla^2 y,\\ \Delta F &= -(1-2p)\theta y^{-2+2p}|\nabla y|^2+\theta y^{-1+2p}\Delta y.\end{aligned}\tag{2-32}$$

As a result, we see from (2-32) that

$$\begin{aligned}&2z\lambda D_y F|\nabla v|^2-2\lambda(\nabla v\cdot\nabla^2 F\cdot\nabla v)\\ &=2z\lambda\theta y^{-1+2p}|\nabla y|^2|\nabla v|^2-2\lambda\theta y^{-1+2p}(\nabla v\cdot\nabla^2 y\cdot\nabla v)+2(1-2p)\lambda\theta y^{-2+2p}(D_y v)^2\\ &\geqslant 2\lambda\theta y^{-1+2p}[\nabla v\cdot(\eta z|\nabla y|^2 I-\nabla^2 y)\cdot\nabla v]+2(1-2p)\lambda\theta y^{-2+2p}(D_y v)^2\\ &\qquad+2(1-\eta)z\lambda\theta y^{-1+2p}(D_y v)^2,\end{aligned}\tag{2-33}$$

for some $0<\eta<1$ whose value will be chosen later.

Applying the Hardy inequality (with $q=-1+p$ and $q=-\frac{1}{2}+p$), we see that

$$\begin{aligned}&2(1-2p)\lambda\theta y^{-2+2p}(D_y v)^2+2(1-\eta)z\lambda\theta y^{-1+2p}(D_y v)^2\\ &\geqslant \nabla\cdot J_H+\tfrac{1}{2}(1-2p)(3-2p)^2\lambda\theta y^{-4+2p}|\nabla y|^4v^2+2(1-\eta)(1-p)^2 z\lambda\theta y^{-3+2p}|\nabla y|^4 v^2\\ &\qquad-(1-2p)(3-2p)\lambda\theta y^{-3+2p}\Delta y|\nabla y|^2v^2-C'\lambda\theta y^{-2+2p}v^2,\end{aligned}\tag{2-34}$$

where the vector field J_H is given by

$$J_H:=(1-2p)(3-2p)\lambda\theta y^{-3+2p}\nabla y|\nabla y|^2v^2+2(1-\eta)(1-p)z\lambda\theta y^{-2+2p}\nabla y|\nabla y|^2v^2.\tag{2-35}$$

In particular, we have collected all terms of order y^{-2+2p} or better into the final negative term in the right-hand side of (2-34). Furthermore, any term containing $\nabla y\cdot\nabla^2 y\cdot\nabla y$ can be included in this negative term by default, since by Definition 2.1 both $|\nabla y|^2=1$ and $\nabla y\cdot\nabla^2 y\cdot\nabla y=0$ in the region $d_\Gamma\leqslant d_0$.

Combining now (2-29) with (2-33)–(2-35) yields

$$\begin{aligned}&\tfrac{1}{4}e^{-2\lambda F}|(\partial_t+\Delta_{\sigma,y})u|^2-(\partial_t J^t+\nabla\cdot J)\\ &\geqslant 2\lambda\theta y^{-1+2p}[\nabla v\cdot(\eta z|\nabla y|^2 I-\nabla^2 y)\cdot\nabla v]+\tfrac{1}{2}(1-2p)(3-2p)^2\lambda\theta y^{-4+2p}|\nabla y|^4v^2\\ &\qquad+2(1-\eta)(1-p)^2z\lambda\theta y^{-3+2p}|\nabla y|^4v^2-(1-2p)(3-2p)\lambda\theta y^{-3+2p}\Delta y|\nabla y|^2v^2+\mathcal{A}v^2\\ &\qquad-C'\lambda\theta y^{-2+2p}v^2,\end{aligned}\tag{2-36}$$

where the vector field J in (2-18) can now be given explicitly by

$$\begin{aligned}J&:=J_0+J_H\\ &=\nabla v\partial_t v+2\lambda\nabla v(\nabla F\cdot\nabla v)-\lambda\nabla F|\nabla v|^2+\lambda(\Delta F-2zD_yF)v\nabla v-\tfrac{1}{2}\lambda\nabla(\Delta F-2zD_yF)v^2\\ &\qquad+(1-2p)(3-2p)\lambda\theta y^{-3+2p}\nabla y|\nabla y|^2v^2+2(1-\eta)(1-p)z\lambda\theta y^{-2+2p}\nabla y|\nabla y|^2v^2\\ &\qquad+\lambda\mathcal{A}_0\nabla F v^2.\end{aligned}\tag{2-37}$$

Recalling that y satisfies Definition 2.1, we then have, for any $\xi\in\mathbb{R}^n$,

$$\eta z|\nabla y|^2|\xi|^2-\xi\cdot\nabla^2 y\cdot\xi\geqslant\begin{cases}\eta z|\xi|^2, & d_\Gamma\leqslant d_0,\\ \left(\frac{1}{2}\eta z-\varepsilon'\right)|\xi|^2, & d_0<d_\Gamma<2d_0,\\ \varepsilon|\xi|^2, & d_\Gamma\geqslant 2d_0.\end{cases}\tag{2-38}$$

In particular, letting ε' be sufficiently small, and choosing

$$\eta := \frac{4\varepsilon'}{z} \in (0,1), \tag{2-39}$$

we obtain from (2-38) that

$$\eta z|\nabla y|^2|\xi|^2 - \xi \cdot \nabla^2 y \cdot \xi \geqslant C|\xi|^2. \tag{2-40}$$

Furthermore, the same concavity properties (2-2) also yield the following in Ω:

$$-\Delta y \geqslant \begin{cases} 0, & d_\Gamma \leqslant d_0, \\ -\varepsilon' n, & d_0 < d_\Gamma < 2d_0, \\ \varepsilon n, & d_\Gamma \geqslant 2d_0. \end{cases} \tag{2-41}$$

From (2-36) and (2-40), we now conclude

$$\begin{aligned} &\tfrac{1}{4}e^{-2\lambda F}|(\partial_t + \Delta_{\sigma,y})u|^2 - (\partial_t J_t + \nabla \cdot J) \\ &\geqslant C\lambda\theta y^{-1+2p}|\nabla v|^2 + \tfrac{1}{2}(1-2p)(3-2p)^2\lambda\theta y^{-4+2p}|\nabla y|^4 v^2 \\ &\qquad + 2(1-\eta)(1-p)^2 z\lambda\theta y^{-3+2p}|\nabla y|^4 v^2 - (1-2p)(3-2p)\lambda\theta y^{-3+2p}\Delta y|\nabla y|^2 v^2 + \mathcal{A}v^2 \\ &\qquad - C\lambda\theta y^{-2+2p}v^2. \end{aligned} \tag{2-42}$$

Step 3. The zeroth order terms. It remains to estimate the zero-order coefficient $\mathcal{A}$. First, for $\mathcal{A}_0$, note from (2-22) and (2-32) that

$$\mathcal{A}_0 = \sigma y^{-2} + \lambda^2\theta^2 y^{-2+4p}|\nabla y|^2 + 2z\lambda\theta y^{-1+2p}|\nabla y|^2 + \frac{1}{2p}\lambda\theta' y^{2p}. \tag{2-43}$$

Using that

$$|\theta'| \lesssim \theta^2, \quad |\theta''| \lesssim \theta^3, \tag{2-44}$$

we then compute that

$$-\tfrac{1}{2}\partial_t \mathcal{A}_0 \geqslant -C'\lambda^2\theta^3 y^{-2+2p}. \tag{2-45}$$

Next, using (2-32) and (2-43) we expand

$$\begin{aligned} -\lambda\nabla F \cdot \nabla\mathcal{A}_0 &= -\lambda\theta y^{-1+2p} D_y \mathcal{A}_0 \\ &\geqslant 2\sigma\lambda\theta y^{-4+2p}|\nabla y|^2 + 2(1-2p)\lambda^3\theta^3 y^{-4+6p}|\nabla y|^4 - \lambda^3\theta^3 y^{-3+6p}(\nabla y \cdot \nabla^2 y \cdot \nabla y) \\ &\qquad + 2z(1-2p)\lambda^2\theta^2 y^{-3+4p}|\nabla y|^4 - C'\lambda^2\theta^2 y^{-2+2p}, \end{aligned} \tag{2-46}$$

as well as

$$\begin{aligned} -2z\lambda D_y F \mathcal{A}_0 &= -2z\lambda\theta y^{-1+2p}|\nabla y|^2 \mathcal{A}_0 \\ &\geqslant -2\sigma z\lambda\theta y^{-3+2p}|\nabla y|^2 - 2z\lambda^3\theta^3 y^{-3+6p}|\nabla y|^4 - C'\lambda^2\theta^2 y^{-2+2p}. \end{aligned} \tag{2-47}$$

Lastly, observe from (2-32) that

$$\begin{aligned} &\tfrac{1}{2}\lambda\Delta(\Delta F - 2zD_y F) \\ &= \tfrac{1}{2}\lambda\theta\Delta[-(1-2p)y^{-2+2p}|\nabla y|^2 + y^{-1+2p}\Delta y - 2zy^{-1+2p}|\nabla y|^2] \\ &\geqslant -(1-2p)(1-p)(3-2p)\lambda\theta y^{-4+2p}|\nabla y|^4 + 2(1-2p)(1-p)\lambda\theta y^{-3+2p}|\nabla y|^2\Delta y \\ &\qquad - 2z(1-2p)(1-p)\lambda\theta y^{-3+2p}|\nabla y|^4 - C'\lambda\theta y^{-2+2p}. \end{aligned} \tag{2-48}$$

Thus, combining (2-30) and (2-45)–(2-48) yields

$$\begin{aligned}\mathcal{A} \geqslant {} & [2\sigma|\nabla y|^{-2} - (1-2p)(1-p)(3-2p)]\lambda\theta y^{-4+2p}|\nabla y|^4 \\ & - [2\sigma z|\nabla y|^{-2} + 2z(1-2p)(1-p)]\lambda\theta y^{-3+2p}|\nabla y|^4 + 2(1-2p)(1-p)\Delta y|\nabla y|^{-2}\lambda\theta y^{-3+2p}|\nabla y|^4 \\ & + 2\lambda^3\theta^3[(1-2p) - zy]y^{-4+6p}|\nabla y|^4 + 2z(1-2p)\lambda^2\theta^2 y^{-3+4p}|\nabla y|^4 - C'\lambda^2\theta^3 y^{-2+2p}. \end{aligned} \tag{2-49}$$

Putting (2-49) together with our estimate (2-42), we then have

$$\begin{aligned} & \tfrac{1}{4}e^{-2\lambda F}|(\partial_t + \Delta_{\sigma,y})u|^2 - (\partial_t J_t + \nabla\cdot J) \\ & \geqslant C\lambda\theta y^{-1+2p}|\nabla v|^2 + 2\big(p^2 - 2p + \sigma|\nabla y|^{-2} + \tfrac{3}{4}\big)\lambda\theta y^{-4+2p}|\nabla y|^4 v^2 \\ & \quad + 2z[p - \eta(1-p) - \sigma|\nabla y|^{-2}]\lambda\theta y^{-3+2p}|\nabla y|^4 v^2 - (1-2p)\lambda\theta y^{-3+2p}\Delta y|\nabla y|^2 v^2 \\ & \quad + 2\lambda^3\theta^3[(1-2p) - zy]y^{-4+6p}|\nabla y|^4 v^2 + 2z(1-2p)\lambda^2\theta^2 y^{-3+4p}|\nabla y|^4 v^2 \\ & \quad - C'\lambda^2\theta^3 y^{-2+2p}v^2. \end{aligned} \tag{2-50}$$

Choosing ε' sufficiently small, so that (2-39) implies

$$p - \eta(1-p) \geqslant \tfrac{1}{2}p + C\varepsilon,$$

and recalling (2-14), (2-20), and (2-41), we conclude that

$$\begin{aligned} & \tfrac{1}{4}e^{-2\lambda F}|(\partial_t + \Delta_{\sigma,y})u|^2 - (\partial_t J_t + \nabla\cdot J) \\ & \geqslant C\lambda\theta y^{-1+2p}|\nabla v|^2 + C\lambda^3\theta^3 y^{-4+6p}|\nabla y|^4 v^2 + 2\big(p^2 - 2p + \sigma|\nabla y|^{-2} + \tfrac{3}{4}\big)\lambda\theta y^{-4+2p}|\nabla y|^4 v^2 \\ & \quad + z(p - 2\sigma|\nabla y|^{-2})\lambda\theta y^{-3+2p}|\nabla y|^4 v^2 - C'\lambda^2\theta^3 y^{-3+4p}v^2. \end{aligned} \tag{2-51}$$

We now claim that (2-51) implies

$$\begin{aligned} & \tfrac{1}{4}e^{-2\lambda F}|(\partial_t + \Delta_{\sigma,y})u|^2 - (\partial_t J_t + \nabla\cdot J) \\ & \qquad \geqslant C\lambda\theta y^{-1+2p}|\nabla v|^2 + C(\lambda^3\theta^3 y^{-4+6p} + \lambda\theta y^{-3+2p})|\nabla y|^4 v^2 - C'\lambda^2\theta^3 y^{-3+4p}v^2. \end{aligned} \tag{2-52}$$

First, when $\sigma \leqslant 0$, we have that (2-52) follows from (2-14), (2-51), and the inequalities

$$\begin{aligned} 2\sigma|\nabla y|^{-2}\lambda\theta y^{-4+2p}|\nabla y|^4 v^2 &\geqslant 2\sigma\lambda\theta y^{-4+2p}|\nabla y|^4 v^2 - C'\lambda\theta y^{-2+2p}v^2, \\ 2\big(p^2 - 2p + \sigma + \tfrac{3}{4}\big)\lambda\theta y^{-4+2p}|\nabla y|^4 v^2 &\geqslant 0, \\ z(p - 2\sigma|\nabla y|^{-2})\lambda\theta y^{-3+2p}|\nabla y|^4 v^2 &\geqslant zp\lambda\theta y^{-3+2p}|\nabla y|^4. \end{aligned}$$

(The first inequality above follows, since $|\nabla y|^{-2} - 1$ vanishes near Γ and is bounded from below on Ω by a negative constant.) On the other hand, the case $\sigma > 0$ follows from (2-14), (2-20), (2-51), and the inequalities

$$\begin{aligned} 2\big(p^2 - 2p + \tfrac{3}{4}\big)\lambda\theta y^{-4+2p}|\nabla y|^4 v^2 \geqslant 0, \\ 2\sigma\lambda\theta y^{-4+2p}|\nabla y|^2 v^2 - z2\sigma\lambda\theta y^{-3+2p}|\nabla y|^2 v^2 \geqslant 4p\sigma\lambda\theta y^{-4+2p}|\nabla y|^2 v^2. \end{aligned}$$

Combining the above two cases completes the proof of (2-52).

Step 4. Completion of the proof. Since x_* is the only critical point of y, it follows that $|\nabla y|$ is bounded away from zero on $\Omega \setminus B_\delta(x_*)$, and hence (2-52) becomes

$$\begin{aligned} e^{-2\lambda F} &|(\partial_t + \Delta_{\sigma,y})u|^2 - 4(\partial_t J_t + \nabla \cdot J) \\ &\geqslant C\lambda\theta y^{-1+2p}|\nabla v|^2 + C(\lambda^3\theta^3 y^{-4+6p} + \lambda\theta y^{-3+2p})\mathbb{1}_{\Omega\setminus B_\delta(x_*)} v^2 - C'\lambda^2\theta^3 y^{-3+4p} v^2. \end{aligned}$$

Furthermore, on $\Omega \setminus B_\delta(x_*)$, the negative term in the right-hand side of the above can be absorbed into the positive terms by taking λ sufficiently large, and hence

$$\begin{aligned} e^{-2\lambda F} &|(\partial_t + \Delta_{\sigma,y})u|^2 - 4(\partial_t J_t + \nabla \cdot J) \\ &\geqslant C\lambda\theta y^{-1+2p}|\nabla v|^2 + C(\lambda^3\theta^3 y^{-4+6p} + \lambda\theta y^{-3+2p})\mathbb{1}_{\Omega\setminus B_\delta(x_*)} v^2 - C'\lambda^2\theta^3 y^{-3+4p}\mathbb{1}_{B_\delta(x_*)} v^2. \end{aligned} \tag{2-53}$$

The desired estimate (2-15) now follows from (2-53) by (2-19), and by noting that

$$\begin{aligned} e^{-2\lambda F} y^{-1+2p}|\nabla u|^2 &\leqslant C y^{-1+2p}|\nabla v|^2 + C\lambda^2\theta^2 y^{-3+6p}|\nabla y|^2 v^2 \\ &\leqslant C y^{-1+2p}|\nabla v|^2 + C\lambda^2\theta^2 y^{-4+6p}\mathbb{1}_{\Omega\setminus B_\delta(x_*)} v^2 + C'\lambda^2\theta^2 y^{-3+4p}\mathbb{1}_{B_\delta(x_*)} v^2. \end{aligned}$$

It remains to prove the inequalities (2-17) and (2-18). For the latter bound, we apply (2-19), (2-32), (2-37), and (2-43) to obtain

$$\begin{aligned} \nabla y \cdot J - \partial_t v D_y v &\leqslant 2\lambda\theta y^{-1+2p}(D_y v)^2 - \lambda\theta y^{-1+2p}|\nabla v|^2 + C\lambda\theta y^{-2+2p}|v||D_y v| + C\lambda\theta y^{-3+2p} v^2 \\ &\leqslant C\lambda\theta y^{-1+2p}(D_y v)^2 + C\lambda\theta y^{-3+2p} v^2 \\ &\leqslant C e^{-2\lambda F}\lambda\theta y^{-1+2p}(D_y v)^2 + C e^{-2\lambda F}\lambda^3\theta^3 y^{-3+2p} u^2, \end{aligned}$$

whenever $d_\Gamma < d_0$ (so that $|\nabla y|^2 = 1$ by Definition 2.1). Notice, in particular, that terms containing derivatives of v in directions other than along ∇y are nonpositive and hence can be omitted. The desired (2-18) now follows from the above, (2-16), (2-19), and (2-44). Similarly, for (2-17), we estimate

$$|J^t| \leqslant C|\nabla v|^2 + C\lambda^2\theta^2 y^{-2} v^2 \leqslant C e^{-2\lambda F}|\nabla u|^2 + C e^{-2\lambda F}\lambda^2\theta^2 y^{-2} u^2,$$

where we applied (2-19), (2-31), (2-32), and (2-43). □

2.3. ***The global Carleman estimate.*** In this subsection, we will state and prove the precise version our main global Carleman estimate. Before doing so, we must first improve the pointwise estimate (2-15) by eliminating the negative term in the right-hand side that is supported near the critical point of the boundary defining function. This is accomplished below by summing two instances of (2-15), using two boundary defining functions with distinct critical points.

Lemma 2.8. *Fix $T > 0$, and let $\sigma, p \in \mathbb{R}$ satisfy* (2-14). *There exist $C, \varepsilon, \varepsilon', \lambda_0 > 0$ (depending on $T, \Omega, d_0, \sigma, p$) and an $(\varepsilon, \varepsilon')$-boundary defining pair (y_1, y_2) such that, for all $u \in C^2([0, T] \times \Omega)$ and $\lambda \geqslant \lambda_0$,*

$$\begin{aligned} \sum_{j=1}^{2} e^{-2\lambda F_j} &|(\pm\partial_t + \Delta_{\sigma,y_j})u|^2 - 4\sum_{j=1}^{2}(\partial_t J_j^t + \nabla\cdot J_j) \\ &\geqslant C\sum_{j=1}^{2} e^{-2\lambda F_j}\big[\lambda\theta y_j^{-1+2p}|\nabla u|^2 + (\lambda^3\theta^3 y_j^{-4+6p} + \lambda\theta y_j^{-3+2p})u^2\big], \end{aligned} \tag{2-54}$$

where F_j $(j=1,2)$ is given by

$$F_j(t,x) := \theta(t)\Big(\frac{1}{2p}y_j(x)^{2p}+\beta_j\Big), \qquad \theta(t) := \frac{1}{t(T-t)}, \tag{2-55}$$

for appropriately chosen $\beta_j > 0$, where the scalars J_j^t satisfy

$$|J_j^t| \leqslant Ce^{-2\lambda F_j}|\nabla u|^2 + Ce^{-2\lambda F_j}\lambda^2\theta^2 y_j^{-2}u^2, \tag{2-56}$$

and where the vector fields J_j satisfy, sufficiently near Γ,

$$\nabla y_j \cdot J_j - e^{-2\lambda F_j}\partial_t u D_{y_j}u \leqslant Ce^{-2\lambda F_j}\lambda\theta y_j^{-1+2p}(D_{y_j}u)^2 + Ce^{-2\lambda F_j}\lambda^3\theta^3 y_j^{-3+2p}u^2. \tag{2-57}$$

Proof. Lemma 2.4 yields a $(\varepsilon,\varepsilon')$-boundary defining (y_1,y_2) satisfying the properties of Definition 2.3, for any sufficiently small ε and ε'. In particular, y_j $(j=1,2)$ has a unique critical point $x_j\in\Omega$, with $d_\Gamma(x_j) > 2d_0$, at which it attains its maximum $R_j := y_j(x_j)$. Since x_j is the (unique) global maximum of y_j, and since $x_1\neq x_2$, there exist $\delta>0$, $0<r_1<R_1$, and $0<r_2<R_2$ such that

$$B_\delta(x_1)\cap B_\delta(x_2)=\varnothing, \quad \{r_1\leqslant y_1\leqslant R_1\}\cap\{y_2\leqslant r_2\}\supseteq B_\delta(x_1), \quad \{r_2\leqslant y_2\leqslant R_2\}\cap\{y_1\leqslant r_1\}\supseteq B_\delta(x_2). \tag{2-58}$$

See Figure 1 for an illustration of this setting.

We can thus apply Lemma 2.7 with $y=y_j$, our given p,σ, the above δ, and sufficiently large $\lambda>0$. Summing both estimates, we derive

$$\begin{aligned}\sum_{j=1}^{2} e^{-2\lambda F_j}|(\pm\partial_t+\Delta_{\sigma,y_j}u)|^2 - 4\sum_{j=1}^{2}(\partial_t J_j^t+\nabla\cdot J_j)\\ \geqslant C\lambda\theta\sum_{j=1}^{2} e^{-2\lambda F_j}y_j^{-1+2p}|\nabla u|^2 - C'\lambda^2\theta^3\sum_{j=1}^{2} e^{-2\lambda F_j}y_j^{-3+4p}\mathbb{1}_{B_\delta(x_j)}u^2\\ + C\sum_{j=1}^{2} e^{-2\lambda F_j}(\lambda^3\theta^3 y_j^{-4+6p}+\lambda\theta y_j^{-3+2p})\mathbb{1}_{\Omega\setminus B_\delta(x_j)}u^2.\end{aligned} \tag{2-59}$$

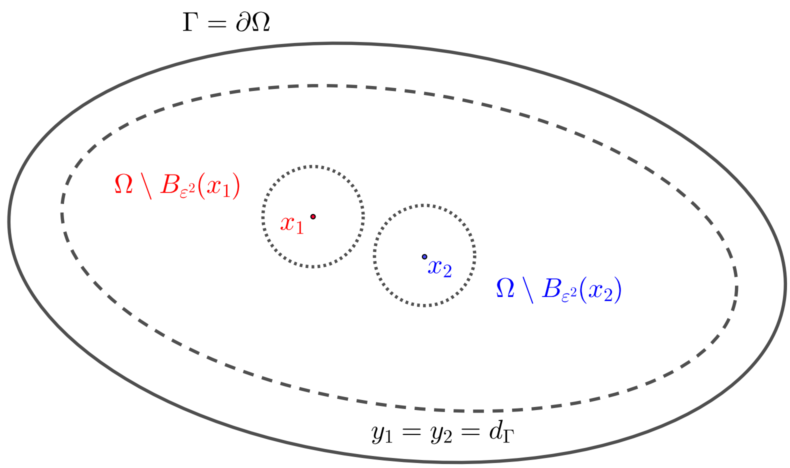

Figure 1. The domain Ω with convex boundary Γ is depicted together with balls centered at the critical points x_1, x_2 of two good boundary defining functions y_1, y_2. In a neighborhood of Γ, these functions agree with the distance to the boundary d_Γ.

Furthermore, we write the Carleman weights F_j as

$$F_j(t,x) = \theta(t) f_j(y_j(x)), \quad f_j(r) := \frac{1}{2p} r^{2p} + \beta_j,$$

and we choose $\beta_1, \beta_2 > 0$ to satisfy

$$\beta_2 - \beta_1 := \frac{1}{2p}(r_1^{2p} - r_2^{2p}).$$

Notice that with the above choice, we have

$$f_1(r_1) = f_2(r_2). \tag{2-60}$$

Then, for each $j = 1, 2$ and $j^* := 3 - j$, we have that

$$\begin{aligned} e^{-2\lambda F_j} y_j^{-3+4p} \mathbb{1}_{B_\delta(x_j)} \leqslant e^{-2\lambda\theta(t) f_j(r_j)} y_j^{-4+6p} \mathbb{1}_{B_\delta(x_j)} &\leqslant C e^{-2\lambda\theta(t) f_{j^*}(r_{j^*})} y_{j^*}^{-4+6p} \mathbb{1}_{B_\delta(x_j)} \\ &\leqslant C e^{-2\lambda F_{j^*}} y_{j^*}^{-4+6p} \mathbb{1}_{\Omega \setminus B_\delta(x_{j^*})}, \end{aligned} \tag{2-61}$$

with $C > 0$ independent of λ. (Here, the first and third steps in (2-61) follow from (2-58) and the monotonicity of f_1 and f_2, while the second step is a consequence of (2-60) and the fact that both y_j, y_{j^*} are bounded away from 0 on $B_\delta(x_j)$.)

Applying (2-61) and taking λ large enough, the negative term in the right-hand side of (2-59) can be absorbed in the subsequent positive term, and we arrive at

$$\begin{aligned} \sum_{j=1}^{2} e^{-2\lambda F_j} |(\pm\partial_t + \Delta_{\sigma,y_j})u|^2 - 4\sum_{j=1}^{2} (\partial_t J_j^t + \nabla\cdot J_j) \\ \geqslant C \sum_{j=1}^{2} e^{-2\lambda F_j} \big[\lambda\theta y_j^{-1+2p} |\nabla u|^2 + (\lambda^3\theta^3 y_j^{-4+6p} + \lambda\theta y_j^{-3+2p}) \mathbb{1}_{\Omega\setminus B_\delta(x_j)} u^2\big]. \end{aligned}$$

Finally, the desired (2-54) follows by noting that the factor $\mathbb{1}_{\Omega\setminus B_\delta(x_j)}$ in the above can be removed — this is because Ω is covered by $\Omega \setminus B_\delta(x_1)$ and $\Omega \setminus B_\delta(x_2)$, and both y_1, y_2 are bounded away from zero on $B_\delta(x_1) \cup B_\delta(x_2)$. □

We can now state our main global Carleman estimate:

Theorem 2.9. *Fix $T > 0$, and let $\sigma, p \in \mathbb{R}$ satisfy* (2-14). *Then, there exist constants $C, \varepsilon, \varepsilon', \lambda_0 > 0$ (depending on $T, \Omega, d_0, \sigma, p$) and an $(\varepsilon, \varepsilon')$-boundary defining pair (y_1, y_2) such that the following Carleman estimate holds*:

$$\begin{aligned} C \sum_{j=1}^{2} \int_{[0,T]\times\Omega} e^{-2\lambda F_j} \big[\lambda\theta y_j^{-1+2p} |\nabla u|^2 + (\lambda^3\theta^3 y_j^{-4+6p} + \lambda\theta y_j^{-3+2p}) u^2\big] \\ \leqslant \limsup_{\delta\searrow 0} \sum_{j=1}^{2} \int_{[0,T]\times\{y_j=\delta\}} e^{-2\lambda F_j} \big[\lambda\theta y_j^{-1+2p} (D_{y_j} u)^2 + \lambda^3\theta^3 y_j^{-3+2p} u^2\big] \\ + \limsup_{\delta\searrow 0} \sum_{j=1}^{2} \left| \int_{[0,T]\times\{y_j=\delta\}} e^{-2\lambda F_j} \partial_t u D_{y_j} u \right| + \sum_{j=1}^{2} \int_{[0,T]\times\Omega} e^{-2\lambda F_j} |(\pm\partial_t + \Delta_{\sigma,y_j})u|^2, \end{aligned} \tag{2-62}$$

for all $\lambda \geqslant \lambda_0$ *and for all* $u \in C^2([0, T] \times \Omega)$ *having finite energy,*

$$\sup_{t \in [0,T]} \int_{\{t\} \times \Omega} (|\nabla u|^2 + d_\Gamma^{-2} u^2) < \infty, \tag{2-63}$$

and where both F_j $(j = 1, 2)$ *and* θ *are defined as in* (2-55).

Proof. Let C, ε, ε', λ_0, (y_1, y_2) be chosen as in Lemma 2.8. Integrating the pointwise estimate (2-54) over the domain $[0, T] \times \{y_j > \delta\}$ and applying both the fundamental theorem of calculus (in t) and the divergence theorem (in x) yields

$$\begin{aligned} C \sum_{j=1}^{2} \int_{[0,T] \times \{y_j > \delta\}} e^{-2\lambda F_j} \big[\lambda \theta y_j^{-1+2p} |\nabla u|^2 + (\lambda^3 \theta^3 y_j^{-4+6p} + \lambda \theta y_j^{-3+2p}) u^2\big] \\ \leqslant \sum_{j=1}^{2} \int_{[0,T] \times \{y_j > \delta\}} e^{-2\lambda F_j} |(\pm \partial_t + \Delta_{\sigma, y_j}) u|^2 + 4 \sum_{j=1}^{2} \int_{\{T\} \times \{y_j > \delta\}} |J_j^t| + 4 \sum_{j=1}^{2} \int_{\{0\} \times \{y_j > \delta\}} |J_j^t| \\ + 4 \sum_{j=1}^{2} \int_{[0,T] \times \{y_j = \delta\}} (\nabla y_j \cdot J_j). \end{aligned} \tag{2-64}$$

By (2-57), there exists $C' > 0$ (with the same dependencies as before) with

$$\begin{aligned} \int_{[0,T] \times \{y_j = \delta\}} (\nabla y_j \cdot J_j) \leqslant C' \int_{[0,T] \times \{y_j = \delta\}} e^{-2\lambda F_j} \lambda \theta y_j^{-1+2p} (D_{y_j} u)^2 + C' \int_{[0,T] \times \{y_j = \delta\}} e^{-2\lambda F_j} \lambda^3 \theta^3 y_j^{-3+2p} u^2 \\ + C' \left| \int_{[0,T] \times \{y_j = \delta\}} e^{-2\lambda F_j} \partial_t u D_{y_j} u \right|, \end{aligned} \tag{2-65}$$

for $j = 1, 2$. For the remaining boundary integrals for J_j^t, note that

$$\lambda^k \theta^k e^{-\lambda F_j} \leqslant \lambda^k \theta^k e^{-\lambda \theta \beta_j}$$

converges uniformly to 0 as $t \nearrow T$ and $t \searrow 0$, for any $k \geqslant 0$. The above, combined with (2-56) and (2-63), imply that the terms of (2-64) containing J_1^t, J_2^t vanish:

$$4 \sum_{j=1}^{2} \int_{\{T\} \times \{y_j < \delta\}} |J_j^t| = 4 \sum_{j=1}^{2} \int_{\{0\} \times \{y_j < \delta\}} |J_j^t| = 0. \tag{2-66}$$

Combining (2-64)–(2-66) and then letting $\delta \searrow 0$ results in (2-62). □

Remark 2.10. While the final boundary term in (2-62) (involving $\partial_t u$) is expected to vanish in our applications of Theorem 2.9, it has to be treated especially delicately. Thus is due to the presence of $\partial_t u$, which counts for two spatial derivatives in the context of parabolic equations, and which makes this the least regular boundary term. In particular, we will have to take full advantage of the structure of our heat operator in order to ensure that this term is well-defined and finite.

3. Boundary observability

As an application of Theorem 2.9, we present in this section a boundary observability result for critically singular (backwards) heat equations. Throughout, we let Ω, Γ, d_Γ, and the constant d_0 be as in previous sections.

Before stating our key results, we must first develop the requisite well-posedness theory for our singular heat operators. For this, we will also have to treat the more general inhomogeneous extension of Problem (O):

Problem (OI). *Given final data u_T on Ω, and forcing term F on $(0, T) \times \Omega$, solve the following final-boundary value problem for u*:

$$\begin{aligned} (\partial_t + \Delta_\sigma + X \cdot \nabla + V)u &= F \quad \text{on } (0, T) \times \Omega, \\ u(T) &= u_T \quad \text{on } \Omega, \\ u &= 0 \quad \text{on } (0, T) \times \Gamma, \end{aligned} \tag{3-1}$$

where $\sigma \in \left(-\frac{3}{4}, 0\right)$, and where the lower-order coefficients satisfy $(X, V) \in \mathcal{Z}$.

Our analysis of Problem (OI) is closely connected to the setting studied in [Biccari and Zuazua 2016] (but only for subcritical σ). Since we are dealing with boundary rather than interior observability, here we must deal more carefully with boundary asymptotics. Moreover, the presence of lower-order terms in (3-1) complicates the analysis. As a result, we provide abridged proofs of several key results for completeness.

Remark 3.1. We note that all the theory in this section applies to the *forward* heat equation as well, with the final data u_T replaced by initial data u_0 at $t = 0$. Indeed, this can be obtained by applying the time transformation $t \mapsto T - t$.

For future convenience, we also use Lemma 2.4 to fix the following:

Setting (boundary defining function). Fix a boundary defining function (Definition 2.1) $y \in C^4(\Omega)$. (The associated constants ε, ε' are not relevant.)

The above is mainly for technical simplification, as this allows us to replace d_Γ, which can fail to be differentiable away from Γ, by a smoother quantity.

Remark 3.2. Equation (3-1) can now be rewritten as

$$\partial_t u + y^{-\kappa} \nabla \cdot [y^{2\kappa} \nabla (y^{-\kappa} u)] + X \cdot \nabla u + V_y u = F, \tag{3-2}$$

where the modified potential V_y is given by

$$V_y = V - \kappa y^{-1} \Delta y \phi + \kappa (1 - \kappa)(|\nabla y|^2 y^{-2} - d_\Gamma^{-2})\phi. \tag{3-3}$$

Note in particular that $(X, V_y) \in \mathcal{Z}$. In the upcoming analysis, it will often be more convenient to express Δ_σ in terms of "y-twisted" derivatives, $y^\kappa \nabla y^{-\kappa}$ and $y^{-\kappa} \nabla y^\kappa$.

3.1. ***Elliptic and semigroup theory.*** The first task is to establish the elliptic and semigroup properties for the singular operator $\Delta_\sigma + X \cdot \nabla + V$.

The following Hardy inequality will play a crucial role in our analysis:

Proposition 3.3. *For any $\phi \in H^1_0(\Omega)$,*

$$\frac{1}{4} \int_\Omega d_\Gamma^{-2} \phi^2 \leqslant \int_\Omega |\nabla \phi|^2. \tag{3-4}$$

Remark 3.4. See [Brezis and Marcus 1997; Marcus et al. 1998] for details on Proposition 3.3. We mention that the explicit constant $\frac{1}{4}$ in (3-4) is only valid when Γ is convex; for more general Ω and Γ, one still has (3-4), but with $\frac{1}{4}$ replaced by a possibly smaller positive constant.

Corollary 3.5. *The following holds for any $\sigma \in \left(-\frac{3}{4}, 0\right)$ and $\phi \in H^1_0(\Omega)$,*

$$\|\phi\|_{H^1(\Omega)} \simeq \|y^\kappa \nabla (y^{-\kappa} \phi)\|_{L^2(\Omega)} + \|\phi\|_{L^2(\Omega)}, \tag{3-5}$$

where the constants depend on Ω and σ.

Proof. Half of (3-5) is an immediate consequence of (3-4):

$$\|y^\kappa \nabla (y^{-\kappa} \phi)\|_{L^2(\Omega)} \lesssim \|\nabla \phi\|_{L^2(\Omega)} + \|y^{-1} \phi\|_{L^2(\Omega)} \lesssim \|\nabla \phi\|_{L^2(\Omega)}.$$

For the reverse inequality, we integrate by parts to obtain, for $\phi \in C^\infty_0(\Omega)$,

$$\begin{aligned} \int_\Omega |\nabla \phi|^2 &\leqslant \int_\Omega \phi(-\Delta \phi - \sigma y^{-2} \phi) \\ &\leqslant -\int_\Omega \phi(y^{-\kappa} \nabla \cdot [y^{2\kappa} \nabla (y^{-\kappa} \phi)]) + [\|\nabla \phi\|_{L^2(\Omega)} + \|\phi\|_{L^2(\Omega)}] \|\phi\|_{L^2(\Omega)} \\ &\leqslant \int_\Omega |y^\kappa \nabla (y^{-\kappa} \phi)|^2 + [\|\nabla \phi\|_{L^2(\Omega)} + \|\phi\|_{L^2(\Omega)}] \|\phi\|_{L^2(\Omega)}. \end{aligned}$$

The result now follows from the above via approximation. □

Remark 3.6. One can in fact show, using (3-4), that (3-5) holds for all $\sigma < \frac{1}{4}$.

Next, we show that $\Delta_\sigma + X \cdot \nabla + V$ generates an appropriate semigroup, from which one can derive well-posedness properties for Problem (OI):

Proposition 3.7. *Fix $\sigma \in \left(-\frac{3}{4}, 0\right)$ and $(X, V) \in \mathcal{Z}$, and consider the operator*

$$A_\sigma := \Delta_\sigma + X \cdot \nabla + V, \tag{3-6}$$

which we view as an unbounded operator on $L^2(\Omega)$,

$$A_\sigma : \mathfrak{D}(A_\sigma) \to L^2(\Omega), \quad \mathfrak{D}(A_\sigma) := \{\phi \in H^1_0(\Omega) \mid A_\sigma \phi \in L^2(\Omega)\}.$$

Then, there exists $\gamma \geqslant 0$ such that:

- *$\lambda I - A_\sigma$ is invertible for any $\lambda > \gamma$, and*

$$\|(\lambda I - A_\sigma)^{-1} f\|_{L^2(\Omega)} \leqslant (\lambda - \gamma)^{-1} \|f\|_{L^2(\Omega)}, \quad f \in L^2(\Omega). \tag{3-7}$$

- $-A_\sigma$ *generates a* γ*-contractive semigroup* $t \mapsto e^{-tA_\sigma}$ *on* $L^2(\Omega)$*; that is,*

$$\|e^{-tA_\sigma}\phi\|_{L^2(\Omega)} \leqslant e^{\gamma t}\|\phi\|_{L^2(\Omega)}, \quad t > 0, \quad \phi \in L^2(\Omega). \tag{3-8}$$

Furthermore, if $\phi \in \mathfrak{D}(A_\sigma)$*, then* $\phi \in H^2_{\text{loc}}(\Omega)$*, and*

$$\|y^{-\kappa}\nabla[y^{2\kappa}\nabla(y^{-\kappa}\phi)]\|_{L^2(\Omega)} + \|\nabla\phi\|_{L^2(\Omega)} \lesssim \|A_\sigma\phi\|_{L^2(\Omega)} + \|\phi\|_{L^2(\Omega)}, \tag{3-9}$$

with the constant of the inequality depending only on Ω, σ, X, V.

Proof sketch. First, by the computations in Remark 3.2, we have

$$A_\sigma = y^{-\kappa}\nabla\cdot(y^{2\kappa}\nabla y^{-\kappa}) + X\cdot\nabla + V_y. \tag{3-10}$$

We begin with the resolvent estimate (3-7). Note $-A_\sigma$ can be associated with the bilinear form $\mathcal{B}_\sigma : H^1_0(\Omega)\times H^1_0(\Omega) \to \mathbb{R}$, given by

$$\mathcal{B}_\sigma(\phi,\psi) := \int_\Omega \bigl[y^\kappa\nabla(y^{-\kappa}\phi)\cdot y^\kappa\nabla(y^{-\kappa}\psi) - (X\cdot\nabla\phi)\psi - V_y\phi\psi\bigr]. \tag{3-11}$$

By Definition 1.5 and (3-5), there exist $c > 0$ and $\gamma \geqslant 0$ such that

$$\mathcal{B}_\sigma(\phi,\phi) \geqslant c\|\phi\|^2_{H^1(\Omega)} - \gamma\|\phi\|^2_{L^2(\Omega)}. \tag{3-12}$$

In particular, when $\lambda > \gamma$, the Lax–Milgram theorem and (3-12) imply that for any $f \in L^2(\Omega)$, there exists a unique $\phi \in H^1_0(\Omega)$ such that

$$\lambda\int_\Omega \phi\psi + \mathcal{B}_\sigma(\phi,\psi) = \int_\Omega f\psi, \quad \psi \in H^1_0(\Omega). \tag{3-13}$$

Applying an integration by parts to (3-13), we see that $f = (\lambda I - A_\sigma)\phi$ (at least in a weak sense). Moreover, setting $\psi := \phi$ in (3-13) and recalling (3-12) yields

$$(\lambda-\gamma)\|\phi\|^2_{L^2(\Omega)} \leqslant \|f\|_{L^2(\Omega)}\|\phi\|_{L^2(\Omega)},$$

from which the resolvent inequality (3-7) immediately follows.

The next step is to obtain the H^2-estimate (3-9). The H^1-bound

$$\|\nabla\phi\|_{L^2(\Omega)} \lesssim \|A_\sigma\phi\|_{L^2(\Omega)} + \|\phi\|_{L^2(\Omega)} \tag{3-14}$$

is a consequence of (3-11), (3-12), and an integration by parts. Moreover, interior regularity for A_σ follows from standard elliptic theory (see [Evans 2010, Section 6.3]), since all the coefficients of A_σ are bounded on any compact subset of Ω. In particular, $\phi \in \mathfrak{D}(A_\sigma)$ implies $\phi \in H^2_{\text{loc}}(\Omega)$, and hence it suffices to bound $y^{-\kappa}\nabla[y^{2\kappa}\nabla(y^{-\kappa}\phi)]$ in (3-9) while assuming that ϕ is supported sufficiently near Γ.

Let $\not\nabla$ and $\not\Delta$ denote the gradient and Laplacian on the level sets of y, respectively. The informal idea is then to integrate by parts the identity

$$\int_\Omega A_\sigma\phi\not\Delta\phi = \int_\Omega \bigl\{y^{-\kappa}\nabla\cdot[y^{2\kappa}\nabla(y^{-\kappa}\phi)] + X\cdot\nabla\phi + V_y\phi\bigr\}\not\Delta\phi. \tag{3-15}$$

In particular, estimating lower-order terms using Definition 1.5 and (3-4), and noting that $\not\nabla\phi$ and $\not\nabla^2\phi$ have zero trace on Γ, we obtain the estimate

$$
\begin{aligned}
&\|y^{-\kappa}\not\nabla[y^{2\kappa}\nabla(y^{-\kappa}\phi)]\|^2_{L^2(\Omega)}\\
&\lesssim \|A_\sigma\phi\|_{L^2(\Omega)}\|\not\Delta\phi\|_{L^2(\Omega)}+\|\phi\|_{L^2(\Omega)}\|y^{-\kappa}\not\nabla[y^{2\kappa}\nabla(y^{-\kappa}\phi)]\|_{L^2(\Omega)}+\|\phi\|^2_{H^1(\Omega)}+\|y^{-1}\phi\|_{L^2(\Omega)}\|\not\Delta\phi\|_{L^2(\Omega)}\\
&\lesssim [\|A_\sigma\phi\|_{L^2(\Omega)}+\|\phi\|_{H^1(\Omega)}]\big\|y^{-\kappa}\not\nabla[y^{2\kappa}\nabla(y^{-\kappa}\phi)]\big\|_{L^2(\Omega)}+\|\phi\|^2_{H^1(\Omega)}.
\end{aligned}
$$

(Formally, there is not enough regularity to carry out the above manipulations, and one must approximate, e.g., by replacing $\not\Delta\phi$ in (3-15) with appropriate difference quotients; see [Evans 2010, Section 6.3].) The above then implies

$$\|y^{-\kappa}\not\nabla[y^{2\kappa}\nabla(y^{-\kappa}\phi)]\|^2_{L^2(\Omega)}\lesssim\|A_\sigma\phi\|^2_{L^2(\Omega)}+\|\phi\|^2_{H^1(\Omega)}. \tag{3-16}$$

In addition, for normal derivatives, we bound, using (3-4), (3-6), and (3-16),

$$
\begin{aligned}
\|y^{-\kappa}D_y[y^{2\kappa}D_y(y^{-\kappa}\phi)]\|_{L^2(\Omega)}&\lesssim\|A_\sigma\phi\|_{L^2(\Omega)}+\|\not\Delta\phi\|_{L^2(\Omega)}+\|\phi\|_{H^1(\Omega)}\\
&\lesssim\|A_\sigma\phi\|_{L^2(\Omega)}+\|\phi\|_{H^1(\Omega)}.
\end{aligned}\tag{3-17}
$$

The desired estimate (3-9) now follows by combining (3-14), (3-16), and (3-17).

It remains to prove the semigroup property for $-A_\sigma$. By the Hille–Yosida theorem (see, e.g., the discussions in [Evans 2010, Section 7.4]), this is a consequence of (3-7), provided we show that A_σ is closed and densely defined. The latter property holds, since $\mathfrak{D}(A_\sigma)$ contains $C_0^\infty(\Omega)$ and hence is dense in $L^2(\Omega)$.

Finally, to see that A_σ is closed, consider a sequence (ϕ_k) in $\mathfrak{D}(A_\sigma)$ such that

$$\lim_{k\to\infty}\phi_k=\phi,\qquad\lim_{k\to\infty}A_\sigma\phi_k=\psi, \tag{3-18}$$

with both limits in $L^2(\Omega)$. Then, all the ϕ_k's lie in $H^2_{\mathrm{loc}}(\Omega)$, and (3-9) yields that

$$\|y^{-\kappa}\nabla[y^{2\kappa}\nabla(y^{-\kappa}(\phi_k-\phi_l))]\|_{L^2(\Omega)}+\|\nabla(\phi_k-\phi_l)\|_{L^2(\Omega)}\lesssim\|A_\sigma\phi_k-A_\sigma\phi_l\|_{L^2(\Omega)}+\|\phi_k-\phi_l\|_{L^2(\Omega)},$$

for any $k,l\in\mathbb{N}$. Since the right-hand side of the above goes to zero as $k,l\to\infty$ by (3-18), then (ϕ_k) is a Cauchy sequence in a weighted H^2-space, and

$$\lim_{k\to\infty}\nabla\phi_k=\nabla\phi,\qquad\lim_{k\to\infty}y^{-\kappa}\nabla[y^{2\kappa}\nabla(y^{-\kappa}\phi_k)]=y^{-\kappa}\nabla[y^{2\kappa}\nabla(y^{-\kappa}\phi)].$$

The above then implies $\psi=A_\sigma\phi$, and hence A_σ is indeed closed. □

Remark 3.8. Hardy's inequality ensures the usual Sobolev space $H^1_0(\Omega)$ suffices for working at the level of first derivatives. However, the situation changes for second derivatives, as the left-hand side of (3-9) is no longer comparable to the H^2-norm.

3.2. ***Strict solutions.*** Following the discussions in [Biccari 2019; Biccari and Zuazua 2016], we now define two notions of solutions of (3-1), and we state the corresponding well-posedness results:

Definition 3.9. Given $u_T \in L^2(\Omega)$ and $F \in L^2((0,T)\times\Omega)$, we call

$$u \in C^0([0,T]; L^2(\Omega)) \cap L^2((0,T); H_0^1(\Omega))$$

a *mild solution* of Problem (OI) if and only if the following holds:

$$u(t) = e^{(T-t)A_\sigma} u_T - \int_t^T e^{(s-t)A_\sigma} F(s)\, ds, \quad t \in [0,T]. \tag{3-19}$$

Proposition 3.10. *Suppose $u_T \in L^2(\Omega)$ and $F \in L^2((0,T)\times\Omega)$. Then, there is a unique mild solution u to Problem* (OI). *Furthermore, u satisfies the estimate*

$$\|u\|^2_{L^\infty([0,T];L^2(\Omega))} + \|y^\kappa \nabla(y^{-\kappa}u)\|^2_{L^2((0,T)\times\Omega)} \lesssim \|u_T\|^2_{L^2(\Omega)} + \|F\|^2_{L^2((0,T)\times\Omega)}, \tag{3-20}$$

with the constant of the inequality depending only on Ω, σ, X, V.

Proof sketch. Both existence and uniqueness are immediate from (3-19). For (3-20), we only consider when $u_T \in \mathfrak{D}(A_\sigma)$ (so that $u(t) \in \mathfrak{D}(A_\sigma)$ and $\partial_t u(t) \in L^2(\Omega)$ for every $t \in [0,T)$); the general case then follows by approximation.

By the fundamental theorem of calculus, (3-2), and integrations by parts,

$$\begin{aligned}
&\|u(T)\|^2_{L^2(\Omega)} - \|u(t)\|^2_{L^2(\Omega)} \\
&\qquad = 2\int_t^T \int_\Omega u\big\{F - y^{-\kappa}\nabla\cdot[y^{2\kappa}\nabla(y^{-\kappa}u)] - X\cdot\nabla u - V_y u\big\}\big|_{t=s}\, ds \\
&\qquad = 2\int_t^T \int_\Omega Fu|_{t=s}\, ds + 2\int_t^T\int_\Omega |y^\kappa\nabla(y^{-\kappa}u)|^2\big|_{t=s}\, ds + \int_t^T\int_\Omega (\nabla\cdot X - 2V_y)u^2\big|_{t=s}\, ds,
\end{aligned}$$

for any $t \in [0,T)$. Rearranging and recalling Definition 1.5, we obtain that

$$\begin{aligned}
&\|u(t)\|^2_{L^2(\Omega)} + 2\int_t^T\int_\Omega |y^\kappa\nabla(y^{-\kappa}u(s))|^2\, ds \\
&\qquad\qquad \leqslant \|u_T\|^2_{L^2(\Omega)} + \int_t^T \big[\|F(s)\|_{L^2(\Omega)} + \|y^{-1}u(s)\|_{L^2(\Omega)}\big]\|u(s)\|_{L^2(\Omega)}\, ds.
\end{aligned}$$

Applying (3-4), (3-5), and absorbing then yields,

$$\|u(t)\|^2_{L^2(\Omega)} + \|u\|^2_{L^2((0,T);H^1(\Omega))} \lesssim \|u_T\|^2_{L^2(\Omega)} + \|F\|^2_{L^2((0,T)\times\Omega)} + \int_t^T \|u(s)\|^2_{L^2(\Omega)}\, ds,$$

and the result follows from Gronwall's inequality. □

Definition 3.11. Given $u_T \in H_0^1(\Omega)$ and $F \in L^2((0,T)\times\Omega)$, we call

$$u \in C^0([0,T]; H_0^1(\Omega)) \cap H^1((0,T); L^2(\Omega)) \cap L^2((0,T); \mathfrak{D}(A_\sigma))$$

a *strict solution* of Problem (OI) if and only if:

- $(\partial_t + \Delta_\sigma + X\cdot\nabla + V)u = F$ almost everywhere on $(0,T)\times\Omega$.
- $u(T) = u_T$ holds as an equality in $H_0^1(\Omega)$.

Proposition 3.12. *Suppose $u_T \in H_0^1(\Omega)$ and $F \in L^2((0,T)\times\Omega)$. Then, the mild solution u from Proposition 3.10 is also the unique strict solution to Problem* (OI). *Furthermore, u satisfies the energy inequality*

$$\|u\|^2_{L^\infty([0,T];H^1(\Omega))} + \|y^{-\kappa}\nabla[y^{2\kappa}\nabla(y^{-\kappa}u)]\|^2_{L^2((0,T)\times\Omega)} \lesssim \|u_T\|^2_{H^1(\Omega)} + \|F\|^2_{L^2((0,T)\times\Omega)}, \tag{3-21}$$

again with the constant depending only on Ω, σ, X, V.

Proof sketch. That the mild solution is also the strict solution is immediate. For (3-21), we again need only consider $u_T \in \mathfrak{D}(A_\sigma)$.

By the fundamental theorem of calculus, integrations by parts, and (3-2),

$$\begin{aligned}
&\|y^\kappa\nabla(y^{-\kappa}u(T))\|^2_{L^2(\Omega)} - \|y^\kappa\nabla(y^{-\kappa}u(t))\|^2_{L^2(\Omega)} \\
&= -2\int_t^T\int_\Omega \partial_t u y^{-\kappa}\nabla\cdot[y^{2\kappa}\nabla(y^{-\kappa}u)]\big|_{t=s}\,ds \\
&= 2\int_t^T\int_\Omega (-F + X\cdot\nabla u + V_y u)y^{-\kappa}\nabla\cdot[y^{2\kappa}\nabla(y^{-\kappa}u)]\big|_{t=s}\,ds + 2\int_t^T\int_\Omega |y^{-\kappa}\nabla\cdot[y^{2\kappa}\nabla(y^{-\kappa}u)]|^2\big|_{t=s}\,ds.
\end{aligned}$$

Rearranging the above and applying Hardy's inequality then yields

$$\|u\|^2_{L^\infty([0,T];H^1(\Omega))} + \|y^{-\kappa}\nabla\cdot[y^{2\kappa}\nabla(y^{-\kappa}u)]\|^2_{L^2((0,T)\times\Omega)} \lesssim \|u_T\|^2_{H^1(\Omega)} + \|F\|^2_{L^2((0,T)\times\Omega)}.$$

The desired (3-21) now follows from the above and from (3-9). □

Remark 3.13. While our well-posedness theory only applies when the lower-order coefficients X and V are time-independent, this restriction is not essential. In fact, one can also treat time-dependent X and V using a Galerkin method approach; see [Warnick 2013], which develops this theory for critically singular hyperbolic equations.

3.3. ***The Neumann trace.*** From now on, we will focus mainly be on strict solutions to Problem (OI), which are particularly relevant as this level of regularity is sufficient to define and control the Neumann boundary trace.

Proposition 3.14. *Fix $u_T \in H_0^1(\Omega)$ and $F \in L^2((0,T)\times\Omega)$, and let u denote the strict solution to Problem* (OI) *(with this u_T and F). Then, the Neumann trace $\mathcal{N}_\sigma u$ is well-defined in $L^2((0,T)\times\Gamma)$ and satisfies the bound*

$$\|\mathcal{N}_\sigma u\|^2_{L^2((0,T)\times\Gamma)} \lesssim \|u_T\|^2_{H^1(\Omega)} + \|F\|^2_{L^2((0,T)\times\Omega)}, \tag{3-22}$$

where the constant in the above depends on Ω, σ, X, V.

Furthermore, the following limit holds in $L^2((0,T)\times\Gamma)$:

$$\lim_{d_\Gamma\to 0} d_\Gamma^{-1+\kappa}u = \frac{1}{1-2\kappa}\mathcal{N}_\sigma u. \tag{3-23}$$

Proof. For any $x \in \Gamma$ and $0 < y_0 < 2d_0$, we let $\eta_{y_0}(x)$ denote the point on the level set $\{y = y_0\}$ that is reached from x along the integral curve of ∇y. Letting dS be the surface measure on Γ, then for any $0 < y_0' < y_0 < 2d_0$,

$$\begin{aligned}
&\int_{(0,T)\times\Gamma} \big[y^{2\kappa} D_y(y^{-\kappa}u)|_{(t,\eta_{y_0}(x))} - y^{2\kappa} D_y(y^{-\kappa}u)|_{(t,\eta_{y_0'}(x))}\big]^2 \, dS(x)\, dt \\
&\qquad = \int_{(0,T)\times\Gamma} \biggl(\int_{y_0'}^{y_0} D_y[y^{2\kappa} D_y(y^{-\kappa}u)]|_{(t,\eta_y(x))} dy\biggr)^2 \, dS(x)\, dt \\
&\qquad \leqslant \int_{y_0'}^{y_0} y^{2\kappa}\, dy \cdot \int_{(0,T)\times\Gamma} \int_{y_0'}^{y_0} \big|y^{-\kappa} D_y[y^{2\kappa} D_y(y^{-\kappa}u)]|_{(t,\eta_y(x))}\big|^2 \, dy\, dS(x)\, dt \\
&\qquad \lesssim (1+2\kappa)^{-1} y_0^{1+2\kappa} \cdot \int_0^T \int_\Omega \big|y^{-\kappa} \nabla[y^{2\kappa} \nabla(y^{-\kappa}u(s))]\big|^2 \, ds,
\end{aligned}$$

where we used that $2\kappa > -1$ and that $y = d_\Gamma$ near Γ. By the inequality (3-21), the right-hand side of the above vanishes when $y_0 \searrow 0$, and it hence follows that $\mathcal{N}_\sigma u$ exists as an element of $L^2((0, T) \times \Gamma)$.

Next, let $\chi : \mathbb{R} \to [0, 1]$ be a cutoff function satisfying

$$\chi(s) = \begin{cases} 1 & s < d_0, \\ 0 & s > \tfrac{1}{2} 3d_0. \end{cases}$$

Then, a similar computation as before, again using that $2\kappa > -1$, yields

$$\begin{aligned}
\int_{(0,T)\times\Gamma} (\mathcal{N}_\sigma u)^2 &= \int_{(0,T)\times\Gamma} \biggl(\int_0^{2d_0} D_y[\chi(y) y^{2\kappa} D_y(y^{-\kappa}u)]|_{(t,\eta_y(x))}\, dy\biggr)^2 \, dS(x)\, dt \\
&\lesssim d_0^{1+2\kappa} \int_{(0,T)\times\Gamma} \int_0^{2d_0} \big|y^{-\kappa} D_y[y^{2\kappa} D_y(y^{-\kappa}u)]|_{(t,\eta_y(x))}\big|^2 \, dy\, dS(x)\, dt \\
&\qquad\qquad + d_0^{1+2\kappa} \int_{(0,T)\times\Gamma} \int_0^{2d_0} \big|y^{\kappa} D_y(y^{-\kappa}u)|_{(t,\eta_y(x))}\big|^2 \, dy\, dS(x)\, dt \\
&\lesssim \int_0^T \int_\Omega |y^{-\kappa} \nabla[y^{2\kappa} \nabla(y^{-\kappa}u(s))]|^2 \, ds + \|u\|^2_{L^2((0,T);H^1(\Omega))},
\end{aligned}$$

where we also used (3-5). The bound (3-22) follows from (3-21) and the above.

Next, for (3-23), we first note, for any $0 < y_0 < 2d_0$, that

$$\begin{aligned}
&\int_{(0,T)\times\Gamma} \Bigl(y^{\kappa-1} u|_{(t,\eta_{y_0}(x))} - \frac{1}{1-2\kappa} \mathcal{N}_\sigma u|_{(t,x)}\Bigr)^2 \, dS(x)\, dt \\
&\qquad = \int_{(0,T)\times\Gamma} \biggl[y_0^{2\kappa-1} \int_0^{y_0} D_y(y^{-\kappa}u)|_{(t,\eta_y(x))}\, dy - \frac{1}{1-2\kappa} \mathcal{N}_\sigma u|_{(t,x)}\biggr]^2 \, dS(x)\, dt \\
&\qquad = \int_{(0,T)\times\Gamma} \biggl(y_0^{2\kappa-1} \int_0^{y_0} y^{-2\kappa} \big[y^{2\kappa} D_y(y^{-\kappa}u)|_{(t,\eta_y(x))} - \mathcal{N}_\sigma u|_{(t,x)}\big]\, dy\biggr)^2 \, dS(x)\, dt,
\end{aligned}$$

where we used the boundary condition $u=0$ on Γ from (3-1), and that $\kappa<0$. We next employ Minkowski's inequality on the above to derive

$$\left[\int_{(0,T)\times\Gamma}\left(y^{\kappa-1}u|_{(t,\eta_y(x))}-\frac{1}{1-2\kappa}\mathcal{N}_\sigma u|_{(t,x)}\right)^2 dS(x)\,dt\right]^{\frac{1}{2}}$$
$$\lesssim y_0^{2\kappa-1}\int_0^{y_0} y^{-2\kappa}\left[\int_{(0,T)\times\Gamma}\left(y^{2\kappa}D_y(y^{-\kappa}u)|_{(t,\eta_y(x))}-\mathcal{N}_\sigma u|_{(t,x)}\right)^2 dS(x)\,dt\right]^{\frac{1}{2}} dy$$
$$\lesssim \sup_{0<y<y_0}\left[\int_{(0,T)\times\Gamma}\left(y^{2\kappa}D_y(y^{-\kappa}u)|_{(t,\eta_y(x))}-\mathcal{N}_\sigma u|_{(t,x)}\right)^2 dS(x)\,dt\right]^{\frac{1}{2}}.$$

Since $\mathcal{N}_\sigma u\in L^2((0,T)\times\Gamma)$, its definition (1-3) implies the above converges to 0 as $y_0\searrow 0$. This immediately implies the desired limit (3-23). □

Remark 3.15. With some modification, one can extend the preceding well-posedness theory (Propositions 3.10 and 3.12) and Proposition 3.14 to $0\leqslant\sigma<\frac{1}{4}$.

Next, we prove a technical result, roughly stating that the least regular boundary term in the Carleman estimate (2-62) indeed vanishes in our present setting:

Proposition 3.16. *Let $u_T\in H_0^1(\Omega)$, and let u denote the strict solution to Problem* (O) (*that is*, *Problem* (OI) *without forcing term $F\equiv 0$*). *Then*, *u satisfies*

$$\begin{aligned}\lim_{\delta\searrow 0}\int_{(0,T)\times\{y=\delta\}} e^{-2\lambda\mathcal{F}}\partial_t(y^{-\kappa}u)y^{2\kappa}D_y(y^{-\kappa}u)=0,\\ \lim_{\delta\searrow 0}\int_{(0,T)\times\{y=\delta\}} e^{-2\lambda\mathcal{F}}\partial_t(y^{-\kappa}u)y^{-1+\kappa}u=0,\end{aligned}\tag{3-24}$$

for any $\lambda>0$, where $\mathcal{F}$ denotes the weight

$$\mathcal{F}(t,x):=\frac{1}{t(T-t)}[y(x)^{1+2\kappa}+\beta],\qquad \beta>0.\tag{3-25}$$

Proof sketch. Define the bilinear maps $\mathcal{B}_1,\mathcal{B}_2:H_0^1(\Omega)\to\mathbb{R}$ by

$$\begin{aligned}\mathcal{B}_1(u_T)&:=\lim_{\delta\searrow 0}\int_{(0,T)\times\{y=\delta\}} e^{-2\lambda\mathcal{F}}\partial_t(y^{-\kappa}u)y^{2\kappa}D_y(y^{-\kappa}u),\\ \mathcal{B}_2(u_T)&:=\lim_{\delta\searrow 0}\int_{(0,T)\times\{y=\delta\}} e^{-2\lambda\mathcal{F}}\partial_t(y^{-\kappa}u)y^{-1+\kappa}u,\end{aligned}\tag{3-26}$$

where u is the strict solution to Problem (O) with final data u_T. It then suffices to show that both $\mathcal{B}_1$ and $\mathcal{B}_2$ are everywhere vanishing.

The main step is to show that both $\mathcal{B}_1$ and $\mathcal{B}_2$ are well-defined and finite. The process is similar to the proof of Proposition 3.14, except we need more care with regularity. Somewhat informally, we use the divergence theorem to bound $\mathcal{B}_1$ by

$$
\begin{aligned}
|\mathcal{B}_1(u_T)| &= \left|\lim_{\delta\searrow 0}\int_{(0,T)\times\{y>\delta\}} \nabla\cdot[e^{-2\lambda\mathcal{F}}\partial_t(y^{-\kappa}u)y^{2\kappa}\nabla(y^{-\kappa}u)]\right| \\
&\leqslant \tfrac{1}{2}\limsup_{\delta\searrow 0}\left|\int_{(0,T)\times\{y>\delta\}} e^{-2\lambda\mathcal{F}}\partial_t[|y^\kappa\nabla(y^{-\kappa}u)|^2]\right| + C\int_{(0,T)\times\Omega}|\partial_t u|\big|y^{-\kappa}\nabla\cdot[y^{2\kappa}\nabla(y^{-\kappa}u)]\big| \\
&\qquad + C\int_{(0,T)\times\Omega}|\partial_t u|y^\kappa|y^{2\kappa}D_y(y^{-\kappa}u)| \\
&\lesssim \sup_{t\in[0,T]}\int_\Omega |y^\kappa\nabla(y^{-\kappa}u(t))|^2 + \int_{(0,T)\times\Omega} y^{2\kappa}|y^{2\kappa}D_y(y^{-\kappa}u)|^2 \\
&\qquad + \int_{(0,T)\times\Omega}\big(|\partial_t u|^2 + \big|y^{-\kappa}\nabla\cdot[y^{2\kappa}\nabla(y^{-\kappa}u)]\big|^2\big) \\
&= I_{1,1} + I_{1,2} + I_{1,3},
\end{aligned}
\tag{3-27}
$$

where all constants here and below can depend on Ω, σ, X, V, as well as β, λ, and where we also noted that $\lambda^3 t^{-3}(T-t)^{-3}e^{-2\lambda\mathcal{F}}$ is bounded.

For $I_{1,1}$, we apply Corollary 3.5 and Proposition 3.12, which yield

$$I_{1,1} \lesssim \|u_T\|^2_{H^1(\Omega)}. \tag{3-28}$$

For $I_{1,3}$, we recall the heat equation (1-9), Proposition 3.3, and (3-21) to obtain

$$I_{1,3} \lesssim \|u_T\|^2_{H^1(\Omega)}. \tag{3-29}$$

For $I_{1,2}$, we integrate the pointwise Hardy inequality of Lemma 2.6, with parameters $q := 1+\kappa$ and $v := y^{2\kappa}D_y(y^{-\kappa}u)$, and we recall Propositions 3.12 and 3.14:

$$
\begin{aligned}
I_{1,2} &\lesssim \int_{(0,T)\times\Omega}\big(y^{2+2\kappa}|D_y[y^{2\kappa}D_y(y^{-\kappa}u)]|^2 + y^{1+2\kappa}|y^{2\kappa}D_y(y^{-\kappa}u)|^2\big) \\
&\qquad + \lim_{\delta\searrow 0}\int_{(0,T)\times\{y=\delta\}} y^{1+2\kappa}|y^{2\kappa}D_y(y^{-\kappa}u)|^2 \\
&\lesssim \|u_T\|^2_{H^1(\Omega)} + \int_{(0,T)\times\Omega} y^{1+2\kappa}|y^{2\kappa}D_y(y^{-\kappa}u)|^2.
\end{aligned}
$$

(Formally, the region near the critical point of y, where $|\nabla y| = 0$, can be trivially treated.) Integrating Lemma 2.6 again, now with $q := \frac{3}{2}+\kappa$, yields

$$I_{1,2} \lesssim \|u_T\|^2_{H^1(\Omega)}. \tag{3-30}$$

Combining (3-27)–(3-30), we see that

$$\mathcal{B}_1(u_T) \lesssim \|u_T\|^2_{H^1(\Omega)}.$$

Also, applying the above to differences of final data, we see that $\mathcal{B}_1$ is continuous.

Next, for $\mathcal{B}_2$, we have

$$|\mathcal{B}_2(u_T)| = \frac{1}{2}\left|\int_{(0,T)\times\Gamma} e^{-2\lambda\mathcal{F}}\partial_t(y^{-1}u^2)\right| \lesssim \sup_{t\in[0,T]}\lim_{\delta\searrow 0}\int_{\{y=\delta\}} y^{-1}|u(t)|^2 + \lim_{\delta\searrow 0}\int_{(0,T)\times\{y=\delta\}} y^{2\kappa}u^2.$$

The last term in the above vanishes by Proposition 3.14. For the remaining term, we again integrate Lemma 2.6, with $q=0$, which yields

$$|\mathcal{B}_2(u_T)| \lesssim \sup_{t\in[0,T]} \int_\Omega (|D_y u|^2 + y^{-1}u^2) \lesssim \|u_T\|^2_{H^1(\Omega)},$$

where in the last step, we also applied Propositions 3.3 and 3.12. Like for $\mathcal{B}_1$, the above suffices to imply the finiteness and continuity of $\mathcal{B}_2$.

(Formally, to rigorously show $\mathcal{B}_1(u_T)$, $\mathcal{B}_2(u_T)$ are well-defined, we would need, as in the proof of Proposition 3.14, to estimate differences of the associated integrals over $(0,T)\times\{y=\delta_1\}$ and $(0,T)\times\{y=\delta_2\}$, with $\delta_1,\delta_2\searrow 0$. However, we skip this step here, as the details of this are analogous to the above.)

Finally, by continuity, it suffices to show $\mathcal{B}_1$ and $\mathcal{B}_2$ vanish on a dense subspace of $H^1_0(\Omega)$. For this, we consider the domain $\mathfrak{D}(A_\sigma)$ from Proposition 3.7. Observe in particular that if $u_T\in\mathfrak{D}(A_\sigma)$, then the relations (see (3-19))

$$u(t)=e^{(T-t)A_\sigma}u_T, \qquad \partial_t u(t) = e^{(T-t)A_\sigma}(-A_\sigma u_T)$$

imply that $\partial_t u$ is a mild solution to Problem (O), with final data $-A_\sigma u_T\in L^2(\Omega)$. Also, Proposition 3.10 yields $\partial_t u\in L^2((0,T);H^1_0(\Omega))$, and hence $\mathcal{D}_\sigma(\partial_t u)=0$ as an element of $L^2((0,T)\times\Gamma)$. Applying the above to (3-26), we now have both $\mathcal{B}_1(u_T)=0$ and $\mathcal{B}_2(u_T)=0$ whenever $u_T\in\mathfrak{D}(A_\sigma)$, as desired. □

3.4. *Observability.* Lastly, we state the key observability inequality and unique continuation property satisfied by solutions of Problem (O):

Theorem 3.17. *Let $u_T\in H^1_0(\Omega)$, and let u be the corresponding strict solution to Problem* (O). *Then, the observability estimate*

$$\|u(0)\|^2_{H^1(\Omega)} \lesssim \|\mathcal{N}_\sigma u\|^2_{L^2((0,T)\times\Gamma)} \tag{3-31}$$

holds with the constant of the inequality depending on Ω, σ, X, V.

In particular, if $\mathcal{N}_\sigma u\equiv 0$ on $(0,T)\times\Gamma$, then $u\equiv 0$ on $[0,T]\times\Omega$.

Proof. Applying the global Carleman estimate of Theorem 2.9, with $\sigma:=\kappa(1-\kappa)$ from Problem (O) and with $p:=\kappa+\frac{1}{2}$, so that

$$p\in\left(0,\tfrac{1}{2}\right), \qquad p^2-2p+\tfrac{3}{4}=\sigma,$$

we see that there exists a boundary defining pair (y_1,y_2) (again, the values of the associated constants are not important) such that, for sufficiently large $\lambda>0$,

$$\begin{aligned}
&\sum_{j=1}^2 \int_{(0,T)\times\Omega} \lambda\theta e^{-2\lambda F_j}(|\nabla u|^2 + y_j^{-2}u^2) \\
&\leqslant \limsup_{\delta\searrow 0} \sum_{j=1}^2 \int_{(0,T)\times\{y_j=\delta\}} \lambda^3\theta^3 e^{-2\lambda F_j}[y_j^{2\kappa}(D_{y_j}u)^2 + y_j^{-2+2\kappa}u^2] \\
&\qquad + \limsup_{\delta\searrow 0} \sum_{j=1}^2 \left| \int_{(0,T)\times\{y_j=\delta\}} e^{-2\lambda F_j}\partial_t u D_{y_j} u \right| + \sum_{j=1}^2 \int_{(0,T)\times\Omega} e^{-2\lambda F_j}(\partial_t+\Delta_{\sigma,y_j}u)^2.
\end{aligned} \tag{3-32}$$

In the above, (θ, F_1, F_2) are defined from (y_1, y_2) via (2-55), and the left-hand side of (2-62) was further simplified by recalling that $\kappa < 0$. (While (2-62) holds for classical regular solutions, this can be extended to strict solutions via approximation.)

For the first boundary term in (3-32), we apply Proposition 3.14 to obtain

$$\begin{aligned}\limsup_{\delta\searrow 0}\sum_{j=1}^{2}\int_{(0,T)\times\{y_j=\delta\}} &\lambda^3\theta^3 e^{-2\lambda F_j}[y_j^{2\kappa}(D_{y_j}u)^2 + y_j^{-2+2\kappa}u^2] \\ &\lesssim \limsup_{\delta\searrow 0}\sum_{j=1}^{2}\int_{(0,T)\times\{y_j=\delta\}} \lambda^3\theta^3 e^{-2\lambda F_j}[|y_j^{2\kappa}D_{y_j}(y_j^{-\kappa}u)|^2 + y_j^{-2+2\kappa}u^2] \\ &\lesssim \int_{(0,T)\times\Gamma}(\mathcal{N}_\sigma u)^2, \end{aligned} \tag{3-33}$$

where we also noted in the last step that $\lambda^3\theta^3 e^{-2\lambda F_j}$ is bounded. Moreover, from Proposition 3.16, the remaining boundary term in (3-32) vanishes.

Next, from Definition 1.5 and the definition of y, we have

$$\sum_{j=1}^{2}\int_{(0,T)\times\Omega} e^{-2\lambda F_j}(\partial_t + \Delta_{\sigma,y_j}u)^2 \lesssim \sum_{j=1}^{2}\int_{(0,T)\times\Omega} e^{-2\lambda F_j}(|\nabla u|^2 + y_j^{-2}u^2). \tag{3-34}$$

Thus, combining (3-32)–(3-34) and taking λ sufficiently large yields

$$\sum_{j=1}^{2}\int_{(0,T)\times\Omega} e^{-2\lambda F_j}(|\nabla u|^2 + y_j^{-2}u^2) \lesssim \int_{(0,T)\times\Gamma}(\mathcal{N}_\sigma u)^2. \tag{3-35}$$

Note (3-35) implies unique continuation — if $\mathcal{N}_\sigma u \equiv 0$, then $u \equiv 0$ on $[0, T] \times \Omega$.

Finally, applying the Hardy inequality (3-4) to (3-35), we have

$$\int_0^T e^{-c\lambda\theta(t)}\|u(t)\|_{H^1(\Omega)}\,dt \lesssim \int_{(0,T)\times\Gamma}(\mathcal{N}_\sigma u)^2, \quad c > 0.$$

Applying the inequality (3-21) on each interval $(0, t)$ (with $F \equiv 0$) in the left-hand side of the above, we can estimate the H^1-norm of $u(t)$ from below by the H^1-norm of $u(0)$. Since $e^{-c\lambda\theta}$ is clearly integrable on $(0, T)$, then (3-31) follows. □

4. Boundary controllability

In this section, we prove our main boundary controllability result for the forward heat equation by applying the Neumann regularity (Proposition 3.14) and boundary observability (Theorem 3.17) for the backward heat equation. In particular, here we are primarily concerned with the setting of Problem (C):

$$\begin{aligned} (-\partial_t + \Delta_\sigma + Y\cdot\nabla + W)v &= 0 \quad \text{on } (0,T)\times\Omega, \\ v(0) &= v_0 \quad \text{on } \Omega, \\ \mathcal{D}_\sigma v &= f \quad \text{on } (0,T)\times\Gamma. \end{aligned}$$

As usual, we adopt the same setting as described in previous sections.

4.1. ***Regular solutions.*** The first step is to briefly discuss how solutions of Problem (C) with nonzero Dirichlet data are constructed for sufficiently regular data.

Proposition 4.1. *Given* $v_0 \in H^1_0(\Omega)$ *and* $f \in C^\infty_0((0,T)\times\Gamma)$, *there exists*

$$v \in C^0([0,T];H^1_{\mathrm{loc}}(\Omega)) \cap H^1((0,T)\times L^2(\Omega)) \cap L^2((0,T);H^2_{\mathrm{loc}}(\Omega))$$

that solves Problem (C) *in the following sense*:

- $(-\partial_t + \Delta_\sigma + Y\cdot\nabla + W)v = 0$ *almost everywhere on* $(0,T)\times\Omega$.
- $v(0) = v_0$ *holds as an equality in* $H^1_{\mathrm{loc}}(\Omega)$.
- $\mathcal{D}_\sigma v = f$ *holds in the trace sense in* $C^0([0,T];L^2(\Gamma))$.

Moreover, if $u_T \in H^1_0(\Omega)$ *and* $F \in L^2((0,T)\times\Omega)$, *and if* u *is the corresponding strict solution of Problem* (OI), *with lower-order coefficients given by*

$$(X,V) := (-Y, W - \nabla\cdot Y) \in \mathcal{Z}, \tag{4-1}$$

then the following identity holds:

$$\int_{(0,T)\times\Omega} Fv = \int_\Omega u_T v(T) - \int_\Omega u(0)v_0 + \int_{(0,T)\times\Gamma} \mathcal{N}_\sigma u f. \tag{4-2}$$

Proof sketch. For convenience, we adopt the shorthand

$$B_\sigma := \Delta_\sigma + Y\cdot\nabla + W. \tag{4-3}$$

First, we construct a suitable extension $v_f : (0,T)\times\Omega \to \mathbb{R}$ of f:

- We extend f to a sufficiently small neighborhood $(0,T)\times U_\Gamma$ of $(0,T)\times\Gamma$ by defining it to be constant along the integral curves of ∇y at each time. Calling this extension f_Γ, we then define, on $(0,T)\times U_\Gamma$, the function

$$v_f := y^\kappa f_\Gamma - \frac{1}{2\kappa} y^{1+\kappa}(\kappa Y\cdot\nabla y + yW_y) f_\Gamma \in C^2((0,T)\times U_\Gamma). \tag{4-4}$$

- v_f is then extended arbitrarily to all of $(0,T)\times\Omega$ as a C^2-function.

Furthermore, observe that since $f \in C^\infty_0((0,T)\times\Gamma)$, we can also arrange such that v_f smoothly extends to $t=0$ by the condition $v_f|_{t=0} \equiv 0$.

The key observation is that $(-\partial_t + B_\sigma)v_f$ lies in $L^2((0,T)\times\Omega)$. To confirm this, we need only check that (4-4) has this property on $(0,T)\times U_\Gamma$, on which we can assume $y = d_\Gamma$. For the first term on the right-hand side of (4-4), we have

$$\begin{aligned}(-\partial_t + B_\sigma)(y^\kappa f_\Gamma) &= y^{-\kappa}\nabla\cdot(y^{2\kappa}\nabla f_\Gamma) + Y\cdot\nabla(y^\kappa f_\Gamma) + W_y y^\kappa f_\Gamma + O(y^\kappa)\\ &= 2\kappa y^{\kappa-1}\nabla y\cdot\nabla f_\Gamma + y^{\kappa-1}(\kappa Y\cdot\nabla y + yW_y) f_\Gamma + O(y^\kappa),\end{aligned}$$

since f_Γ and its derivatives are bounded up to Γ by definition. As $\nabla y\cdot\nabla f_\Gamma$ vanishes (again by the definition of f_Γ), we hence obtain

$$(-\partial_t + B_\sigma)(y^\kappa f_\Gamma) = y^{\kappa-1}(\kappa Y\cdot\nabla y + yW_y) f_\Gamma + O(y^\kappa). \tag{4-5}$$

In addition, since Y and yW_y are C^2 at Γ (by Definition 1.5), we have

$$
\begin{aligned}
(-\partial_t + B_\sigma)\Big[-\frac{1}{2\kappa} y^{1+\kappa}(\kappa Y\cdot\nabla y + yW_y) f_\Gamma\Big] &= -\frac{1}{2\kappa}[y^{-\kappa}\nabla\cdot(y^{2\kappa}\nabla y)](\kappa Y\cdot\nabla y + yW_y) f_\Gamma + O(y^\kappa) \\
&= -y^{\kappa-1}(\kappa Y\cdot\nabla y + yW_y) f_\Gamma + O(y^\kappa). \qquad (4\text{-}6)
\end{aligned}
$$

Summing (4-5) and (4-6), and recalling that $\kappa \in \left(-\frac{1}{2}, 0\right)$, we conclude that

$$(-\partial_t + B_\sigma) v_f = O(y^\kappa) \in L^2((0,T)\times\Omega). \qquad (4\text{-}7)$$

Next, we define v_h as the strict solution to the following problem:

$$
\begin{aligned}
(-\partial_t + B_\sigma) v_h &= -(-\partial_t + B_\sigma) v_f && \text{on } (0,T)\times\Omega, \\
v_h(T) &= v_0 && \text{on } \Omega, \\
v_h &= 0 && \text{on } (0,T)\times\Gamma.
\end{aligned} \qquad (4\text{-}8)
$$

Note that the existence of v_h follows from Proposition 3.12 (adapted to the forward heat equation — see Remark 3.1) along with (4-7). Finally, observe that

$$v := v_h + v_f, \qquad (4\text{-}9)$$

which lies in the required space, suffices as our desired solution to Problem (C).

Lastly, given u_T, F, and u as in the hypotheses, we write

$$
\begin{aligned}
\int_{(0,T)\times\Omega} Fv &= \int_{(0,T)\times\Omega} \big(\partial_t u + y^{-\kappa}\nabla\cdot[y^{2\kappa}\nabla(y^{-\kappa}u)] + X\cdot\nabla u + V_y u\big) v \\
&= I_1 + I_2 + I_3 + I_4, \qquad (4\text{-}10)
\end{aligned}
$$

and we integrate each term on the right-hand side of (4-10) by parts. First,

$$
\begin{aligned}
I_1 &= \int_{(0,T)\times\Omega} u(-\partial_t v) + \int_\Omega u(T)v(T) - \int_\Omega u(0)v(0) \\
&= \int_{(0,T)\times\Omega} u(-\partial_t v) + \int_\Omega u_T v(T) - \int_\Omega u(0) v_0. \qquad (4\text{-}11)
\end{aligned}
$$

To see that the right-hand side of (4-11) is well-defined, we consider, for instance,

$$\int_\Omega u_T v(T) = \int_\Omega u_T v_h(T) + \int_\Omega u_T v_f(T).$$

Note that both terms on the right-hand side are finite, since $u_T, v_h, v_f \in L^2(\Omega)$ by Proposition 3.12, (4-4), and the assumption $\kappa > -\frac{1}{2}$; the remaining term involving $u(0)v_0$ is treated similarly. Next, observe from (3-3) and (4-1) that

$$
\begin{aligned}
I_3 + I_4 &= \int_{(0,T)\times\Omega} u(Y\cdot\nabla v + W_y v) - \int_{(0,T)\times\Gamma} (Y\cdot\nabla y)\Big[\lim_{y\searrow 0} y^\kappa u\Big]\mathcal{D}_\sigma v \\
&= \int_{(0,T)\times\Omega} u(Y\cdot\nabla v + W_y v), \qquad (4\text{-}12)
\end{aligned}
$$

where the boundary term in (4-12) vanishes due to (3-23).

For the remaining term I_2, we first obtain

$$I_2 = -\int_{(0,T)\times\Omega} y^\kappa \nabla(y^{-\kappa} u) \cdot y^\kappa \nabla(y^{-\kappa} v) + \int_{(0,T)\times\Gamma} \mathcal{N}_\sigma u \mathcal{D}_\sigma v$$
$$= -\int_{(0,T)\times\Omega} y^\kappa \nabla(y^{-\kappa} u) \cdot y^\kappa \nabla(y^{-\kappa} v) + \int_{(0,T)\times\Gamma} \mathcal{N}_\sigma u f,$$

where we note that $\mathcal{N}_\sigma u$ is well-defined by Proposition 3.14, and where we also note that $y^\kappa \nabla(y^{-\kappa} u)$, $y^\kappa \nabla(y^{-\kappa} v_h)$, and $y^\kappa \nabla(y^{-\kappa} v_f)$ all lie in $C([0, T]; L^2(\Omega))$, by Corollary 3.5, Proposition 3.12, and (4-4). Integrating by parts again then yields

$$I_2 = \int_{(0,T)\times\Omega} u \nabla \cdot [y^{2\kappa} \nabla(y^{-\kappa} v)] + \int_{(0,T)\times\Gamma} \mathcal{N}_\sigma u f - \int_{(0,T)\times\Gamma} \mathcal{D}_\sigma u \mathcal{N}_\sigma v. \tag{4-13}$$

We claim the last term in the right-hand side of (4-13) vanishes. However, treating this (informally written) term properly requires additional comments:

- For the Neumann trace "$\mathcal{N}_\sigma v$", we first notice from Proposition 3.14 that $\mathcal{N}_\sigma v_h$ is well-defined, with a finite value on $(0, T) \times \Gamma$. Also, from (4-4), we see directly that $\mathcal{N}_\sigma v_f$ (or, more accurately, $y^{2\kappa} D_y(y^{-\kappa} v_f)$ in the limit $y \to 0$) blows up like $O(y^{2\kappa})$ at $(0, T) \times \Gamma$.
- By the second part of Proposition 3.14, the Dirichlet trace $\mathcal{D}_\sigma u$ exists and vanishes to order $O(y^{1-\kappa})$ at $(0, T) \times \Gamma$.

Thus, the informally stated product "$\mathcal{D}_\sigma u \mathcal{N}_\sigma v$" vanishes at $(0, T) \times \Gamma$ like $O(y^{1+\kappa})$, which is a positive power of y since $\kappa > -\frac{1}{2}$.

Combining (3-3) and (4-10)–(4-13) then yields

$$\int_{(0,T)\times\Omega} F v = \int_{(0,T)\times\Omega} u(-\partial_t v + B_\sigma v) + \int_{(0,T)\times\Gamma} \mathcal{N}_\sigma u f + \int_\Omega u_T v(T) - \int_\Omega u(0) v_0,$$

and the desired identity (4-2) follows from the equation satisfied by v. □

Remark 4.2. In proving Proposition 4.1, the extension $v_f := d_\Gamma^\kappa f_\Gamma$ may have seemed natural at first glance. However, this v_f runs into issues, since $(-\partial_t + B_\sigma) v_f$ fails to lie in $L^2((0, T) \times \Omega)$. As a result, one requires the extra correction term in (4-4) to ensure v_f is sufficiently well-behaved near the boundary. In fact, this correction term also motivates the boundary conditions imposed in Definition 1.5.

4.2. ***Weak solutions.*** The next task is to derive, using the identity (4-2), a well-posedness theory for Problem (C) that is dual to that of Problem (OI).

Definition 4.3. Given $v_0 \in H^{-1}(\Omega)$ and $f \in L^2((0, T) \times \Gamma)$, we call

$$v \in C^0([0, T]; H^{-1}(\Omega)) \cap L^2((0, T) \times \Omega)$$

a *weak* (or *transposition*) *solution* of Problem (C) if and only if for any $F \in L^2((0, T) \times \Omega)$,

$$\int_{(0,T)\times\Omega} F v = -\int_\Omega u(0) v_0 + \int_{(0,T)\times\Gamma} \mathcal{N}_\sigma u f, \tag{4-14}$$

where u is the strict solution to Problem (OI) with the above F, with $u_T \equiv 0$, and with lower-order coefficients X and V given by (4-1).

Proposition 4.4. *Given $v_0 \in H^{-1}(\Omega)$ and $f \in L^2((0,T)\times\Gamma)$, there exists a unique weak solution v of Problem* (C). *In addition, v satisfies*

$$\|v\|^2_{L^\infty([0,T];H^{-1}(\Omega))} + \|v\|^2_{L^2((0,T)\times\Omega)} \lesssim \|v_0\|^2_{H^{-1}(\Omega)} + \|f\|^2_{L^2((0,T)\times\Gamma)}, \tag{4-15}$$

where the constant depends on Ω, σ, Y, W.

Proof sketch. Define the linear functional $S : L^2((0,T)\times\Omega) \to \mathbb{R}$ by

$$SF := -\int_\Omega u(0)v_0 + \int_{[0,T]\times\Gamma} \mathcal{N}_\sigma u f,$$

where u is the strict solution to Problem (OI) with the above F, with $u_T \equiv 0$, and with X and V given by (4-1). Observe that S is bounded, since

$$\begin{aligned} |SF|^2 &\lesssim \|u(0)\|^2_{H^1(\Omega)}\|v_0\|^2_{H^{-1}(\Omega)} + \|\mathcal{N}_\sigma u\|^2_{L^2((0,T)\times\Gamma)}\|f\|^2_{L^2((0,T)\times\Gamma)} \\ &\lesssim (\|v_0\|^2_{H^{-1}(\Omega)} + \|f\|^2_{L^2((0,T)\times\Gamma)})\|F\|^2_{L^2((0,T)\times\Omega)}, \end{aligned} \tag{4-16}$$

where in the last step, we applied (3-21) and (3-22). By the Riesz representation theorem, there exists a unique $v \in L^2((0,T)\times\Omega)$ such that

$$\int_{(0,T)\times\Omega} Fv = SF.$$

In particular, v satisfies the desired identity (4-14).

In addition, the representation theorem and (4-16) also imply the estimate

$$\|v\|^2_{L^2((0,T)\times\Omega)} \lesssim \|v_0\|^2_{H^{-1}(\Omega)} + \|f\|^2_{L^2((0,T)\times\Gamma)},$$

hence it remains only to obtain the $C^0([0,T]; H^{-1}(\Omega))$-estimate for v. For this, we fix any $\tau \in (0,T]$ and $u_\tau \in H^1_0(\Omega)$, and we let u be the strict solution of

$$\begin{aligned} (\partial_t + \Delta_\sigma u + X\cdot\nabla + V)u &= 0 \quad \text{on } (0,\tau)\times\Omega, \\ u(\tau) &= u_\tau \quad \text{on } \Omega, \\ u &= 0 \quad \text{on } (0,\tau)\times\Gamma. \end{aligned} \tag{4-17}$$

For sufficiently regular v_0 and f, uniqueness yields that v must be equal to that of Proposition 4.1. As a result, the identity (4-2) yields

$$\int_\Omega u_\tau v(\tau) = \int_\Omega u(0)v_0 - \int_{(0,T)\times\Gamma} \mathcal{N}_\sigma u f.$$

The estimate (3-21) then implies

$$\begin{aligned} \left|\int_\Omega u_\tau v(\tau)\right| &\leqslant \|u(0)\|_{H^1(\Omega)}\|v_0\|_{H^{-1}(\Omega)} + \|\mathcal{N}_\sigma u\|_{L^2((0,T)\times\Gamma)}\|f\|_{L^2((0,T)\times\Gamma)} \\ &\lesssim \|u_\tau\|_{H^1(\Omega)}\big[\|v_0\|_{H^{-1}(\Omega)} + \|f\|_{L^2((0,T)\times\Gamma)}\big], \end{aligned}$$

and the desired $C^0([0,T]; H^{-1}(\Omega))$-estimate for v follows. Finally, the general case $v_0 \in H^{-1}(\Omega)$ follows via an approximation argument. □

4.3. *Null controllability.* We can now turn our attention to the main null control result. The first step is to properly characterize the desired null control:

Proposition 4.5. *Fix any $v_0 \in H^{-1}(\Omega)$. Then, $f \in L^2((0,T)\times\Gamma)$ is a null control for Problem* (C) (*that is, the weak solution v to Problem* (C), *with the above v_0 and f, satisfies $v(T)=0$*) *if and only if for any $u_T \in H_0^1(\Omega)$,*

$$0 = \int_{(0,T)\times\Gamma} \mathcal{N}_\sigma u f - \int_\Omega u(0) v_0,$$

where u is the strict solution of Problem (O), *with (X, V) as in* (4-1).

Proof. For sufficiently regular v_0 and f, this follows from the identity (4-2) (with $F \equiv 0$). The general case then follows by approximation. □

Theorem 4.6. *Problem* (C) *is boundary null controllable — more specifically, given any $v_0 \in H^{-1}(\Omega)$, there is a null control $f \in L^2((0,T)\times\Gamma)$ for Problem* (C).

Proof. Consider the following seminorm on $H_0^1(\Omega)$,

$$\|u_T\|_{\mathfrak{N}} := \|\mathcal{N}_\sigma u\|_{L^2((0,T)\times\Gamma)}, \quad u_T \in H_0^1(\Omega), \tag{4-18}$$

where u is the strict solution of Problem (O), with u_T as above and with (X, V) as in (4-1). Theorem 3.17 implies that (4-18) defines a norm, and we can now define $\mathfrak{N}$ to be the Hilbert space completion of $H_0^1(\Omega)$ with respect to (4-18).

Consider now the functional $I_\sigma : H_0^1(\Omega) \to \mathbb{R}$ given by

$$I_\sigma(u_T) := \frac{1}{2}\int_{(0,T)\times\Gamma} |\mathcal{N}_\sigma u|^2 - \int_\Omega u(0) v_0, \tag{4-19}$$

with u as before. The observability inequality (3-31) then implies I_σ extends to a continuous functional on $\mathfrak{N}$, and this continuity also implies the estimate

$$I_\sigma(u_T) \geqslant c\|u_T\|_{\mathfrak{N}}^2 - C\|v_0\|_{H^{-1}(\Omega)}^2, \quad u_T \in \mathfrak{N},$$

with $c, C > 0$. In particular, I_σ is coercive, hence I_σ has a minimizer $u_T^* \in \mathfrak{N}$.

Let $\{u_{T,j}\}$ be a sequence in $H_0^1(\Omega)$ with $u_{T,j} \to u_T^*$ in $\mathfrak{N}$, and let $\{u_j\}$ be the corresponding solutions to Problem (O). By (3-31) and (4-18), there exist functions $f \in L^2((0,T)\times\Gamma)$ and $u_0 \in H_0^1(\Omega)$ such that

$$\|f - \mathcal{N}_\sigma u_j\|_{L^2((0,T)\times\Gamma)} \to 0, \quad \|u_0 - u_j(0)\|_{H_0^1(\Omega)} \to 0.$$

Finally, taking the first variation of I_σ and recalling the above limits, we therefore obtain, for any $u_T \in H_0^1(\Omega)$ (and with u as before),

$$0 = \lim_{h\to 0} \frac{1}{h}[I_\sigma(u_T^* + h u_T) - I_\sigma(u_T^*)] = \int_{(0,T)\times\Gamma} \mathcal{N}_\sigma u f - \int_\Omega u(0) v_0.$$

As a result, by Proposition 4.5, the above f is the desired null control. □

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FOCUSING DYNAMICS OF 2D BOSE GASES IN THE INSTABILITY REGIME

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We consider the dynamics of a 2D Bose gas with an interaction potential of the form $N^{2\beta-1}w(N^{\beta}\cdot)$ for $\beta \in \left(0, \frac{3}{2}\right)$. The interaction may be chosen to be negative and large, leading to the instability regime where the corresponding focusing cubic nonlinear Schrödinger equation (NLS) may blow up in finite time. We show that to leading order, the N-body quantum dynamics can be effectively described by the NLS prior to the blow-up time. Moreover, we prove the validity of the Bogoliubov approximation, where the excitations from the condensate are captured in a norm approximation of the many-body dynamics.

1. Introduction

Since the pioneering work of Bose [1924] and Einstein [1925], and especially after the experimental realization of the Bose–Einstein condensation [Anderson et al. 1995; Davis et al. 1995], there has been a remarkable effort to understand the macroscopic behavior of interacting Bose gases from first principles. From the mathematical point of view, the theory of interacting Bose gases goes back to Bogoliubov [1947], who proposed an effective method to transform a weakly interacting Bose gas to a noninteracting one, subject to a modification of the kinetic operator due to the interaction effect. While the original work of Bogoliubov focuses on the spectral property of bosonic systems towards a microscopic explanation for Landau's criteria of superfluidity, his ideas are also applicable to quantum dynamics. In the present paper, we will justify Bogoliubov's approximation in the dynamical setting for a class of Bose gases with attractive interactions.

In the presence of large attractive interaction potentials, blow-up phenomena have been observed in experiments with ultracold Bose gases [Bradley et al. 1995; Cornish et al. 2000; Donley et al. 2001]. In these experimental settings, first a repulsive interaction was used to prepare an initial state, and then the interaction was switched to attractive by means of Feshbach resonances. When the strength of the attractive interaction was increased beyond a critical threshold, a blow-up process happened, where a large fraction of the condensate was lost [Roberts et al. 2001]. Heuristically, this behavior can be explained by describing the condensate by the solution of a focusing cubic nonlinear Schrödinger equation (NLS), which may exhibit a finite-time blow-up.

In the present work, we will focus on the instability regime for dilute Bose gases in two dimensions, where the corresponding NLS is mass-critical. Before the blow-up time, we give a rigorous derivation of Bose–Einstein condensation and Bogoliubov's theory; in particular, we prove that the many-body dynamics are effectively described by the solution of the NLS, and that the kinetic energy of the system

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diverges in finite time. To our knowledge, this is the first result of this kind for dilute Bose gases in the instability regime.

1.1. ***Mathematical setting.*** In the framework of many-body quantum physics, the dynamics of a system of N (spinless) bosons in $\mathbb{R}^2$ can be described by the linear N-body Schrödinger equation

$$\begin{cases} \mathrm{i}\partial_t \Psi_N(t) = H_N \Psi_N(t), \\ \Psi_N(0) = \Psi_{N,0}, \end{cases} \tag{1-1}$$

where the wave function $\Psi_N(t)$ belongs to $L^2_s(\mathbb{R}^{2N})$, the space of square integrable functions of N variables in $\mathbb{R}^2$ satisfying the bosonic symmetry

$$\Psi_N(t, x_1, \dots, x_N) = \Psi_N(t, x_{\sigma(1)}, \dots, x_{\sigma(N)}) \quad \text{for all } \sigma \in S_N \text{ and } x_i \in \mathbb{R}^2, \tag{1-2}$$

where S_N denotes the set of all permutations of $\{1, \dots, N\}$. We will work on a nonrelativistic system with short-range interactions, where the underlying Hamiltonian is typically given by

$$H_N = \sum_{j=1}^{N} (-\Delta_j) + \frac{1}{N-1} \sum_{1 \le j < k \le N} w_N(x_j - x_k), \tag{1-3}$$

where

$$w_N(x) = N^{2\beta} w(N^\beta x), \quad \beta > 0, \tag{1-4}$$

with a real-valued, even and bounded potential w. We do not impose any positivity condition on w; in particular, the attractive case $w \le 0$ is allowed.

When w is bounded, the Hamiltonian H_N is self-adjoint on $L^2_s(\mathbb{R}^{2N})$ with the same domain as the noninteracting Hamiltonian. Therefore, the linear Schrödinger equation (1-1) has a unique global solution $\Psi_N(t) = e^{-\mathrm{i}tH_N}\Psi_N(0)$ with $t \in \mathbb{R}$, for every initial state $\Psi_N(0) \in L^2_s(\mathbb{R}^{2N})$. The major challenge in the analysis of (1-1) is that the relevant dimension grows fast as $N \to \infty$, making it very difficult to extract helpful information about the quantum system. Therefore, in practice, it is desirable to obtain collective descriptions by reasonable approximations, based on suitable assumptions on the initial state. In the present work, we will assume that the initial state exhibits the Bose–Einstein condensation (BEC), and that the particles outside of the BEC have bounded kinetic energy. These assumptions allow a rigorous derivation of effective nonlinear equations describing the BEC and the excitations which are computable by numerical methods.

Roughly speaking, Bose–Einstein condensation (BEC) is the phenomenon where many particles occupy a common quantum state. In particular, this is the case when the N-body wave function is approximately given by a factorized state, namely

$$\Psi_N(t, x_1, x_2, \dots, x_N) \approx \varphi(t, x_1)\varphi(t, x_2) \cdots \varphi(t, x_N) \tag{1-5}$$

in an appropriate sense. Here the normalized function $\varphi(t, \cdot) \in L^2(\mathbb{R}^2)$ describes the condensate, and its evolution is governed by the cubic nonlinear Schrödinger equation (NLS)

$$\begin{cases} \mathrm{i}\partial_t \varphi(t, x) = \big(-\Delta_x + b\,|\varphi(t, x)|^2 - \mu(t)\big)\varphi(t, x), \\ \varphi(0, x) = \varphi_0(x), \end{cases} \tag{1-6}$$

where

$$b = \int_{\mathbb{R}^2} w, \quad \mu(t) = \tfrac{1}{2} b \int_{\mathbb{R}^2} |\varphi(t,x)|^4 \, \mathrm{d}x. \tag{1-7}$$

The equation (1-6) can be formally obtained from (1-1) using the assumption (1-5) and the fact that $w_N(x) = N^{2\beta} w(N^\beta x) \to b\delta(x)$ weakly.

The coupling constant $b = \int w$ plays a crucial role in (1-6). The focusing case $b < 0$ and the defocusing case $b > 0$ correspond to rather different physical situations. In particular, we are interested in the focusing case where the NLS (1-6) may blow up in finite time, even if the initial datum $\varphi(0)$ is smooth. The possibility of the finite-time blow up is closely related to instability, which we will explain below.

1.2. ***Stability vs. instability.*** Since the 2D cubic NLS (1-6) is mass critical, it is well-known from [Weinstein 1983] that the possibility of the finite-time blow up for H^1-solution depends not only on the sign of the interaction, but also on its strength. To be precise, let us denote the critical interaction strength as the optimal constant $a^* > 0$ in the Gagliardo–Nirenberg interpolation inequality

$$\Big(\int_{\mathbb{R}^2} |\nabla f(x)|^2 \, \mathrm{d}x\Big)\Big(\int_{\mathbb{R}^2} |f(x)|^2 \, \mathrm{d}x\Big) \geq \tfrac{1}{2} a^* \int_{\mathbb{R}^2} |f(x)|^4 \, \mathrm{d}x \quad \text{for all } f \in H^1(\mathbb{R}^2). \tag{1-8}$$

Equivalently, $a^* = \|Q\|_{L^2}^2$ where Q is the unique positive solution of

$$-\Delta Q + Q - Q^3 = 0 \quad \text{in } \mathbb{R}^2$$

(see [McLeod and Serrin 1987; Kwong 1989]). From [Weinstein 1983, Theorems 3.1 and 4.2], we have two distinct regimes:

- *NLS stability regime*: $b > -a^*$. The NLS (1-6) has a unique global solution for all initial data $\varphi_0 \in H^1(\mathbb{R}^2)$ satisfying $\|\varphi_0\|_{L^2} = 1$.
- *NLS instability regime*: $b < -a^*$. A finite-time blow up occurs, for example, if the initial data $\varphi_0 \in H^1(\mathbb{R}^2) \cap L^2(\mathbb{R}^2; |x|^2 \, \mathrm{d}x)$ satisfy $\|\varphi_0\|_{L^2} = 1$ and

$$\int_{\mathbb{R}^2} |\nabla \varphi_0(x)|^2 \, \mathrm{d}x + \tfrac{1}{2} b \int_{\mathbb{R}^2} |\varphi_0(x)|^4 \, \mathrm{d}x < 0. \tag{1-9}$$

In the instability regime, we refer to [Merle and Raphael 2004] for the universality of the blow-up profile, [Merle and Raphael 2005] for a precise description of the solutions near the blow-up time, and [Merle and Raphael 2003; 2006; Raphael 2005] for works on the blow-up rate. We also refer to [Merle 1993] for a complete characterization of the minimal-mass blow-up solutions in the special case $b = -a^*$.

Unlike the NLS (1-6), for the N-body quantum dynamics (1-1), the solution $\Psi_N(t)$ exists globally for every L^2-initial datum. Nevertheless, we can still discuss stability and instability regimes by considering the boundedness of the energy per particle.

- *Many-body stability regime*: The system is stable of the second kind if

$$H_N \geq -CN \tag{1-10}$$

for some constant $C > 0$ independent of N (see [Lieb and Seiringer 2010]). In principle, (1-10) is stronger than the NLS stability. By testing (1-10) against factorized states, we see that $\int w \geq -a^*$. However, the condition $\int w \geq -a^*$, or even $\int |w_-| < a^*$ with $w_- = \min\{w, 0\}$ the negative part of w, does not imply the many-body stability (1-10), except if $\beta \leq \frac{1}{2}$ [Lewin 2015]. The range of β guaranteeing (1-10) can be improved for trapped systems; see [Lewin et al. 2016; 2017; 2018; Nam and Rougerie 2020].

- *Many-body instability regime*: If $\int w < -a^*$, then (1-10) fails to hold. More precisely, we have

$$H_N \geq -CN^{1+2\beta}, \tag{1-11}$$

and the optimality of (1-11) can be seen by testing against factorized states and using $\|w_N\|_{L^\infty} \sim CN^{2\beta}$. In particular, (1-11) allows the energy per particle to diverge to $-\infty$ as $N \to \infty$, which is consistent with blow up of the NLS (1-6).

Our goal is to make a rigorous connection from the many-body Schrödinger equation (1-1) to the NLS (1-6) in the instability regime.

1.3. *Derivation of NLS from many-body dynamics.* The rigorous derivation of the NLS from the many-body Schrödinger equation (1-1) has been studied since the 1970s, initiated by Hepp [1974], Ginibre and Velo [1979] and Spohn [1980], and has gained renewed interest since the 2000s with important developments including the derivation of the Gross–Pitaevskii equation in 3D by Erdős, Schlein and Yau [Erdős et al. 2009; 2010]. We refer to [Benedikter et al. 2016] for a pedagogical introduction to the subject and a detailed discussion of the literature. In particular, in the defocusing case ($w \geq 0$), we refer to [Kirkpatrick et al. 2011; Jeblick et al. 2019] for the derivation of the 2D NLS (1-6) and [Chen and Holmer 2017; Boßmann 2020] for the derivation of the effectively 2D dynamics of strongly confined 3D systems.

In the focusing case ($w \leq 0$) in 2D, most of the existing works in the literature are based on the stability condition $\int |w_-| < a^*$. In this case, the focusing NLS (1-6) is globally well-posed, and its derivation from the many-body equation (1-1) was given by Chen and Holmer [2017] and Jeblick and Pickl [2018] under the technical addition of a trapping potential like $V(x) = |x|^s$, enabling them to use the many-body stability (1-10) for $0 < \beta < (s+1)/(s+2)$ by [Lewin et al. 2017]. Since the stability (1-10) was later extended to trapped systems for $0 < \beta < 1$ [Nam and Rougerie 2020], the approaches in [Chen and Holmer 2017; Jeblick and Pickl 2018] are conceptually applicable for that range of β. After that, Nam and Napiórkowski [2019] removed the trapping potential and derived (1-6) for all $0 < \beta < 1$, still under the crucial assumption $\int |w_-| < a^*$.

In the present paper, we will give a novel derivation of the focusing NLS (1-6) which covers arbitrarily negative potentials w and all $\beta \in \left(0, \frac{3}{2}\right)$. Without the stability condition $\int |w_-| < a^*$, one only has the very weak bound (1-11) instead of (1-10), and to our knowledge, the derivation of the NLS (1-6) prior to the blow-up time is only available for $\beta < \frac{1}{2}$, following the methods in [Pickl 2010; Chen and Holmer 2017; Nam and Napiórkowski 2017a; 2019; Jeblick and Pickl 2018; Chong 2021]. Although we do not expect our extended range $\beta \in \left(0, \frac{3}{2}\right)$ to be optimal, it is sufficiently large and in particular covers the physical setting of dilute Bose gases where $\beta > \frac{1}{2}$. Actually, we will derive (1-6) from a stronger result, namely a norm approximation of the many-body quantum dynamics also describing the fluctuations around the condensate in the spirit of Bogoliubov's theory. That result requires further notation and explanation, which we defer to the next section.

We conjecture that our results hold for all $\beta \in (0,\infty)$, and also for $\beta = \beta_N \to 0$ slowly such that $\lim_{N\to\infty} \log(N^\beta)/N = 0$. The latter scaling regime was considered in [Caraci 2021] for the repulsive case $w \geq 0$. For the repulsive potential $w \geq 0$, it is also possible to consider the critical scaling regime with $w_N(x) = e^{2N} w(N^\beta x)$. In this so-called Gross–Pitaevskii regime, it was proved in [Jeblick et al. 2019] that the correlations at short distance leads to a subtle correction to the leading order where the coupling constant b in (1-6) must be replaced by the zero-scattering energy of w. It is natural to expect a similar result for the attractive case $w \leq 0$, but this remains an open problem.

It is also interesting to consider the derivation of the focusing NLS in one and in three dimensions. In three dimensions, the focusing cubic NLS always has finite-time blow-up for all strength of the interaction, and the asymptotic behavior of the many-body quantum dynamics has been established for $0 < \beta < \frac{1}{3}$ in [Nam and Napiórkowski 2017a; Chong 2021]. It remains open to understand the case $\beta > \frac{1}{3}$. In one dimension, the focusing cubic NLS is globally well-posed (it is mass subcritical), and the norm approximation of the many-body quantum dynamics for all $\beta > 0$ has been derived in [Nam and Napiórkowski 2019]. It is possible to obtain the finite-time blow-up in one dimension by considering a quantum system with three-body interactions, and we expect that the techniques introduced in the present paper is also helpful for the corresponding problem (see, e.g., [Nguyen and Ricaud 2024] for a related model in the stationary setting).

Finally, we refer to [Michelangeli and Schlein 2012] for a pioneering study on the rigorous understanding of the many-body dynamical instability for bosons. This work is based on a different setting where the particles have a relativistic dispersion law and an attractive potential of the form $|x|^{-1}$, ensuring that the corresponding Hartree theory has finite-time blow-up for a sufficiently large interaction coupling constant. On one hand, the general idea of proving the instability by Fock space from [Michelangeli and Schlein 2012] is very helpful for us (see, in particular, Corollary 4). On the other hand, on the technical side, the analysis in [Michelangeli and Schlein 2012] does not extend to our case. More precisely, while the N-independent interaction potential considered in [Michelangeli and Schlein 2012] places the system in a mean-field regime, controlling the N-dependent potential will be the main task of our approach.

2. Main results

Recall that we consider the Schrödinger equation (1-1) with the Hamiltonian H_N given in (1-3), where $w_N(x) = N^{2\beta} w(N^\beta x)$ as in (1-4). We will give rigorous descriptions of the macroscopic behavior of the many-body dynamics $\Psi_N(t) = e^{-itH_N}\Psi_{N,0}$ when $N \to \infty$, including the NLS (1-6) as the leading-order approximation, and a norm approximation in $L^2_s(\mathbb{R}^{2N})$ as the second-order approximation.

We always impose the following condition on the interaction potential:

Assumption 1. Let $w \in L^\infty(\mathbb{R}^2)$ be compactly supported and $w(x) = w(-x) \in \mathbb{R}$.

We do not put any assumption on the sign and the size of w.

2.1. ***Derivation of the NLS.*** Let us recall the following well-known result concerning the NLS (1-6) (see, e.g., [Cazenave 2003, Theorem 4.10.1]):

Lemma 2. *For every $b \in \mathbb{R}$ and $\varphi_0 \in H^1(\mathbb{R}^2)$ with $\|\varphi_0\|_{L^2} = 1$, there exists a unique solution*

$$\varphi \in C([0, T_{\max}), H^1(\mathbb{R}^2))$$

of (1-6) *with a unique maximal time $T_{\max} \in (0, \infty]$. Moreover, if $T_{\max} < \infty$, then*

$$\lim_{t \nearrow T_{\max}} \|\varphi(t)\|_{H^1} = \infty. \tag{2-1}$$

For nontrivial interactions w, the many-body quantum state $\Psi_N(t)$ is not expected to be close to the factorized state $\varphi(t)^{\otimes N}$ in norm (see Theorem 5 below). Therefore, the leading-order approximation (1-5) has to be understood in an average sense, which can be formulated properly in terms of reduced density matrices. For every normalized vector $\Psi_N \in L^2_s(\mathbb{R}^{2N})$, its one-body density matrix $\gamma^{(1)}_{\Psi_N}$ is a nonnegative operator on $L^2(\mathbb{R}^2)$ with kernel

$$\gamma^{(1)}_{\Psi_N}(x; y) = \int_{\mathbb{R}^{2(N-1)}} \Psi_N(x, x_2, \ldots, x_N) \overline{\Psi_N(y, x_2, \ldots, x_N)} \, \mathrm{d}x_2 \cdots \mathrm{d}x_N. \tag{2-2}$$

Equivalently, it can be obtained by taking the partial trace

$$\gamma^{(1)}_{\Psi_N} = \mathrm{Tr}_{2\to N} |\Psi_N\rangle\langle\Psi_N|. \tag{2-3}$$

Clearly, if $\Psi_N = \varphi^{\otimes N}$, then $\gamma^{(1)}_{\Psi_N} = |\varphi\rangle\langle\varphi|$ (the rank-one projection onto $\varphi \in L^2(\mathbb{R}^2)$). In general, the approximation

$$\gamma^{(1)}_{\Psi_N} \approx |\varphi\rangle\langle\varphi| \tag{2-4}$$

with respect to the trace norm is an appropriate interpretation of (1-5). Our first main result is a rigorous derivation of the NLS (1-6) from (1-1).

Theorem 3 (NLS evolution of the condensate). *Let $\beta \in \left(0, \frac{3}{2}\right)$, $0 < \alpha_1 < \min\left(\beta, \frac{1}{8}, \frac{1}{16}(3 - 2\beta)\right)$ and let w satisfy Assumption 1. Let $\varphi(t)$ be the solution of* (1-6) *on the maximal time interval* $[0, T_{\max})$ *as in Lemma 2 with initial datum $\varphi_0 \in H^4(\mathbb{R}^2)$, $\|\varphi_0\|_{L^2} = 1$. Let $\Psi_N(t)$ be the solution of* (1-1) *with a normalized initial state $\Psi_{N,0} \in L^2_s(\mathbb{R}^{2N})$ satisfying*

$$N \, \mathrm{Tr}((1 - \Delta) q \gamma^{(1)}_{\Psi_{N,0}} q) \le C, \quad q = 1 - |\varphi_0\rangle\langle\varphi_0|, \tag{2-5}$$

for some constant $C > 0$. Then for every $t \in [0, T_{\max})$, we have Bose–Einstein condensation in the state $\varphi(t)$, i.e.,

$$\mathrm{Tr} \left| \gamma^{(1)}_{\Psi_N(t)} - |\varphi(t)\rangle\langle\varphi(t)| \right| \le C_t N^{-\alpha_1} \tag{2-6}$$

for sufficiently large N, where C_t is independent of N and continuous on $[0, T_{\max})$.

The initial condition (2-5) means that at the time $t = 0$, the total kinetic energy of all excited particles outside the condensate φ_0 is bounded. Thus, there are only few excitations, which is a key assumption allowing us to control the fluctuations around the condensate $\varphi(t)$ for all $t \in [0, T_{\max})$ by using an energy method. The kinetic bound (2-5) has been proven for the ground state or low-lying excited states of trapped systems with suitable repulsive interactions; see, e.g., [Seiringer 2011; Lewin et al. 2015b].

In Theorem 3 we do not make any assumption on the sign of the potential w, but our result is mostly interesting in the focusing case $w \le 0$. It substantially extends the result in [Nam and Napiórkowski 2019] where the NLS (1-6) was derived under the stability condition $\int |w_-| < a^*$ and the smaller range $\beta \in (0,1)$ (see also [Chen and Holmer 2017; Jeblick and Pickl 2018] for earlier related results). Without the stability condition, the derivation of the NLS (1-6) prior to the blow-up time is only available for $\beta < \frac{1}{2}$, for instance by following the methods in Pickl 2010; Chen and Holmer 2017; Nam and Napiórkowski 2017a; 2019; Jeblick and Pickl 2018; Chong 2021] and using the uniform-in-N bounds on the Hartree equation which we prove in Lemma 10.

The speed of the divergence of C_t as $t \to T_{\max}$ depends on the solution of the NLS in Lemma 2, but it is beyond the scope of this paper to investigate the quantitative behavior of this nonlinear problem.

The following statement is a direct consequence of Theorem 3 and the definition of $T_{\max}$ in Lemma 2.

Corollary 4 (Many-body blow up). *We keep the same assumptions as in Theorem 3, and assume additionally that $T_{\max} < \infty$. Then there is a sequence $N(t) \in \mathbb{N}$ such that $N(t) \to \infty$ as $t \nearrow T_{\max}$ and such that*

$$\lim_{t \nearrow T_{\max}} \frac{1}{N(t)} \Big\langle \Psi_{N(t)}(t), \sum_{j=1}^{N(t)} (-\Delta_j) \Psi_{N(t)}(t) \Big\rangle = \lim_{t \nearrow T_{\max}} \operatorname{Tr}(-\Delta \gamma^{(1)}_{\Psi_N(t)}) = \infty. \tag{2-7}$$

The implication of Corollary 4 follows from a well-known argument (see [Michelangeli and Schlein 2012, Remark 2]): for every $t \in [0, T_{\max})$, the trace convergence in Theorem 3 and Fatou's lemma imply that

$$\liminf_{N \to \infty} \operatorname{Tr}((1-\Delta)\gamma^{(1)}_{\Psi_N}(t)) \ge \operatorname{Tr}\big((1-\Delta)|\varphi(t)\rangle\langle\varphi(t)|\big) = \|\varphi(t)\|^2_{H^1(\mathbb{R}^2)}. \tag{2-8}$$

Therefore, if $T_{\max} < \infty$, then the one-body blow-up condition (2-1) implies the many-body blow-up result (2-7). Note that (2-8) is only an inequality, hence the reverse direction, which would imply that the many-body blow-up phenomenon does not occur at any fixed time $t \in [0, T_{\max})$, cannot be deduced from Theorem 3. We expect that this holds true, but a proof would require some additional analysis, which we will not pursue in the present work. Moreover, it is an open question whether the number of the excitations blows up as $t \to T_{\max}$.

We will derive Theorem 3 from a stronger result, namely the norm convergence of the many-body dynamics (see Theorem 5 below). On the technical side, it would be interesting if one could prove Theorem 3 directly using an analysis at the level of density matrices, but we do not see how to achieve this (without going to the norm approximation).

2.2. ***Norm approximation.*** Let us now discuss the fluctuations around the condensate. For this purpose, we first introduce the Hartree-type equation

$$\begin{cases} i\partial_t u_N(t,x) = \big(-\Delta_x + (w_N * |u_N(t,\cdot)|^2)(x) - \mu_N(t)\big) u_N(t,x) =: h(t) u_N(t,x), \\ \qquad\qquad u_N(0,x) = \varphi_0(x), \end{cases} \tag{2-9}$$

with

$$\mu_N(t) = \tfrac{1}{2} \iint_{\mathbb{R}^2 \times \mathbb{R}^2} |u_N(t,x)|^2 w_N(x-y) |u_N(t,y)|^2 \, dx \, dy. \tag{2-10}$$

The Hartree dynamics (2-9) plays the same role as the NLS dynamics (1-6) in the leading-order description, but using the former is slightly more natural for the second-order approximation (see Lewin et al. 2015a;

Nam and Napiórkowski 2017a; 2017b; 2019; Brennecke et al. 2019] for a similar choice). In particular, (2-9) has a unique global solution, and $\|u_N(t)\|_{H^1}$ is bounded uniformly in N and locally in time when $t \in [0, T_{\max})$, with $T_{\max}$ given in Lemma 2. Moreover, since $u_N(t) \to \varphi(t)$ in $L^2(\mathbb{R}^2)$ as $N \to \infty$, the convergence (2-6) remains true if $\varphi(t)$ is replaced by $u_N(t)$ (see Lemma 10 for the details).

To describe the excitations around the condensate, it is convenient to switch to a Fock space setting where the number of particles is not fixed. Let us introduce the one-body excited space

$$\mathfrak{H}_\perp(t) = \{u_N(t)\}^\perp \subset \mathfrak{H} = L^2(\mathbb{R}^2) \tag{2-11}$$

and the (bosonic) Fock spaces over $\mathfrak{H}_\perp$

$$\mathcal{F}_\perp^{\le N}(t) = \bigoplus_{k=0}^{N} \bigotimes_{\text{sym}}^{k} \mathfrak{H}_\perp \subset \mathcal{F}_\perp(t) = \bigoplus_{k\ge 0} \bigotimes_{\text{sym}}^{k} \mathfrak{H}_\perp \subset \mathcal{F} = \bigoplus_{k\ge 0} \bigotimes_{\text{sym}}^{k} \mathfrak{H}. \tag{2-12}$$

Note that $\mathcal{F}_\perp(t)$ and its subspace $\mathcal{F}_\perp^{\le N}(t)$ are time-dependent via $u_N(t)$, and they are naturally embedded in the full Fock space $\mathcal{F}$ over $\mathfrak{H}$.

Let us recall the standard second quantization formalism, where the creation and annihilation operators on $\mathcal{F}$, $a^\dagger(f)$ and $a(f)$, are defined by

$$(a^\dagger(f)\boldsymbol{\chi})^{(k)}(x_1, \dots, x_k) = \frac{1}{\sqrt{k}} \sum_{j=1}^{k} f(x_j)\chi^{(k-1)}(x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_k) \quad \text{for all } k \ge 1, \tag{2-13a}$$

$$(a(f)\boldsymbol{\chi})^{(k)}(x_1, \dots, x_k) = \sqrt{k+1} \int_{\mathbb{R}^2} \mathrm{d}x\, \overline{f(x)}\chi^{(k+1)}(x_1, \dots, x_k, x) \quad \text{for all } k \ge 0 \tag{2-13b}$$

for all $f \in L^2(\mathbb{R}^2)$ and $\boldsymbol{\chi} = (\chi^{(k)})_{k=0}^\infty \in \mathcal{F}$. It is also convenient to introduce the operator-valued distributions $a_x^\dagger$, a_x by

$$a^\dagger(f) = \int \mathrm{d}x\, f(x) a_x^\dagger, \quad a(f) = \int \mathrm{d}x\, \overline{f(x)} a_x, \tag{2-14}$$

which satisfy the canonical commutation relations

$$[a_x, a_y^\dagger] = \delta(x-y), \quad [a_x, a_y] = [a_x^\dagger, a_y^\dagger] = 0. \tag{2-15}$$

Using this language, we define the second quantization of one- and two-body operators as

$$\begin{aligned} \mathrm{d}\Gamma_1(T) &= 0 \oplus \bigoplus_{k\ge 1} \sum_{j=1}^{k} T_j = \iint T(x; x') a_x^\dagger a_{x'}\, \mathrm{d}x\, \mathrm{d}x', \\ \mathrm{d}\Gamma_2(S) &= 0 \oplus 0 \oplus \bigoplus_{k\ge 2} \sum_{1\le i<j\le k} S_{ij} = \tfrac{1}{2} \iiiint S(x, y; x', y') a_x^\dagger a_y^\dagger a_{x'} a_{y'}\, \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}x'\, \mathrm{d}y', \end{aligned} \tag{2-16}$$

for $T(x, x')$ and $S(x, y; x, y')$ the kernels of the operators T on $\mathfrak{H}$ and S on $\mathfrak{H}^2$ (see, e.g., [Solovej 2014, Section 7]). In this language, the Hamiltonian (1-3) can be expressed equivalently as

$$H_N = \mathrm{d}\Gamma_1(-\Delta) + \frac{1}{N-1} \mathrm{d}\Gamma_2(w_N) \tag{2-17}$$

on $\mathfrak{H}^N$. We also introduce the number operator on Fock space $\mathcal{F}$,

$$\mathcal{N} = \mathrm{d}\Gamma_1(\mathbb{1}), \tag{2-18}$$

where $\mathbb{1}$ this is the identity operator on $\mathfrak{H}$, and define the cut-off functions

$$\mathbb{1}^{\leq m} = \mathbb{1}(\mathcal{N} \leq m), \quad \mathbb{1}^{>m} = \mathbb{1}(\mathcal{N} > m) \qquad \text{for all } m \in (0, \infty). \tag{2-19}$$

Following the approach in [Lewin et al. 2015a; 2015b], the N-body dynamics $\Psi_N(t) \in L^2_s(\mathbb{R}^{2N})$ can be decomposed as

$$\Psi_N(t) = \sum_{k=0}^{N} u_N(t)^{\otimes(N-k)} \otimes_s \phi_N^{(k)}(t) = \sum_{k=0}^{N} \frac{a^\dagger(u_N(t))^{\otimes(N-k)}}{\sqrt{(N-k)!}} \phi_N^{(k)}(t) \tag{2-20}$$

for $\otimes_s$ the symmetric tensor product and where the vector

$$\Phi_N(t) = (\phi_N^{(k)}(t))_{k=0}^N \in \mathcal{F}_\perp^{\leq N}(t) \subset \mathcal{F}_\perp(t) \tag{2-21}$$

describes the excitations around the condensate $u_N(t)$ (see Section 3 for details).

Our goal is to approximate the N-body dynamics $\Phi_N(t)$ by the solution $\Phi(t)$ of the simpler evolution equation

$$\begin{cases} \mathrm{i}\partial_t \Phi(t) = \mathbb{H}(t)\Phi(t), \\ \quad \Phi(0) = \Phi_0, \end{cases} \tag{2-22}$$

where $\mathbb{H}(t)$ denotes the Bogoliubov Hamiltonian

$$\mathbb{H}(t) = \mathrm{d}\Gamma_1(h(t) + K_1(t)) + \tfrac{1}{2}\biggl(\iint K_2(t,x,y) a_x^\dagger a_y^\dagger \,\mathrm{d}x\,\mathrm{d}y + \text{h.c.} \biggr). \tag{2-23}$$

In (2-23), $h(t)$ is defined in the Hartree equation (2-9), and

$$K_1(t) = q(t)\widetilde{K}_1(t)q(t), \quad K_2(t) = q(t) \otimes q(t)\widetilde{K}_2(t), \tag{2-24}$$

where

$$q(t) = 1 - p(t) = 1 - |u_N(t)\rangle\langle u_N(t)| \tag{2-25}$$

and the kernel of the operator $\widetilde{K}_1(t)$ and the function $\widetilde{K}_2(t) \in \mathfrak{H}^2$ are given by

$$\begin{aligned} \widetilde{K}_1(t,x,y) &= u_N(t,x) w_N(x-y) \overline{u_N(y)}, \\ \widetilde{K}_2(t,x,y) &= u_N(t,x) w_N(x-y) u_N(y). \end{aligned} \tag{2-26}$$

The effective generator $\mathbb{H}(t)$ emerges from the Bogoliubov approximation when we write H_N in the second quantization formalism, then implement the c-number substitution $a(u_N), a^\dagger(u_N) \mapsto \sqrt{N}$, and finally keep only the terms that are quadratic in creation and annihilation operators. Note that $\mathbb{H}(t)$ is an operator on the full Fock space $\mathcal{F}$ since $h(t)$ does not leave $\mathfrak{H}_\perp(t)$ invariant, but it does not contradict the fact that $\Phi(t) \in \mathcal{F}_\perp(t)$ (see, e.g., [Lewin et al. 2015a] for a detailed explanation). Moreover, $\mathbb{H}(t)$ is N-dependent, although we do not make this explicit in the notation. The Bogoliubov equation (2-22) is globally well-posed (see Lemma 7).

Now we are ready to state our second main result.

Theorem 5 (Bogoliubov excitations from the condensate). *Let $\beta \in \big(0, \frac{3}{2}\big)$, $0 < \alpha_2 < \min\big(\frac{1}{8}, \frac{1}{16}(3-2\beta)\big)$ and let w satisfy Assumption 1. Let $u_N(t)$ be the solution of the Hartree equation* (2-9) *with initial datum $\varphi_0 \in H^4(\mathbb{R}^2)$, $\|\varphi_0\| = 1$. Let $\Phi(t) = (\phi^{(k)}(t))_{k=0}^{\infty} \in \mathcal{F}_{\perp}(t)$ be the solution of the Bogoliubov equation* (2-22) *with initial datum $\Phi_0 = (\phi_0^{(k)})_{k=0}^{\infty} \in \mathcal{F}_{\perp}(0)$ satisfying $\|\Phi_0\| = 1$ and*

$$\langle \Phi_0, \mathrm{d}\Gamma_1(1-\Delta)\Phi_0\rangle \le C \tag{2-27}$$

for some constant $C \ge 0$. Let $\Psi_N(t)$ the solution of the Schrödinger equation (1-1) *with initial datum*

$$\Psi_{N,0} = \sum_{k=0}^{N} {\varphi_0}^{\otimes(N-k)} \otimes_s \phi_0^{(k)} = \sum_{k=0}^{N} \frac{a^{\dagger}(\varphi_0)^{\otimes(N-k)}}{\sqrt{(N-k)!}} \phi_0^{(k)}. \tag{2-28}$$

Then, for all $t \in [0, T_{\max})$, we have the norm approximation

$$\Big\| \Psi_N(t) - \sum_{k=0}^{N} u_N(t)^{\otimes(N-k)} \otimes_s \phi^{(k)}(t) \Big\| \le C_t N^{-\alpha_2}, \tag{2-29}$$

where the constant C_t is independent of N and continuous in $t \in [0, T_{\max})$.

Under the decomposition (2-28), the kinetic condition (2-5) is equivalent to condition (2-27) in Theorem 5 (see Remark 6 below). Strictly speaking, the state $\Phi_{N,0}$ in (2-28) is not normalized in $L^2_s(\mathbb{R}^{2N})$, but the condition (2-27) ensures that

$$1 \ge \|\Psi_{N,0}\|^2 = 1 - \|\mathbb{1}_{\{\mathcal{N}>N\}}\Phi_0\|^2 \ge 1 - \langle \Phi_0, (\mathcal{N}/N)\Phi_0\rangle \ge 1 - CN^{-1}. \tag{2-30}$$

In the mean-field regime $\beta = 0$, the norm approximation in the form (2-29) was first given in [Lewin et al. 2015a], and higher-order corrections to Bogoliubov's theory were recently derived in [Boßmann et al. 2021]. For repulsive interaction $w \ge 0$, the validity of Bogoliubov's theory in 3D was extended to $0 < \beta < 1$ in [Brennecke et al. 2019] and $\beta = 1$ in [Caraci et al. 2025] (see also [Nam and Napiórkowski 2017a; 2017b] for earlier results). We expect that the ideas from these works in 3D apply to handle the repulsive case in 2D as well, possibly allowing a larger value of β in 2D. Our result is mainly interesting in the attractive case $w \le 0$ in 2D, where the validity of Bogoliubov's theory was known only for $0 < \beta < 1$ in the stability regime $\int |w_-| > -a^*$ [Nam and Napiórkowski 2019].

There have been many works devoted to the dynamics around the coherent states in Fock space, initiated in [Hepp 1974; Ginibre and Velo 1979; Grillakis et al. 2010; 2011; Boccato et al. 2017]. Our method is also applicable to this setting, but we skip the details. We refer to [Lewin et al. 2015a] for a detailed comparison between the N-body setting and the Fock space situation, and [Benedikter et al. 2016] for further results.

The ideas of our proof are explained in the next section, and the full technical details are provided afterwards.

Notation. We will use $C > 0$ for a general constant which may depend on w and φ_0 and which may vary from line to line. We also use the notation C_t to highlight the time dependence. When it is unambiguous, we abbreviate the L^2-norm and the corresponding inner product by $\|\cdot\|$ and $\langle\cdot,\cdot\rangle$, respectively.

3. Proof strategy

In this section we explain the main ingredients of the proof. We will focus on Theorem 5, which implies Theorem 3. Our approach is based on Bogoliubov's approximation where the fluctuations around the condensate are effectively described by an evolution equation with a quadratic generator in Fock space. The main mathematical challenge is to justify this approximation by rigorous estimates. Let us first give an overview of the proof strategy, and then we come to the detailed setting.

As an important input of Bogoliubov's theory [1947], we expect that most particles are in the condensate $u_N(t)$, which is governed by the Hartree equation (2-9). The first step in our analysis is to establish several uniform-in-N bounds for the Hartree dynamics, which is nontrivial due to the instability issue. These one-body estimates require a careful adaptation of the analysis of the NLS (1-6) in [Cazenave 2003], which will be discussed in Section 4. In the following, we will focus on the many-body aspects of the proof.

In order to extract the excitations, namely the particles outside the condensate, from the N-body wave function $\Psi_N(t)$, we use the unitary transformation $U_N(t)$ introduced in [Lewin et al. 2015b]. This is a mathematical tool to implement Bogoliubov's c-number substitution [1947], resulting in the evolution $\Phi_N(t) = U_N(t)\Psi_N(t)$ on the excited Fock space $\mathcal{F}_\perp^{\leq N}(t)$ where the generator $\mathcal{G}_N(t)$ was computed explicitly in [Lewin et al. 2015a]. Thus, we can rewrite (2-29) in terms of excitations as

$$\|\Phi_N(t) - \Phi(t)\|^2 \leq C_t N^{-\alpha_2} \tag{3-1}$$

for all $t \in [0, T_{\max})$, where $\Phi(t)$ is the solution to the Bogoliubov equation (2-22).

The main difficulty in proving (3-1) is the lack of the stability of the second kind (1-10). More precisely, with an arbitrarily negative potential w, we do not expect to have a good lower bound for the generator $\mathcal{G}_N(t)$ of $\Phi_N(t)$, which in turn prevents us from obtaining a good kinetic bound for $\Phi_N(t)$. A key observation in [Nam and Napiórkowski 2019] is that a weaker version of the stability (1-10) holds if we restrict to a space of few excitations. Rigorously, for the truncated dynamics $\Phi_{N,M}(t) \in \mathcal{F}_\perp^{\leq M}(t)$ which is associated to the generator $\mathbb{1}^{\leq M}\mathcal{G}_N(t)\mathbb{1}^{\leq M}$ with a parameter $M = N^{1-\delta}$, $\delta \in (0,1)$, it was proved in [Nam and Napiórkowski 2019] that $\Phi_{N,M}$ satisfies an essentially uniform kinetic bound, and hence $\|\Phi_{N,M}(t) - \Phi(t)\|$ can be controlled efficiently (see Lemma 7 below).

Thus, by the triangle inequality, the main missing ingredient for (3-1) is a good estimate for the norm $\|\Phi_N(t) - \Phi_{N,M}(t)\|$. For this term, we cannot use the analysis in [Nam and Napiórkowski 2019], which crucially relies on the stability condition $\int |w_-| < a^*$. The main novelty of the present paper is the introduction of a new method which does not require any information about the full dynamics Φ_N. This kind of idea was previously used in [Nam and Napiórkowski 2017a], where various propagation bounds were established by Cauchy–Schwarz inequalities of the form

$$|\langle \Phi_N, A\Phi_{N,M}\rangle| \leq \|\Phi_N\|\,\|A\Phi_{N,M}\|. \tag{3-2}$$

However, this approach is insufficient to handle the dilute regime where $\beta > \frac{1}{2}$ because the Hilbert–Schmidt norm of the operator with integral kernel $w_N(x-y)u_N(x)u_N(y)$ diverges as N^β. An alternative would be to follow the approach in [Nam and Napiórkowski 2019], which avoids the Cauchy–Schwarz argument described above and uses a different strategy, relying on the a priori estimate $\langle \Phi_N, \, \mathrm{d}\Gamma_1(1-\Delta)\Phi_N\rangle \le C_{t,\varepsilon}(N + N^{2\beta})$ ([Nam and Napiórkowski 2019, Lemma 10]. However, in the instability regime, we do not have the a priori bound (1-10) but only (1-11). This leads to the much weaker kinetic estimate $\langle \Phi_N, \, \mathrm{d}\Gamma_1(1-\Delta)\Phi_N\rangle \le C N^{1+2\beta}$, which is not sufficient to close the argument in [Nam and Napiórkowski 2019] for $\beta > \frac{1}{2}$.

To improve the Cauchy–Schwarz argument, we write $1 = \mathcal{W}^{-1}\mathcal{W}$ with a suitable weight $\mathcal{W} > 0$ — eventually we choose $\mathcal{W} = \big(1 + \mathrm{d}\Gamma_2(|w_N|)\big)^{1/2}$; see (3-22) — and split (3-2) into

$$|\langle \Phi_N, A\Phi_{N,M}\rangle| \le |\langle \Phi_N, \mathcal{W}^{-1} A \mathcal{W}\Phi_{N,M}\rangle| + \big|\langle \Phi_N, \mathcal{W}^{-1}[\mathcal{W}, A]\Phi_{N,M}\rangle\big|. \tag{3-3}$$

The first term on the right-hand side of (3-3) looks similar to $|\langle \Phi_N, A\Phi_{N,M}\rangle|$ but it is easier to bound by the Cauchy–Schwarz inequality provided that we can bound $\|A^*\mathcal{W}^{-1}\Phi_N\|$ in terms of $\|\Phi_N\|$ in an average sense. For the second term on the right-hand side, we gain some cancelation due to the commutator $[\mathcal{W}, A]$, which eventually ensures that $\|\mathcal{W}^{-1}[\mathcal{W}, A]\Phi_{N,M}\|$ is much smaller than $\|A\Phi_{N,M}\|$.

Now let us provide further details of the above ingredients.

3.1. ***Reformulation of the Schrödinger equation.*** Our starting point is a reformulation of the Schrödinger equation (1-1), following the method in [Lewin et al. 2015a; 2015b].

Let $u_N(t)$ be the Hartree evolution in (2-9). To factor out the contribution of the condensate, we use the excitation map $U_N(t) : \mathfrak{H}^N(t) \to \mathcal{F}_\perp^{\le N}(t)$ defined by

$$U_N(t) = \bigoplus_{k=0}^{N} q(t)^{\otimes k}\left(\frac{a(u_N(t))^{N-k}}{\sqrt{(N-k)!}}\right), \tag{3-4}$$

where $q(t) = 1 - |u_N(t)\rangle\langle u_N(t)|$ as in (2-25). It was proven in [Lewin et al. 2015b] that $U_N(t)$ is a unitary transformation and its inverse is given by (2-20), namely

$$U_N(t)^*\Phi = \sum_{k=0}^{N} u_N(t)^{\otimes(N-k)} \otimes_s \phi^{(k)} = \sum_{k=0}^{N} \frac{a^\dagger(u_N(t))^{\otimes(N-k)}}{\sqrt{(N-k)!}}\phi^{(k)}$$

for all $\Phi = (\phi_k)_{k=0}^N \in \mathcal{F}_\perp^{\le N}(t)$. Heuristically, the mapping U_N provides an efficient way of focusing on the fluctuations around the Hartree state $u_N(t)^{\otimes N}$; in particular, $U_N(t)u_N(t)^{\otimes N} = \Omega$ is the vacuum of $\mathcal{F}_\perp(t)$.

It was also proven in [Lewin et al. 2015b] that, for $f, g \in \mathfrak{H}_\perp(t)$, we have these identities on $\mathcal{F}_\perp^{\le N}(t)$:

$$\begin{aligned} U_N a^\dagger(u_N)a(u_N)U_N^* &= N - \mathcal{N}, \\ U_N a^\dagger(f)a(u_N)U_N^* &= a^\dagger(f)\sqrt{N-\mathcal{N}}, \\ U_N a^\dagger(u_N)a(g)U_N^* &= \sqrt{N-\mathcal{N}}a(g), \\ U_N a^\dagger(f)a(g)U_N^* &= a^\dagger(f)a(g). \end{aligned} \tag{3-5}$$

If Bose–Einstein condensation holds, then, in an average sense, $\mathcal{N} \ll N$ in $\mathcal{F}_\perp^{\le N}(t)$. Therefore, (3-5) can be interpreted as a rigorous implementation of Bogoliubov's c-number substitution [1947], where $a(u_N)$ and $a^\dagger(u_N)$ are formally replaced by the scalar number $\sqrt{N}$.

Remark 6. From (3-5) we have $U_N^* \, \mathrm{d}\Gamma_1(qAq) U_N = \mathrm{d}\Gamma_1(qAq)$ for any operator A on $\mathfrak{H}$. Consequently, (2-5) is equivalent to (2-27).

Now we consider the transformed dynamics

$$\Phi_N(t) = U_N(t)\Psi_N(t). \tag{3-6}$$

The Schrödinger equation (1-1) can be written in the equivalent form

$$\begin{cases} \mathrm{i}\partial_t \Phi_N(t) = \mathcal{G}_N(t)\Phi_N(t), \\ \Phi_N(0) = U_N(0)^* \Psi_{N,0}. \end{cases} \tag{3-7}$$

Here, the generator $\mathcal{G}_N(t)$ can be computed explicitly, using the second-quantized form (2-17) and the rules (3-5) (see [Lewin et al. 2015a, Appendix B]), as

$$\mathcal{G}_N(t) = (\mathrm{i}\partial_t U_N(t))U_N^*(t) + U_N(t) H_N U_N^*(t) = \tfrac{1}{2}\sum_{j=0}^{4} \mathbb{1}^{\le N}(\mathbb{G}_j + \mathbb{G}_j^*)\mathbb{1}^{\le N} \tag{3-8}$$

with

$$\mathbb{G}_0 = \mathrm{d}\Gamma_1(h) + \mathrm{d}\Gamma_1(K_1)\frac{N-\mathcal{N}}{N-1} + \mathrm{d}\Gamma_1(q(t)(h+\Delta)q(t))\frac{1-\mathcal{N}}{N-1}, \tag{3-9a}$$

$$\mathbb{G}_1 = -2a^\dagger\big(q(t)(w_N * |u_N(t)|^2)u_N(t)\big)\frac{\mathcal{N}\sqrt{N-\mathcal{N}}}{N-1}, \tag{3-9b}$$

$$\mathbb{G}_2 = \iint K_2(t,x,y)a_x^\dagger a_y^\dagger \,\mathrm{d}x\,\mathrm{d}y \frac{\sqrt{(N-\mathcal{N})(N-\mathcal{N}-1)}}{N-1}, \tag{3-9c}$$

$$\mathbb{G}_3 = \iiiint (q(t)\otimes q(t) w_N \mathbb{1}\otimes q(t))(x,y;x',y') u_N(t,x) a_x^\dagger a_y^\dagger a_{y'} \,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}x'\,\mathrm{d}y' \,\frac{\sqrt{N-\mathcal{N}}}{N-1}, \tag{3-9d}$$

$$\mathbb{G}_4 = \frac{1}{N-1}\,\mathrm{d}\Gamma_2(q(t)\otimes q(t) w_N q(t)\otimes q(t)). \tag{3-9e}$$

Recall that $h(t)$ is given in (2-9), and $K_1(t)$ and $K_2(t)$ are given in (2-24). In the above notation, w_N denotes the function $w_N : \mathbb{R}^2 \to \mathbb{R}$ in $\mathbb{G}_1(t)$, and the two-body multiplication operator $w_N(x-y)$ in $\mathbb{G}_3(t)$ and $\mathbb{G}_4(t)$.

3.2. ***Simplified equations.*** Following Bogoliubov's heuristic ideas [1947], we consider a simplification of (3-7), where only the quadratic terms $\mathbb{G}_0$ and $\mathbb{G}_2$ in the generator are kept. This leads to the Bogoliubov equation (2-22), whose well-posedness is well-known; see, e.g., [Nam and Napiórkowski 2019, Lemma 5].

Lemma 7 (Bogoliubov dynamics). *Let w satisfy Assumption 1, let $u_N(t)$ be the Hartree evolution in* (2-9) *with initial state $\varphi_0 \in H^4(\mathbb{R}^2)$, and let $\Phi_0 \in \mathcal{F}_\perp(0)$ be a normalized vector satisfying* (2-27). *Then the Bogoliubov equation* (2-22) *with initial condition Φ_0 has a unique global solution*

$$\Phi \in C([0,\infty),\mathcal{F}) \cap L^\infty_{\mathrm{loc}}\big((0,\infty),\mathcal{Q}(\mathrm{d}\Gamma_1(1-\Delta))\big)$$

and $\Phi(t) \in \mathcal{F}_\perp(t)$ for all $t > 0$. Moreover, for every $t \in [0, T_{\max})$ and $\varepsilon > 0$, we have

$$\langle \Phi(t), \mathrm{d}\Gamma_1(1-\Delta)\Phi(t)\rangle \le C_{t,\varepsilon} N^\varepsilon, \tag{3-10}$$

where $T_{\max}$ is given in Lemma 2 and the constant $C_{t,\varepsilon}$ is independent of N.

Proof. The global well-posedness of $\Phi(t)$ is shown in [Lewin et al. 2015a, Theorem 7]. The kinetic bound (3-10) follows from the analysis in [Nam and Napiórkowski 2019, Lemma 5] and the uniform bounds of $u_N(t)$, which will be given later in Lemma 10. □

In order to estimate the difference $\|\Phi_N(t) - \Phi(t)\|$, we follow [Nam and Napiórkowski 2019] and introduce the truncated dynamics $\Phi_{N,M}(t) \in \mathcal{F}_\perp^{\leq M}(t)$, which solve the equation

$$\begin{cases} i\partial_t \Phi_{N,M}(t) = \mathbb{1}^{\leq M} \mathcal{G}_N(t) \mathbb{1}^{\leq M} \Phi_{N,M}(t), \\ \qquad \Phi_{N,M}(0) = \mathbb{1}^{\leq M} \Phi_0. \end{cases} \tag{3-11}$$

As explained in [Nam and Napiórkowski 2019], the main advantage of (3-11) is that the truncated generator is stable, namely

$$\mathbb{1}^{\leq M} \mathcal{G}_N(t) \mathbb{1}^{\leq M} \geq \tfrac{1}{2}\, d\Gamma_1(-\Delta) - C_{t,\varepsilon} N^\varepsilon \tag{3-12}$$

for all $t \in [0, T_{\max})$ and $M \ll N$. This allows us to establish an efficient kinetic bound for $\Phi_{N,M}(t)$, which is not available for Φ_N. Consequently, it is much easier to compare $\Phi_{N,M}(t)$ with the Bogoliubov dynamics. We collect some known properties of $\Phi_{N,M}(t)$ in the following lemma.

Lemma 8 (Truncated dynamics). *We keep the assumptions of Lemma 7. Let $M = N^{1-\delta}$ for some constant $\delta \in (0,1)$. Then* (3-11) *has a unique global solution $\Phi_{N,M}(t) \in \mathcal{F}_\perp^{\leq M}(t)$ with $t \in [0,\infty)$. Moreover, for every $t \in [0, T_{\max})$ and $\varepsilon = \varepsilon(\delta) > 0$, we have*

$$\langle \Phi_{N,M}(t), d\Gamma_1(1-\Delta)\Phi_{N,M}(t)\rangle \leq C_{t,\varepsilon} N^\varepsilon \tag{3-13}$$

and

$$\|\Phi_{N,M}(t) - \Phi(t)\|^2 \leq C_{t,\varepsilon} N^\varepsilon \left(\sqrt{\frac{M}{N}} + \frac{1}{M} \right). \tag{3-14}$$

Proof. The global well-posedness of $\Phi_{N,M}(t)$ follows from the general method in [Lewin et al. 2015a, Theorem 7] (see also [Nam and Napiórkowski 2019, Section 6]). Given the uniform bounds of $u_N(t)$ in Lemma 10, the bounds (3-13) and (3-14) follow from the arguments in Lemmas 11 and 15 in [Nam and Napiórkowski 2019], respectively. □

3.3. ***From the truncated to the full dynamics.*** Given Lemma 8, the missing piece for the proof of Theorem 5 is an estimate for $\|\Phi_N(t) - \Phi_{N,M}(t)\|$. The main new ingredient of the present paper is the following bound:

Proposition 9. *We keep the assumptions of Lemma 7. Let $M = N^{1-\delta}$ for some constant $\delta \in (0,1)$. Let Φ_N and $\Phi_{N,M}$ be solutions of* (3-7) *and* (3-11), *with initial data $\Phi_N(0) = \mathbb{1}^{\leq N}\Phi_0$, $\Phi_{N,M}(0) = \mathbb{1}^{\leq M}\Phi_0$, respectively. Then for every $t \in [0, T_{\max})$ and every $\varepsilon > 0$, we have*

$$\|\Phi_N(t) - \Phi_{N,M}(t)\|^2 \leq C_{t,\varepsilon} N^\varepsilon \left(\frac{1}{\sqrt{M}} + \frac{N^\beta}{M^{3/2}} \right). \tag{3-15}$$

Eventually, we will take $\delta > 0$ small, hence the condition $\beta < \frac{3}{2}$ is needed to ensure that the error term $N^\beta / M^{3/2}$ on the right-hand side of (3-15) is negligible.

In order to prove Proposition 9, by norm conservation of $\|\Phi_N(t)\|$ and $\|\Phi_{N,M}(t)\|$, it suffices to show that $\langle\Phi_N(t), \Phi_{N,M}(t)\rangle$ is close to 1. For technical reasons, it is more convenient to consider $\langle\Phi_N(t), f_M^2\Phi_{N,M}(t)\rangle$ with f_M a smoothened of version $\mathbb{1}^{\le M}$. To be precise, we fix a smooth function $f:\mathbb{R}\to[0,1]$ such that $f(s)=1$ for $s\le\frac{1}{2}$ and $f(s)=0$ for $s\ge 1$, and define the operator f_M on $\mathcal{F}$ by

$$f_M = f\left(\frac{\mathcal{N}}{M}\right). \tag{3-16}$$

We will deduce Proposition 9 from a Grönwall argument and the estimate

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}\langle\Phi_N(t), f_M^2\Phi_{N,M}(t)\rangle\right| \le C_{t,\varepsilon}N^{\varepsilon}\left(\frac{1}{\sqrt{M}}+\frac{N^{\beta}}{M^{3/2}}\right). \tag{3-17}$$

It remains to explain the proof of (3-17). Let us drop the time dependence from the notation where it is unambiguous. From (3-7) and (3-11), we have

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}\langle\Phi_N(t), f_M^2\Phi_{N,M}(t)\rangle\right| = \left|\Im\langle\Phi_N, [\mathcal{G}_N, f_M^2]\Phi_{N,M}\rangle\right| \tag{3-18}$$

since $\Phi_{N,M}\in\mathcal{F}_\perp^{\le M}$ and $f_M^2\mathbb{1}^{\le M}=f_M^2$. Then it is straightforward to decompose $\mathcal{G}_N$ into the sum of $\mathbb{G}_j$ as in (3-8). Since f_M is a function of $\mathcal{N}$, only the particle number nonpreserving terms $\mathbb{G}_1$, $\mathbb{G}_2$ and $\mathbb{G}_3$ contribute to the commutator.

One of the most difficult terms is the quadratic one $\left|\langle\Phi_N, [\mathbb{G}_2, f_M^2]\Phi_{N,M}\rangle\right|$, where two annihilation operators hit Φ_N. Since $\mathbb{G}_2$ only changes the number of particles by at most 2, the commutator with f_M^2 allows us to gain a factor M^{-1}. Therefore, estimating (3-18) essentially boils down to proving a bound for

$$\frac{1}{M}\left|\iint \mathrm{d}x\,\mathrm{d}y\,u_N(x)u_N(y)w_N(x-y)\langle\Phi_N, a_x^\dagger a_y^\dagger\Phi_{N,M}\rangle\right|. \tag{3-19}$$

In [Nam and Napiórkowski 2019], a variant of this term was estimated using a kinetic bound for Φ_N based on the method in [Lewin 2015] and the stability condition $\int|w_-|<a^*$. In the present paper, since we are considering a general potential w including the instability regime $\int w_- < -a^*$, we only have

$$\langle\Phi_N, \mathrm{d}\Gamma_1(1-\Delta)\Phi_N\rangle \le CN^{1+2\beta}, \tag{3-20}$$

which can be deduced from a variant of the energy lower bound (1-11). However, the latter bound is too weak, and inserting it in the analysis in [Nam and Napiórkowski 2019] produces a solution only for $\beta<\frac{1}{2}$.

Another idea, which can be extracted from the approach in [Nam and Napiórkowski 2017a], is to handle (3-19) by the Cauchy–Schwarz inequality

$$|\langle\Phi_N, a_x^\dagger a_y^\dagger\Phi_{N,M}\rangle| \le \|\Phi_N\|\,\|a_x^\dagger a_y^\dagger\Phi_{N,M}\|. \tag{3-21}$$

(To be precise, a variant of this argument was used in [Nam and Napiórkowski 2017a] to compare Φ_N directly with the Bogoliubov dynamics Φ.) The advantage of (3-21) is that no information about Φ_N is needed. However, since we have to couple (3-21) with the singular potential $w_N(x-y)$ in (3-19), we eventually obtain a large factor $\|w_N\|_{L^\infty}\sim N^{2\beta}$, and the final bound is only good for $\beta<\frac{1}{2}$.

Thus, to cover the extended range $\beta \in \big(0, \frac{3}{2}\big)$, new ideas are needed to handle (3-19). In the present paper, on the one hand, we will not rely on any information of Φ_N; moreover, instead of using directly (3-21) we will further decompose (3-19) by introducing a weight given by

$$\mathcal{R} := \mathrm{d}\Gamma_2(|w_N|) + 1 = \tfrac{1}{2} \int \mathrm{d}x\, \mathrm{d}y\, |w_N(x-y)| a_x^\dagger a_y^\dagger a_x a_y + 1. \tag{3-22}$$

By inserting $1 = \mathcal{R}^{-1/2}\mathcal{R}^{1/2}$, we can write

$$a_x^\dagger a_y^\dagger = \mathcal{R}^{-1/2} a_x^\dagger a_y^\dagger \mathcal{R}^{1/2} + \mathcal{R}^{-1/2}[\mathcal{R}^{1/2}, a_x^\dagger a_y^\dagger]. \tag{3-23}$$

Then, using the triangle inequality we can bound (3-19) by

$$\begin{aligned} &\frac{1}{M} \iint \mathrm{d}x\, \mathrm{d}y\, |u_N(x)|\, |u_N(y)|\, |w_N(x-y)|\, |\langle \Phi_N, \mathcal{R}^{-1/2} a_x^\dagger a_y^\dagger \mathcal{R}^{1/2} \Phi_{N,M}\rangle| \\ &\qquad + \frac{1}{M} \iint \mathrm{d}x\, \mathrm{d}y\, |u_N(x)|\, |u_N(y)|\, |w_N(x-y)|\, \big|\langle \Phi_N, \mathcal{R}^{-1/2}[\mathcal{R}^{1/2}, a_x^\dagger a_y^\dagger] \Phi_{N,M}\rangle\big|. \end{aligned} \tag{3-24}$$

The key point is that although the first term in (3-24) looks similar to (3-19), it is much easier to control. Indeed, by the Cauchy–Schwarz inequality, we have

$$\begin{aligned} &\frac{1}{M} \iint \mathrm{d}x\, \mathrm{d}y\, |u_N(x)|\, |u_N(y)|\, |w_N(x-y)|\, |\langle \Phi_N, \mathcal{R}^{-1/2} a_x^\dagger a_y^\dagger \mathcal{R}^{1/2} \Phi_{N,M}\rangle| \\ &\quad \le \frac{1}{M} \iint \mathrm{d}x\, \mathrm{d}y\, |u_N(x)|\, |u_N(y)|\, |w_N(x-y)|\, \|a_x a_y \mathcal{R}^{-1/2} \Phi_N\|\, \|\mathcal{R}^{1/2}\Phi_{N,M}\| \\ &\quad \le \frac{1}{M} \bigg(\iint \mathrm{d}x\, \mathrm{d}y\, |w_N(x-y)|\, \|a_x a_y \mathcal{R}^{-1/2} \Phi_N\|^2 \bigg)^{1/2} \\ &\qquad\qquad \times \bigg(\iint \mathrm{d}x\, \mathrm{d}y\, |u_N(x)|^2 |u_N(y)|^2 |w_N(x-y)| \bigg)^{1/2} \|\mathcal{R}^{1/2}\Phi_{N,M}\|. \end{aligned} \tag{3-25}$$

Then, by the definition of $\mathcal{R}$, we can bound

$$\begin{aligned} \iint \mathrm{d}x\, \mathrm{d}y\, |w_N(x-y)|\, \|a_x a_y \mathcal{R}^{-1/2}\Phi_N\|^2 &= \big\langle \Phi_N, \mathcal{R}^{-1/2}\, \mathrm{d}\Gamma_2(|w_N|) \mathcal{R}^{-1/2} \Phi_N \big\rangle \\ &\le \|\Phi_N\|^2, \end{aligned} \tag{3-26}$$

without relying on any information on Φ_N. The other factors in (3-25) can be bounded efficiently using $\|w_N\|_{L^1} \le C$ and good estimates on $\Phi_{N,M}$ and u_N, given that $\mathcal{R}$ can essentially be controlled in terms of the kinetic energy; see (5-3). All this allows us to bound (3-25) by $C_{t,\varepsilon} N^\varepsilon / \sqrt{M} \|\Phi_N\|$, which appears as the first error term on the right-hand side of (3-17).

We still have to bound the second term in (3-24). This term looks complicated, but in principle, we gain a huge cancelation from the commutator $[\mathcal{R}^{1/2}, a_x^\dagger a_y^\dagger]$ due to the fact that $\mathcal{R}$ is a "local operator". To make it more transparent, we can use

$$\mathcal{R}^{1/2} = \frac{1}{\pi} \int_0^\infty \frac{1}{\sqrt{s}} \frac{\mathcal{R}}{\mathcal{R}+s}\, \mathrm{d}s \tag{3-27}$$

to write, for any operator B,

$$[\mathcal{R}^{1/2}, B] = \frac{1}{\pi}\int_0^\infty \mathrm{d}s\, \frac{1}{\sqrt{s}}\left[\frac{\mathcal{R}}{\mathcal{R}+s}, B\right] = \frac{1}{\pi}\int_0^\infty \mathrm{d}s\, \frac{\sqrt{s}}{\mathcal{R}+s}[\mathcal{R}, B]\frac{1}{\mathcal{R}+s}. \tag{3-28}$$

In particular, a straightforward computation shows that

$$\begin{aligned}[\mathcal{R}, a_x^\dagger a_y^\dagger] &= \big[\mathrm{d}\Gamma_2(|w_N|), a_x^\dagger a_y^\dagger\big] \\ &= |w_N(x-y)| a_x^\dagger a_y^\dagger + \int \mathrm{d}z\, \big(|w_N(z-x)| + |w_N(z-y)|\big) a_x^\dagger a_y^\dagger a_z^\dagger a_z.\end{aligned} \tag{3-29}$$

Let us take $|w_N(x-y)|a_x^\dagger a_y^\dagger$ from (3-29) and insert it in (3-28). The corresponding contribution from the second term in (3-24) can be controlled by

$$\frac{1}{M}\int_0^\infty \mathrm{d}s\, \sqrt{s} \iint \mathrm{d}x\, \mathrm{d}y\, |u_N(x)|\, |u_N(y)|\, |w_N(x-y)|^2 \left\| a_x a_y \frac{\mathcal{R}^{-1/2}}{\mathcal{R}+s}\Phi_N \right\| \left\| \frac{1}{\mathcal{R}+s}\Phi_{N,M}\right\|. \tag{3-30}$$

The resolvents $(\mathcal{R}+s)^{-1}$ are important in two respects: one the one hand, they provide sufficient decay in s via the estimate $(\mathcal{R}+s)^{-1} \le (1+s)^{-1}$. On the other hand, they compensate for the singular interaction, which is similar to the argument in (3-26) although $|w_N|^2$ is way more singular than $|w_N|$.

To combine these two ideas, we apply the Cauchy–Schwarz inequality on $\mathbb{R}^2 \times \mathbb{R}^2$ to (3-30), where we write

$$|w_N|^2 = |w_N|^{1+\varepsilon/2} |w_N|^{1-\varepsilon/2} \tag{3-31}$$

for $\varepsilon > 0$ small. We estimate the term coming from $|w_N|^{1-\varepsilon/2}$ using

$$\frac{\mathcal{R}^{-1/2}}{\mathcal{R}+s}\,\mathrm{d}\Gamma(|w_N|^{2-\varepsilon})\frac{\mathcal{R}^{-1/2}}{\mathcal{R}+s} \le \frac{\mathcal{R}^{1-\varepsilon}}{(\mathcal{R}+s)^2} \le \frac{1}{(1+s)^{1+\varepsilon}}. \tag{3-32}$$

Here, we used that

$$\mathrm{d}\Gamma_2(|w_N|^{2-\varepsilon}) \le \big(\mathrm{d}\Gamma_2(|w_N|)\big)^{2-\varepsilon} \le \mathcal{R}^{2-\varepsilon}, \tag{3-33}$$

which relies heavily on the locality of $\mathcal{R}$, namely $\mathrm{d}\Gamma_2(|w_N|)$ is the second quantization of a two-body multiplication operator (see Lemma 12). For the term coming from $|w_N|^{1+\varepsilon/2}$, by calculating the L^2-norm of $|w_N|^{1+\varepsilon/2}$, which appears in (3-31), we eventually obtain $C_{t,\varepsilon}N^\varepsilon N^\beta / M^{3/2}$, the second error term on the right-hand side of (3-17). The cubic term $\langle \Phi_N, [\mathbb{G}_3, f_M^2]\Phi_{N,M}\rangle$ can be handled similarly. This completes our overview of the main ingredients of the proof.

In our analysis, the restriction to $\beta < \frac{3}{2}$ seems a purely technical limitation. We conjecture that it could be improved. For example, one would be able to cover all $\beta > 0$ if the higher-moment estimate $\langle \Phi_{N,M}, \mathcal{N}^b \Phi_{N,M}\rangle \le C_{b,\varepsilon}N^\varepsilon$ were established for all $b \ge 1$. At present, however, we are not able to show that, and we will only use the first moment bound ($b = 1$) from Lemma 8.

Organization of the paper. In Section 4, we establish uniform-in-N estimates for the Hartree dynamics. The most technical part of the paper is contained in Section 5 where we prove Proposition 9. From this, we conclude the main results in Section 6.

4. Uniform estimates for Hartree evolution

In this section, we consider the Hartree evolution u_N in (2-9). By Assumption 1, it is globally well-posed in H^k, $k \in \{1, 2, \dots\}$, for any fixed N by [Cazenave 2003, Corollary 6.1.2]. However, it is a priori not clear whether $\|u_N(t)\|_{H^k}$ is bounded uniformly in N for fixed $t \in [0, T_{\max})$. In the following lemma, we prove such uniform bounds for all times prior to the NLS blow-up time $T_{\max}$.

Lemma 10. *Let w satisfy Assumption 1. Let $\varphi_0 \in H^4(\mathbb{R}^2)$ and $T_{\max}$ be as in Lemma 2. Then, for every $T \in [0, T_{\max})$, there exists a constant $C = C(T, \varphi_0) > 0$ such that, for all $t \in [0, T]$ and all N sufficiently large,*

$$\|u_N(t)\|_{L^\infty} \le C\,\|u_N(t)\|_{H^2(\mathbb{R}^2)} \le C, \quad \|\partial_t u_N(t)\|_{H^2(\mathbb{R}^2)} \le C. \tag{4-1}$$

Moreover, for $\varphi(t)$ the solution of the NLS (1-6),

$$\|u_N(t) - \varphi(t)\|_{L^2(\mathbb{R}^2)} \le CN^{-\beta}. \tag{4-2}$$

For interactions satisfying the stability condition $\int_{\mathbb{R}^2} |w_-| < a^*$, (4-1) has been shown in [Nam and Napiórkowski 2019, Lemma 4]. As explained in [Nam and Napiórkowski 2019], the key point is to get the uniform bound $\|u_N(t)\|_{H^1(\mathbb{R}^2)} \le C$, and the rest follows from a rather general argument. In the stability regime considered in [Nam and Napiórkowski 2019], this bound follows immediately from energy conservation and (1-8), namely

$$\begin{aligned}\mathcal{E}[u_N(t)] &= \|\nabla u_N(t)\| + \tfrac{1}{2}\iint \mathrm{d}x\,\mathrm{d}y\,|u_N(t,x)|^2 w_N(x-y)|u_N(t,y)|^2\\ &\ge \|\nabla u_N(t)\| - \tfrac{1}{2}\|(w_N)_-\|_{L^1}\|u_N(t)\|_{L^4}^4\\ &\ge \|\nabla u_N(t)\|^2\left(1 - \frac{\int_{\mathbb{R}^2}|w_-|}{a^*}\right).\end{aligned} \tag{4-3}$$

For a general w in Lemma 10, the estimate (4-3) is not available, hence the estimate of $\|u_N(t)\|_{H^1(\mathbb{R}^2)}$ is more complicated. Instead of studying u_N directly as in [Nam and Napiórkowski 2019], we will focus on the difference

$$\theta_N(t) = u_N(t) - \varphi(t). \tag{4-4}$$

We will bound $\theta_N(t)$ by a bootstrap argument consisting of two steps:

(1) If $\|\theta_N(t)\| \le \delta = \sqrt{a^*/(32\,\|w\|_{L^1})}$, then $\|\nabla\theta_N(t)\| \le C$. This follows from energy conservation and the a priori bound $\|\varphi(t)\|_{H^1(\mathbb{R}^2)} \le C$ on $[0, T]$.

(2) If $\|\theta_N(s)\| \le \delta$ for all $s \in [0, t]$, then $\|\theta_N(t)\| \le N^{-\beta} \ll \delta$ for sufficiently large N. To prove this, we use Step 1 and Gronwall's lemma.

The conclusion thus follows from the continuity of the map $t \mapsto \|\theta_N(t)\|$ and the initial condition $\theta_N(0) = 0$. Now let us go to the details.

Proof of Lemma 10. For simplicity, we consider the solutions $u_N(t)$ and $\varphi(t)$ of (2-9) and (1-6) without the phases $\mu_N(t)$ and $\mu(t)$, respectively. Due to the gauge transformation $u_N \mapsto \exp\{-\mathrm{i}\int_0^t \mu(s)\,\mathrm{d}s\}u_N$, this does not change the N-dependence of the estimates (4-1). Let $\delta = \sqrt{a^*/(32\,\|w\|_{L^1})}$ with a^* as in (1-8).

Step 1. Assume that $\|\theta_N(t)\| \le \delta$ for some $t \in [0, T]$. Using the energy conservation of (2-9) and the fact $\|w_N\|_{L^1} = \|w\|_{L^1}$, we can bound

$$\begin{aligned}\mathcal{E}[u_N(t)] = \mathcal{E}[\varphi_0] &= \|\nabla\varphi_0\|^2 + \tfrac{1}{2}\iint |\varphi_0(x)|^2 w_N(x-y)|\varphi_0(y)|^2\,\mathrm{d}x\,\mathrm{d}y \\ &\le \|\nabla\varphi_0\|^2 + \tfrac{1}{2}\|w\|_{L^1}\|\varphi_0\|_{L^4}^4 \le C. \end{aligned} \tag{4-5}$$

On the other hand, using (1-8) and the assumption $\|\theta_N(t)\| \le \delta$, we can bound

$$\|\theta_N(t)\|_{L^4}^4 \le \frac{2\delta^2}{a^*}\|\nabla\theta_N(t)\|^2 = \frac{1}{16\,\|w\|_{L^1}}\|\nabla\theta_N(t)\|^2.$$

Combining with $\frac{1}{2}\|\nabla\theta_N(t)\|^2 \le \|\nabla u_N(t)\|^2 + \|\nabla\varphi(t)\|^2$, we find that

$$\begin{aligned}\mathcal{E}_N[u_N(t)] &\ge \|\nabla u_N(t)\|^2 - \tfrac{1}{2}\|w\|_{L^1}\|\theta_N(t)+\varphi(t)\|_{L^4}^4 \\ &\ge \big(\tfrac{1}{2}\|\nabla\theta_N(t)\|^2 - \|\nabla\varphi(t)\|^2\big) - 4\,\|w\|_{L^1}\big(\|\theta_N(t)\|_{L^4}^4 + \|\varphi(t)\|_{L^4}^4\big) \\ &\ge \tfrac{1}{4}\|\nabla\theta_N(t)\|^2 - C, \end{aligned} \tag{4-6}$$

where we used that $\|\nabla\varphi(t)\| \le C$ on $[0, T]$. Consequently, (4-5) and (4-6) imply that $\|\nabla\theta_N(t)\|^2 \le C$.

Step 2. Let $s \in [0, t]$ and assume that $\|\theta_N(s)\| \le \delta$. Then, dropping the time dependence from the notation, we find that

$$\begin{aligned}\tfrac{1}{2}\big|\partial_s\|\theta_N(s)\|^2\big| &= \big|\Im\big\langle\theta_N, (w_N * |u_N|^2)\theta_N + \big(w_N * (|u_N|^2 - |\varphi|^2)\big)\varphi + (w_N * |\varphi|^2 - b\,|\varphi|^2)\varphi\big\rangle\big| \\ &\le \|\theta_N\|\,\|\varphi\|_{L^\infty}\big(\big\|w_N * (|u_N|^2 - |\varphi|^2)\big\| + \big\|w_N * |\varphi|^2 - b\,|\varphi|^2\big\|\big) \\ &=: \|\theta_N\|\,\|\varphi\|_{L^\infty}(A_1 + A_2). \end{aligned} \tag{4-7}$$

On the right-hand side of (4-7), we have $\|\theta_N(s)\| \le \delta$ by our assumption, and $\|\varphi(s)\|_{L^\infty} \le C$ since $\varphi(s) \in H^2(\mathbb{R}^2)$ [Cazenave 2003, Theorems 5.3.1 and 5.4.1] and Sobolev's embedding $H^2(\mathbb{R}^2) \subset L^\infty(\mathbb{R}^2)$ [Lieb and Loss 2001, Theorem 8.8 (iii)].

Estimate of A_1. Using

$$\big||u_N|^2 - |\varphi|^2\big| = \big|(|u_N| - |\varphi|)(|u_N| + |\varphi|)\big| \le |\theta_N|^2 + 2\,|\varphi|\,|\theta_N|, \tag{4-8}$$

we can bound

$$A_1 \le \|w_N\|_{L^1}(\|\theta_N\|_{L^4}^2 + 2\,\|\varphi\|_{L^\infty}\|\theta_N\|) \le C\,\|\theta_N\|. \tag{4-9}$$

In the last estimate, we used (1-8) and the bound $\|\nabla\theta_N(t)\|^2 \le C$ from Step 1.

Estimate of A_2. Observing that $b = \widehat{w}_N(0)$ and $\widehat{w}_N(\xi) = \widehat{w}(\xi/N^\beta)$, Plancherel's theorem yields

$$A_2 \le \left\|\frac{\widehat{w}(\cdot/N^\beta) - \widehat{w}(0)}{|\cdot|}\right\|_{L^\infty}\big\||\cdot|\,\widehat{|\varphi|^2}\big\|_{L^2} \le CN^{-\beta}. \tag{4-10}$$

Here, we used $\|\nabla\varphi\| \le C$ and the fact that $\widehat{w}$ is Lipschitz.

In summary, inserting (4-9) and (4-10) in (4-7), we arrive at

$$\partial_s \|\theta_N(s)\|^2 \le C\big(\|\theta_N(s)\|^2 + N^{-2\beta}\big). \tag{4-11}$$

Consequently, we obtain $\|\theta_N(t)\| \le CN^{-\beta}$ by Gronwall's lemma since $\theta_N(0) = 0$.

Conclusion. Define

$$t_N^{\max} = \sup\{t \in [0, T] : \|\theta_N(t)\| \le \delta\}. \tag{4-12}$$

Assume that $t_N^{\max} < T$. By [Cazenave 2003, Theorem 4.10.1], the map $[0, T] \ni t \mapsto \|\theta_N(t)\|$ is continuous, hence $\|\theta_N(s)\| \le \delta$ for $s \in [0, t_N^{\max}]$. By Step 2, this implies that

$$\|\theta_N(t_N^{\max})\| \le CN^{-\beta} < \delta \tag{4-13}$$

for sufficiently large N, which contradicts $t_N^{\max} < T$. Hence, $t_N^{\max} \ge T$, and consequently

$$\|\theta_N(t)\| \le \delta \quad \text{for all } t \in [0, T].$$

By Step 1, we get $\|\nabla\theta_N(t)\|^2 \le C$. Therefore,

$$\|u_N(t)\|_{H^1} \le \|\theta_N(t)\|_{H^1} + \|\varphi(t)\|_{H^1} \le C \quad \text{for all } t \in [0, T]. \tag{4-14}$$

The remaining estimates in (4-1) can be deduced from the H^1-bound as in [Nam and Napiórkowski 2019, Lemma 4], using Duhamel's formula. The bound (4-2) also follows from the above argument, where the error term $N^{-\beta}$ comes from (4-10). □

5. From the truncated to the full dynamics

In this section we prove Proposition 9. As explained in Section 3.3, the key step is to prove the propagation bound (3-17). We use (3-18) and (3-8) to decompose

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}\langle \Phi_N(t), f_M^2 \Phi_{N,M}(t)\rangle\right| \le \sum_{j=1}^{3} \big|\langle \Phi_N, [(\mathbb{G}_j + \mathbb{G}_j^*), f_M^2]\Phi_{N,M}\rangle\big| \tag{5-1}$$

with $\mathbb{G}_j$ given in (3-8). In the next subsections, we will handle the cases $j = 1, 2, 3$ separately, and then conclude (3-17) as well as Proposition 9.

As a preparation, let us collect here two auxiliary estimates which will be used repeatedly in this section. The first one is a simple Sobolev-type estimate.

Lemma 11. *Let $W \in L^s(\mathbb{R}^2)$ with $s \in (1, 2]$ and denote by $W(x - y)$ the corresponding two-body multiplication operator. Then*

$$\mathrm{d}\Gamma_2\big(|W(x-y)|\big) \le C_s \|W\|_{L^s(\mathbb{R}^2)} \mathcal{N}\, \mathrm{d}\Gamma_1(1 - \Delta) \tag{5-2}$$

as operators on $\mathcal{F}$.

In particular, Assumption 1 guarantees that $w \in L^{1+\varepsilon}(\mathbb{R}^2)$ for every $\varepsilon > 0$, hence Lemma 11 implies that

$$\mathrm{d}\Gamma_2\big(|w_N(x-y)|\big) \le C_\varepsilon N^\varepsilon \mathcal{N}\, \mathrm{d}\Gamma_1(1 - \Delta). \tag{5-3}$$

Here we used the fact that

$$\int_{\mathbb{R}^2} |w_N(x)|^\alpha \,\mathrm{d}x = N^{2\beta(\alpha-1)} \int |w(x)|^\alpha \,\mathrm{d}x \quad \text{for all } \alpha > 0. \tag{5-4}$$

Proof. Using Sobolev's embedding $L^{s'}(\mathbb{R}^2) \supset H^1(\mathbb{R}^2)$ with $1/s' + 1/s = 1$ [Lieb and Loss 2001, Theorem 8.8], we have

$$\begin{aligned}\iint \mathrm{d}x\,\mathrm{d}y\, |W(x-y)|\,|f(x,y)|^2 &\le C_s \int \mathrm{d}x\, \|W(x-\cdot\,)\|_{L^s(\mathbb{R}^2)} \|f(x,\cdot\,)\|^2_{H^1(\mathbb{R}^2)} \\ &= C_s \|W\|_{L^s(\mathbb{R}^2)} \langle f, (1-\Delta_y) f\rangle_{L^2(\mathbb{R}^2\times\mathbb{R}^2)} \end{aligned} \tag{5-5}$$

for all $f \in H^1(\mathbb{R}^2 \times \mathbb{R}^2)$. Therefore, we have the two-body inequality

$$|W(x-y)| \le C_s \|W\|_{L^s(\mathbb{R}^2)} (1-\Delta_y) \tag{5-6}$$

for each $y \in \mathbb{R}^2$, which implies the second-quantized form (5-2). □

The second estimate is concerned with the second quantization of a two-body multiplication operator:

Lemma 12. *Let $A \ge 0$ be a multiplication operator on $\mathfrak{H}^2$ such that $A(x,y) = A(y,x)$ and let $s \in [1,\infty)$. Then*

$$\mathrm{d}\Gamma_2(A^s) \le [\mathrm{d}\Gamma_2(A)]^s. \tag{5-7}$$

Proof. On every k-particle sector $\mathfrak{H}^k$, $k \ge 2$, we have

$$\mathrm{d}\Gamma_2(A^s) = \sum_{1\le i<j\le k} A_{ij}^s \le \Bigl(\sum_{1\le i<j\le k} A_{ij}\Bigr)^s = [\mathrm{d}\Gamma_2(A)]^s. \tag{5-8}$$

This concludes the proof since $\mathrm{d}\Gamma_2(A)$ preserves the particle number. □

5.1. *Estimate of the linear terms.* We consider first the linear terms in (5-1).

Lemma 13. *For every $t \in [0, T_{\max})$ and $\varepsilon > 0$, we have*

$$\bigl|\bigl\langle \Phi_N, [(\mathbb{G}_1 + \mathbb{G}_1^*), f_M^2] \Phi_{N,M}\bigr\rangle\bigr| \le C_{t,\varepsilon} \frac{N^\varepsilon}{\sqrt{N}}. \tag{5-9}$$

Proof. From the definition of $\mathbb{G}_1$ in (3-8), we obtain

$$\bigl|\langle \Phi_N, [\mathbb{G}_1, f_M^2]\Phi_{N,M}\rangle\bigr| = 2\,\bigl|\bigl\langle \Phi_N, a^\dagger\bigl(q(t)(w_N * |u_N|^2)u_N\bigr)\omega_1 \Phi_{N,M}\bigr\rangle\bigr| \tag{5-10}$$

with

$$\omega_1 = \frac{\mathcal{N}\sqrt{N-\mathcal{N}}}{N-1}\biggl(f^2\Bigl(\frac{\mathcal{N}}{M}\Bigr) - f^2\Bigl(\frac{\mathcal{N}+1}{M}\Bigr)\biggr), \tag{5-11}$$

where we used that $g(\mathcal{N})a_x^\dagger = a_x^\dagger g(\mathcal{N}+1)$. For f as in (3-16), we have

$$|\omega_1| \le \frac{C\mathcal{N}}{M\sqrt{N}} \mathbb{1}^{\le M} \tag{5-12}$$

in the sense of operators on $\mathcal{F}_{\perp}^{\leq N}(t)$. We will use the simple bound

$$a(v)a^{\dagger}(v) = a^{\dagger}(v)a(v) + \|v\|^2 \leq (\mathcal{N}+1)\|v\|^2, \tag{5-13}$$

where $v = q(t)(w_N * |u_N|^2)u_N$ satisfies

$$\|v\|_{L^2} \leq \big\|(w_N * |u_N|^2)u_N\big\|_{L^2} \leq \|w_N\|_{L^1}\|u_N\|_{L^2}^2\|u_N\|_{L^\infty} \leq C_t \tag{5-14}$$

by Lemma 10. Therefore, by the Cauchy–Schwarz inequality, we deduce from (5-10) and (5-13) that

$$\begin{aligned}\big|\langle\Phi_N, [\mathbb{G}_1, f_M^2]\Phi_{N,M}\rangle\big| &\leq 2\,\|\Phi_N\|\,\big\|a^{\dagger}\big(q(t)(w_N * |u_N|^2)u_N\big)(\mathcal{N}+1)^{-1/2}\big\|_{\mathrm{op}}\|(\mathcal{N}+1)^{1/2}\omega_1\Phi_{N,M}\| \\ &\leq C_t\left\|\frac{(\mathcal{N}+1)^{3/2}}{M\sqrt{N}}\mathbb{1}^{\leq M}\Phi_{N,M}\right\| \leq C_{t,\varepsilon}\frac{N^{\varepsilon}}{\sqrt{N}}.\end{aligned} \tag{5-15}$$

In the last estimate, we used that

$$\|\mathcal{N}^{1/2}\Phi_{N,M}\|^2 = \langle\Phi_{N,M}, \mathcal{N}\Phi_{N,M}\rangle \leq C_{t,\varepsilon}N^{\varepsilon}, \tag{5-16}$$

which follows from the kinetic estimate (3-13) in Lemma 8. Similarly, we also get

$$\big|\langle\Phi_N, [\mathbb{G}_1^*, f_M^2]\Phi_{N,M}\rangle\big| \leq C_{t,\varepsilon}\frac{N^{\varepsilon}}{\sqrt{N}} \tag{5-17}$$

since

$$\big|\langle\Phi_N, [\mathbb{G}_1^*, f_M^2]\Phi_{N,M}\rangle\big| = 2\,\big|\big\langle\Phi_N, a\big(q(t)(w_N * |u_N|^2)u_N\big)\widetilde{\omega}_1\Phi_{N,M}\big\rangle\big|, \tag{5-18}$$

where

$$\widetilde{\omega}_1 = \frac{\mathcal{N}\sqrt{N-\mathcal{N}+1}}{N-1}\left(f^2\left(\frac{\mathcal{N}}{M}\right) - f^2\left(\frac{\mathcal{N}-1}{M}\right)\right) \tag{5-19}$$

as an operator on $\mathcal{F}_{\perp}^{\leq N}$. From (5-15) and (5-17), we obtain (5-9). □

5.2. ***Estimate of the quadratic terms.*** We turn to the quadratic terms in (5-1).

Lemma 14. *For every $t \in [0, T_{\max})$ and $\varepsilon > 0$, we have*

$$\big|\langle\Phi_N, [\mathbb{G}_2, f_M^2]\Phi_{N,M}\rangle\big| \leq C_{t,\varepsilon}\left(\frac{1}{\sqrt{M}} + \frac{N^{\beta}}{M^{3/2}}\right)N^{\varepsilon}, \tag{5-20}$$

$$\big|\langle\Phi_N, [\mathbb{G}_2^*, f_M^2]\Phi_{N,M}\rangle\big| \leq C_{t,\varepsilon}\frac{N^{\varepsilon}}{M}. \tag{5-21}$$

Proof. The bound (5-20) is one of the most difficult estimates in this section. We use the strategy explained in Section 3.3.

Step 1. Let us abbreviate

$$\omega_2 = \frac{\sqrt{(N-\mathcal{N})(N-\mathcal{N}-1)}}{N-1}\left(f^2\left(\frac{\mathcal{N}}{M}\right) - f^2\left(\frac{\mathcal{N}+2}{M}\right)\right) \tag{5-22}$$

as an operator on $\mathcal{F}_{\perp}^{\le N}$. For $N \ge 2$, we have

$$|\omega_2| \le \frac{C}{M}\mathbb{1}^{>M/2}. \tag{5-23}$$

We also observe that in the relevant estimate for $\mathbb{G}_2$, $K_2 = q \otimes q\widetilde{K}_2$ in (2-24) can be replaced by $\widetilde{K}_2$ as for any $\chi, \chi' \in \mathcal{F}_{\perp}(t)$ we have

$$\left\langle \chi, \iint \mathrm{d}x\,\mathrm{d}y\; K_2(x,y)u_N(x)u_N(y)a_x^\dagger a_y^\dagger \chi' \right\rangle = \left\langle \chi, \iint \mathrm{d}x\,\mathrm{d}y\; \widetilde{K}_2(x,y)u_N(x)u_N(y)a_x^\dagger a_y^\dagger \chi' \right\rangle. \tag{5-24}$$

Hence, we can write

$$\langle \Phi_N, [\mathbb{G}_2, f_M^2]\Phi_{N,M}\rangle = \iint \mathrm{d}x\,\mathrm{d}y\; w_N(x-y)u_N(x)u_N(y)\langle \Phi_N, a_x^\dagger a_y^\dagger \omega_2 \Phi_{N,M}\rangle. \tag{5-25}$$

By writing

$$a_x^\dagger a_y^\dagger = \mathcal{R}^{-1/2}a_x^\dagger a_y^\dagger \mathcal{R}^{1/2} + \mathcal{R}^{-1/2}[\mathcal{R}^{1/2}, a_x^\dagger a_y^\dagger] \tag{5-26}$$

with $\mathcal{R} = \mathrm{d}\Gamma_2(|w_N|) + 1$ as in (3-22) and using the triangle inequality, we find that

$$\left|\langle \Phi_N, [\mathbb{G}_2, f_M^2]\Phi_{N,M}\rangle\right| \le \mathcal{E}_1 + \mathcal{E}_2 \tag{5-27}$$

where

$$\mathcal{E}_1 = \iint \mathrm{d}x\,\mathrm{d}y\; |w_N(x-y)|\,|u_N(x)|\,|u_N(y)|\,|\langle \Phi_N, \mathcal{R}^{-1/2}a_x^\dagger a_y^\dagger \mathcal{R}^{1/2}\omega_2\Phi_{N,M}\rangle|, \tag{5-28}$$

$$\mathcal{E}_2 = \iint \mathrm{d}x\,\mathrm{d}y\; |w_N(x-y)|\,|u_N(x)|\,|u_N(y)|\,\left|\langle \Phi_N, \mathcal{R}^{-1/2}[\mathcal{R}^{1/2}, a_x^\dagger a_y^\dagger]\omega_2\Phi_{N,M}\rangle\right|. \tag{5-29}$$

Step 2. Now let us estimate $\mathcal{E}_1$. By the Cauchy–Schwarz inequality,

$$\begin{aligned}\mathcal{E}_1 &\le \iint \mathrm{d}x\,\mathrm{d}y\; |w_N(x-y)|\,|u_N(x)|\,|u_N(y)|\,\|a_x a_y \mathcal{R}^{-1/2}\Phi_N\|\,\|\mathcal{R}^{1/2}\omega_2\Phi_{N,M}\| \\ &\le \left(\iint \mathrm{d}x\,\mathrm{d}y\; |w_N(x-y)|\,|u_N(x)|^2|u_N(y)|^2\right)^{1/2} \\ &\qquad \times \left(\iint \mathrm{d}x\,\mathrm{d}y\; |w_N(x-y)|\,\|a_x a_y\mathcal{R}^{-1/2}\Phi_N\|^2\right)^{1/2} \|\mathcal{R}^{1/2}\omega_2\Phi_{N,M}\|.\end{aligned} \tag{5-30}$$

From Lemma 10, we can bound

$$\iint \mathrm{d}x\,\mathrm{d}y\; |w_N(x-y)|\,|u_N(x)|^2|u_N(y)|^2 \le \|u_N\|_{L^\infty}^2\|u_N\|_{L^2}^2\|w_N\|_{L^1} \le C_t. \tag{5-31}$$

Moreover, (3-26) yields

$$\iint \mathrm{d}x\,\mathrm{d}y\; |w_N(x-y)|\,\|a_x a_y \mathcal{R}^{-1/2}\Phi_N\|^2 \le \|\Phi_N\|^2 \le 1. \tag{5-32}$$

From Lemma 11 and the kinetic estimate in Lemma 8, we get

$$\left\langle \Phi_{N,M}, \mathrm{d}\Gamma_2(|w_N|)\Phi_{N,M}\right\rangle \le C_\varepsilon N^\varepsilon \langle \Phi_{N,M}, M\,\mathrm{d}\Gamma_1(1-\Delta)\Phi_{N,M}\rangle \le C_{t,\varepsilon} M N^{2\varepsilon}. \tag{5-33}$$

Combining this with (5-23) and the fact that $\mathcal{R}$ commutes with ω_2, we find that

$$\|\mathcal{R}^{1/2}\omega_2\Phi_{N,M}\|^2 \le \frac{C}{M^2}\langle\Phi_{N,M},\mathcal{R}\Phi_{N,M}\rangle \le \frac{C_{t,\varepsilon}N^\varepsilon}{M}. \tag{5-34}$$

Inserting (5-31), (5-32) and (5-34) in (5-30), we conclude that

$$\mathcal{E}_1 \le \frac{C_{t,\varepsilon}N^\varepsilon}{\sqrt{M}}\|\Phi_N\| \tag{5-35}$$

for every constant $\varepsilon > 0$.

Step 3. We turn to estimate the second term $\mathcal{E}_2$, which is more involved. Using (3-29) and (3-28), we get

$$\begin{aligned}[\mathcal{R}^{1/2}, a_x^\dagger a_y^\dagger] &= \frac{1}{\pi}\int_0^\infty \mathrm{d}s\,\frac{\sqrt{s}}{\mathcal{R}+s}|w_N(x-y)|a_x^\dagger a_y^\dagger\frac{1}{\mathcal{R}+s}\\ &\quad+\frac{1}{\pi}\int_0^\infty \mathrm{d}s\int \mathrm{d}z\,\frac{\sqrt{s}}{\mathcal{R}+s}\big(|w_N(x-z)|+|w_N(y-z)|\big)a_x^\dagger a_y^\dagger a_z^\dagger a_z\frac{1}{\mathcal{R}+s}.\end{aligned} \tag{5-36}$$

This allows us to write

$$\begin{aligned}\mathcal{E}_2 &= \iint \mathrm{d}x\,\mathrm{d}y\,|w_N(x-y)|\,|u_N(x)|\,|u_N(y)|\,\big|\langle\Phi_N,\mathcal{R}^{-1/2}[\mathcal{R}^{1/2},a_x^\dagger a_y^\dagger]\omega_2\Phi_{N,M}\rangle\big|\\ &\le C(\mathcal{E}_{2,1}+\mathcal{E}_{2,2}),\end{aligned} \tag{5-37}$$

where

$$\mathcal{E}_{2,1} = \int_0^\infty \mathrm{d}s\,\sqrt{s}\iint \mathrm{d}x\,\mathrm{d}y\,|w_N(x-y)|^2|u_N(x)|\,|u_N(y)|\left|\langle\Phi_N,\frac{\mathcal{R}^{-1/2}}{\mathcal{R}+s}a_x^\dagger a_y^\dagger\frac{1}{\mathcal{R}+s}\omega_2\Phi_{N,M}\rangle\right|, \tag{5-38}$$

$$\begin{aligned}\mathcal{E}_{2,2} = \int_0^\infty \mathrm{d}s\,\sqrt{s}\iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,|w_N(x-y)|\,|w_N(x-z)|\,|u_N(x)|\,|u_N(y)|&\\ \times\left|\langle\Phi_N,\frac{\mathcal{R}^{-1/2}}{\mathcal{R}+s}a_x^\dagger a_y^\dagger a_z^\dagger a_z\frac{1}{\mathcal{R}+s}\omega_2\Phi_{N,M}\rangle\right|&.\end{aligned} \tag{5-39}$$

Estimate of $\mathcal{E}_{2,1}$. By the Cauchy–Schwarz inequality, we find for any constant $\varepsilon\in(0,1)$ that

$$\begin{aligned}\mathcal{E}_{2,1} &\le \int_0^\infty \mathrm{d}s\sqrt{s}\iint \mathrm{d}x\,\mathrm{d}y\,|w_N(x-y)|^2|u_N(x)|\,|u_N(y)|\left\|a_xa_y\frac{\mathcal{R}^{-1/2}}{\mathcal{R}+s}\Phi_N\right\|\left\|\frac{1}{\mathcal{R}+s}\omega_2\Phi_{N,M}\right\|\\ &\le \int_0^\infty \mathrm{d}s\,\sqrt{s}\left(\iint \mathrm{d}x\,\mathrm{d}y\,|w_N(x-y)|^{2+\varepsilon}|u_N(x)|^2|u_N(y)|^2\right)^{1/2}\\ &\qquad\times\left(\iint \mathrm{d}x\,\mathrm{d}y\,|w_N(x-y)|^{2-\varepsilon}\left\|a_xa_y\frac{\mathcal{R}^{-1/2}}{\mathcal{R}+s}\Phi_N\right\|^2\right)^{1/2}\left\|\frac{1}{\mathcal{R}+s}\omega_2\Phi_{N,M}\right\|.\end{aligned} \tag{5-40}$$

By Lemma 10, we obtain

$$\begin{aligned}\iint \mathrm{d}x\,\mathrm{d}y\,|w_N(x-y)|^{2+\varepsilon}|u_N(x)|^2|u_N(y)|^2 &\le \|u_N\|_{L^\infty}^2\|u_N\|_{L^2}^2\||w_N|^{2+\varepsilon}\|_{L^1}\\ &\le C_tN^{2\beta(1+\varepsilon)}.\end{aligned} \tag{5-41}$$

Moreover, using that

$$\iint \mathrm{d}x\,\mathrm{d}y\,|w_N(x-y)|^{2-\varepsilon} a_x^\dagger a_y^\dagger a_x a_y = \mathrm{d}\Gamma_2(|w_N|^{2-\varepsilon}) \le \big(\mathrm{d}\Gamma_2(|w_N|)\big)^{2-\varepsilon} \le \mathcal{R}^{2-\varepsilon} \tag{5-42}$$

by Lemma 12, we can bound

$$\begin{aligned}\iint \mathrm{d}x\,\mathrm{d}y\,|w_N(x-y)|^{2-\varepsilon} \Big\| a_x a_y \frac{\mathcal{R}^{-1/2}}{\mathcal{R}+s}\Phi_N \Big\|^2 &= \Big\langle \frac{\mathcal{R}^{-1/2}}{\mathcal{R}+s}\Phi_N, \mathrm{d}\Gamma_2(|w_N|^{2-\varepsilon}) \frac{\mathcal{R}^{-1/2}}{\mathcal{R}+s}\Phi_N \Big\rangle \\ &\le \Big\langle \Phi_N, \frac{\mathcal{R}^{1-\varepsilon}}{(\mathcal{R}+s)^2}\Phi_N \Big\rangle \le \frac{1}{(1+s)^{1+\varepsilon}}. \end{aligned} \tag{5-43}$$

In the last estimate we used that $\mathcal{R} \ge 1$. Moreover, using again the fact that $\mathcal{R}$ commutes with ω_2, we find with (5-23) that

$$\begin{aligned}\Big\| \frac{1}{\mathcal{R}+s}\omega_2 \Phi_{N,M} \Big\|^2 &\le \frac{C}{M^2(1+s)^2} \langle \Phi_{N,M}, \mathbb{1}^{>M/2} \Phi_{N,M} \rangle \\ &\le \frac{C}{M^2(1+s)^2} \Big\langle \Phi_{N,M}, \frac{2\mathcal{N}}{M}\Phi_{N,M} \Big\rangle \le \frac{C_{t,\varepsilon}}{M^3(1+s)^2} N^\varepsilon. \end{aligned} \tag{5-44}$$

Here in the last estimate, we used the kinetic bound in Lemma 8. Inserting (5-41), (5-43) and (5-44) in (5-40) we find that, for every constant $\varepsilon \in (0,1)$,

$$\begin{aligned}\mathcal{E}_{2,1} &\le C_{t,\varepsilon} \int_0^\infty \mathrm{d}s\,\sqrt{s}\sqrt{N^{2\beta(1+\varepsilon)}}\sqrt{\frac{1}{(1+s)^{1+\varepsilon}}}\sqrt{\frac{1}{M^3(1+s)^2}N^\varepsilon} \\ &\le C_{t,\varepsilon}\frac{N^{(1+\varepsilon)\beta+\varepsilon/2}}{M^{3/2}} \int_0^\infty \frac{\mathrm{d}s}{(1+s)^{1+\varepsilon/2}} \le C_{t,\varepsilon}\frac{N^{(1+\varepsilon)\beta+\varepsilon/2}}{M^{3/2}}. \end{aligned} \tag{5-45}$$

Estimate of $\mathcal{E}_{2,2}$. Similarly, for every constant $\varepsilon > 0$ small, by the Cauchy–Schwarz inequality,

$$\begin{aligned}\mathcal{E}_{2,2} &= \int_0^\infty \mathrm{d}s\,\sqrt{s} \iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,|w_N(x-y)|\,|w_N(x-z)|\,|u_N(x)|\,|u_N(y)| \\ &\qquad\qquad \times \Big| \Big\langle \Phi_N, \frac{\mathcal{R}^{-1/2}(\mathcal{N}+1)^{-1/2}}{\mathcal{R}+s} a_x^\dagger a_y^\dagger a_z^\dagger a_z \frac{(\mathcal{N}+3)^{1/2}}{\mathcal{R}+s}\omega_2\Phi_{N,M} \Big\rangle \Big| \\ &\le \|u_N\|_{L^\infty}^2 \int_0^\infty \mathrm{d}s\,\sqrt{s} \iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,|w_N(x-y)|\,|w_N(x-z)| \\ &\qquad\qquad \times \Big\| a_x a_y a_z \frac{\mathcal{R}^{-1/2}(\mathcal{N}+1)^{-1/2}}{\mathcal{R}+s}\Phi_N \Big\| \Big\| a_z \frac{(\mathcal{N}+3)^{1/2}}{\mathcal{R}+s}\omega_2\Phi_{N,M} \Big\| \\ &\le C_t \int_0^\infty \mathrm{d}s\,\sqrt{s} \Big(\iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,|w_N(x-y)|^{2-\varepsilon} \Big\| a_x a_y a_z \frac{\mathcal{R}^{-1/2}(\mathcal{N}+1)^{-1/2}}{\mathcal{R}+s}\Phi_N \Big\|^2 \Big)^{1/2} \\ &\qquad \times \Big(\int \mathrm{d}z\,\Big\| a_z \frac{(\mathcal{N}+3)^{1/2}}{\mathcal{R}+s}\omega_2\Phi_{N,M} \Big\|^2 \int \mathrm{d}x\,|w_N(x-z)|^2 \int \mathrm{d}y\,|w_N(x-y)|^\varepsilon \Big)^{1/2}. \end{aligned} \tag{5-46}$$

In the last estimate, we used the uniform bound $\|u_N\|_{L^\infty} \le C_t$ from Lemma 10. Using again (5-42) and $\mathcal{R} \ge 1$ we find that

$$\begin{aligned}\iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,|w_N(x-y)|^{2-\varepsilon}\left\|a_x a_y a_z \frac{\mathcal{R}^{-1/2}(\mathcal{N}+1)^{-1/2}}{\mathcal{R}+s}\Phi_N\right\|^2 \\ = \left\langle \frac{\mathcal{R}^{-1/2}(\mathcal{N}+1)^{-1/2}}{\mathcal{R}+s}\Phi_N, \mathrm{d}\Gamma_2(|w_N|^{2-\varepsilon})(\mathcal{N}-2)\frac{\mathcal{R}^{-1/2}(\mathcal{N}+1)^{-1/2}}{\mathcal{R}+s}\Phi_N\right\rangle \\ \le \left\langle \Phi_N, \frac{\mathcal{R}^{1-\varepsilon}}{(\mathcal{R}+s)^2}\Phi_N\right\rangle \le \frac{1}{(1+s)^{1+\varepsilon}}. \end{aligned} \tag{5-47}$$

Since w is bounded and compactly supported, we get

$$\int \mathrm{d}x\,|w_N(x-z)|^2 \int \mathrm{d}y\,|w_N(x-y)|^{\varepsilon} \le CN^{2\beta\varepsilon}. \tag{5-48}$$

Moreover, using (5-23) together with $\mathcal{N}^2 \le M\,\mathrm{d}\Gamma_1(1-\Delta)$ on $\mathcal{F}^{\le M}$ and Lemma 8, we have

$$\int \mathrm{d}z\left\|a_z \frac{(\mathcal{N}+3)^{1/2}}{\mathcal{R}+s}\omega_2\Phi_{N,M}\right\|^2 = \frac{C}{M^2}\left\langle \Phi_{N,M}, \frac{\mathcal{N}(\mathcal{N}+3)}{(\mathcal{R}+s)^2}\Phi_{N,M}\right\rangle \tag{5-49}$$

$$\le \frac{C}{M^2(1+s)^2}\langle \Phi_{N,M}, \mathcal{N}^2\Phi_{N,M}\rangle \le \frac{C_{t,\varepsilon}N^{\varepsilon}}{M(1+s)^2}. \tag{5-50}$$

Therefore, we deduce from (5-46) that

$$\mathcal{E}_{2,2} \le C_{t,\varepsilon}\int_0^\infty \mathrm{d}s\,\sqrt{s}\sqrt{\frac{1}{(1+s)^{1+\varepsilon}}}\sqrt{\frac{N^{\varepsilon}}{M(1+s)^2}N^{2\beta\varepsilon}} \le C_{t,\varepsilon}\frac{N^{(\beta+1/2)\varepsilon}}{\sqrt{M}}. \tag{5-51}$$

Putting (5-45) and (5-51) together, we conclude from (5-37) that

$$\mathcal{E}_2 \le C_{t,\varepsilon}\left(\frac{N^{(1+\varepsilon)\beta+\varepsilon/2}}{M^{3/2}} + \frac{N^{(\beta+1/2)\varepsilon}}{\sqrt{M}}\right). \tag{5-52}$$

Conclusion of (5-20). Inserting (5-35) and (5-52) in (5-27), we obtain (5-20).

Step 4. It remains to prove (5-21). Similarly to (5-25), we can write

$$\langle \Phi_N, [\mathbb{G}_2^*, f_M^2]\Phi_{N,M}\rangle = \iint \mathrm{d}x\,\mathrm{d}y\,w_N(x-y)\overline{u_N(x)u_N(y)}\langle \Phi_N, a_x a_y \widetilde{\omega}_2\Phi_{N,M}\rangle \tag{5-53}$$

with

$$\widetilde{\omega}_2 = \frac{\sqrt{(N-\mathcal{N}+2)(N-\mathcal{N}+1)}}{N-1}\left(f^2\left(\frac{\mathcal{N}-2}{M}\right) - f^2\left(\frac{\mathcal{N}}{M}\right)\right) \tag{5-54}$$

as an operator on $\mathcal{F}_\perp^{\le N}$. This term is much easier to estimate than (5-25) since now two annihilators hit $\Phi_{N,M}$. To be precise, we have

$$|\widetilde{\omega}_2| \le \frac{C}{M} \tag{5-55}$$

similarly to (5-23). Therefore, by the Cauchy–Schwarz inequality,

$$\begin{aligned}\big|\langle\Phi_N,[\mathbb{G}_2^*,f_M^2]\Phi_{N,M}\rangle\big| &\le \iint \mathrm{d}x\,\mathrm{d}y\,|w_N(x-y)|\,|u_N(x)|\,|u_N(y)|\,\|\Phi_N\|\,\|a_xa_y\widetilde{\omega}_2\Phi_{N,M}\|\\ &\le \|\Phi_N\|\bigg(\iint \mathrm{d}x\,\mathrm{d}y\,|w_N(x-y)|\,|u_N(x)|^2|u_N(y)|^2\bigg)^{1/2}\\ &\qquad\times\bigg(\iint \mathrm{d}x\,\mathrm{d}y\,|w_N(x-y)|\,\|a_xa_y\widetilde{\omega}_2\Phi_{N,M}\|^2\bigg)^{1/2}\\ &\le C_t\big\langle\Phi_{N,M},\mathrm{d}\Gamma_2(|w_N|)|\widetilde{\omega}_2|^2\Phi_{N,M}\big\rangle^{1/2}\\ &\le \frac{C_{t,\varepsilon}}{M^2}\langle\Phi_{N,M},N^\varepsilon\mathcal{N}\,\mathrm{d}\Gamma_1(1-\Delta)\Phi_{N,M}\rangle^{1/2}\le C_{t,\varepsilon}\frac{N^\varepsilon}{M}.\end{aligned}\tag{5-56}$$

Here we used again (5-31), Lemma 11 and the kinetic estimate in Lemma 8. Thus, (5-21) holds true. This completes the proof of Lemma 14. □

5.3. ***Estimate of the cubic terms.*** Concerning the cubic terms in (5-1), we have the following bounds:

Lemma 15. *Let $\Phi_N\in\mathcal{F}_\perp(t)$, $t\in[0,T_{\max})$ and $\varepsilon>0$. Then*

$$\big|\langle\Phi_N,[\mathbb{G}_3,f_M^2]\Phi_{N,M}\rangle\big|\le C_{t,\varepsilon}\bigg(\frac{1}{\sqrt{N}}+\frac{N^\beta}{M\sqrt{N}}\bigg)N^\varepsilon,\tag{5-57}$$

$$\big|\langle\Phi_N,[\mathbb{G}_3^*,f_M^2]\Phi_{N,M}\rangle\big|\le C_{t,\varepsilon}\frac{N^\varepsilon}{\sqrt{N}}.\tag{5-58}$$

Proof. Again, (5-57) is much more difficult than (5-58). We will proceed similarly to the quadratic terms.

Step 1. Analogously to (5-23), we define

$$\omega_3=\sqrt{1-\frac{\mathcal{N}-1}{N-1}}\bigg(f^2\Big(\frac{\mathcal{N}}{M}\Big)-f^2\Big(\frac{\mathcal{N}+1}{M}\Big)\bigg)\tag{5-59}$$

as an operator on $\mathcal{F}_\perp^{\le N}$, which satisfies

$$|\omega_3|\le\frac{C}{M}\mathbb{1}^{\le M}.\tag{5-60}$$

Moreover, similarly to (5-25) we can write

$$\langle\Phi_N,[\mathbb{G}_3,f_M^2]\Phi_{N,M}\rangle=\frac{1}{\sqrt{N}}\iint\mathrm{d}x\,\mathrm{d}y\,w_N(x-y)u_N(x)\langle\Phi_N,a_x^\dagger a_y^\dagger a_y\omega_3\Phi_{N,M}\rangle.\tag{5-61}$$

By decomposing $a_x^\dagger a_y^\dagger a_y$ as

$$a_x^\dagger a_y^\dagger a_y=\mathcal{R}^{-1/2}a_x^\dagger a_y^\dagger a_y\mathcal{R}^{1/2}+\mathcal{R}^{-1/2}[a_x^\dagger a_y^\dagger a_y,\mathcal{R}^{1/2}],\tag{5-62}$$

we obtain

$$\big|\langle\Phi_N,[\mathbb{G}_3,f_M^2]\Phi_{N,M}\rangle\big|\le\mathcal{E}_3+\mathcal{E}_4,\tag{5-63}$$

where

$$\mathcal{E}_3 = \frac{1}{\sqrt{N}} \iint \mathrm{d}x\, \mathrm{d}y\, |w_N(x-y)|\, |u_N(x)|\, |\langle \Phi_N, \mathcal{R}^{-1/2} a_x^\dagger a_y^\dagger a_y \mathcal{R}^{1/2} \omega_3 \Phi_{N,M}\rangle|, \tag{5-64}$$

$$\mathcal{E}_4 = \frac{1}{\sqrt{N}} \iint \mathrm{d}x\, \mathrm{d}y\, |w_N(x-y)|\, |u_N(x)|\, \big|\langle \Phi_N, \mathcal{R}^{-1/2} [a_x^\dagger a_y^\dagger a_y, \mathcal{R}^{1/2}] \omega_3 \Phi_{N,M}\rangle\big|. \tag{5-65}$$

Step 2. Let us first estimate $\mathcal{E}_3$. By the Cauchy–Schwarz inequality,

$$\begin{aligned}\mathcal{E}_3 &\le \frac{1}{\sqrt{N}} \iint \mathrm{d}x\, \mathrm{d}y\, |w_N(x-y)|\, |u_N(x)|\, \|a_x a_y \mathcal{R}^{-1/2}\Phi_N\|\, \|a_y \mathcal{R}^{1/2}\omega_3 \Phi_{N,M}\| \\ &\le \frac{\|u_N\|_{L^\infty}}{\sqrt{N}} \bigg(\iint \mathrm{d}x\, \mathrm{d}y\, |w_N(x-y)|\, \|a_x a_y \mathcal{R}^{-1/2}\Phi_N\|^2 \bigg)^{1/2} \\ &\qquad\qquad \times \bigg(\iint \mathrm{d}x\, \mathrm{d}y\, |w_N(x-y)|\, \|a_y \mathcal{R}^{1/2}\omega_3 \Phi_{N,M}\|^2 \bigg)^{1/2}. \end{aligned}\tag{5-66}$$

We can simplify the right-hand side using (3-26) and Lemma 10. Moreover, by (5-60) and Lemma 11,

$$|\omega_3|^2 \mathcal{N}\mathcal{R} \le \frac{C_\varepsilon N^\varepsilon}{M^2} \mathcal{N}^2\, \mathrm{d}\Gamma_1(1-\Delta) \le C_\varepsilon N^\varepsilon\, \mathrm{d}\Gamma_1(1-\Delta) \tag{5-67}$$

on $\mathcal{F}^{\le M}$. Combining this with the kinetic bound in Lemma 8, we find that

$$\begin{aligned}\iint \mathrm{d}x\, \mathrm{d}y\, |w_N(x-y)|\, \|a_y \mathcal{R}^{1/2}\omega_3 \Phi_{N,M}\|^2 &= \|w_N\|_{L^1} \langle \Phi_{N,M}, |\omega_3|^2 \mathcal{N}\mathcal{R}\Phi_{N,M}\rangle \\ &\le C_\varepsilon N^{2\varepsilon}\end{aligned}\tag{5-68}$$

for every constant $\varepsilon > 0$. Therefore, we deduce from (5-66) that

$$\mathcal{E}_3 \le \frac{C_{t,\varepsilon} N^\varepsilon}{\sqrt{N}}. \tag{5-69}$$

Step 3. Now we turn to the complicated error term $\mathcal{E}_4$. A direct computation shows that

$$\big[\mathrm{d}\Gamma_2(|w_N|), a_x^\dagger a_y^\dagger a_y\big] = |w_N(x-y)| a_x^\dagger a_y^\dagger a_y + \int \mathrm{d}z\, |w_N(x-z)| a_x^\dagger a_y^\dagger a_z^\dagger a_z a_y, \tag{5-70}$$

and with (3-28) this yields

$$\begin{aligned}[\mathcal{R}^{1/2}, a_x^\dagger a_y^\dagger a_y] &= \frac{1}{\pi} \int_0^\infty \mathrm{d}s\, \frac{\sqrt{s}}{\mathcal{R}+s} |w_N(x-y)| a_x^\dagger a_y^\dagger a_y \frac{1}{\mathcal{R}+s} \\ &\quad + \frac{1}{\pi} \int_0^\infty \mathrm{d}s \int \mathrm{d}z\, \frac{\sqrt{s}}{\mathcal{R}+s} |w_N(x-z)| a_x^\dagger a_y^\dagger a_z^\dagger a_z a_y \frac{1}{\mathcal{R}+s}.\end{aligned}\tag{5-71}$$

Thus, by the triangle inequality and the bound $\|u_N\|_{L^\infty} \le C_t$ from Lemma 10, we can split

$$\begin{aligned}\mathcal{E}_4 &= \frac{1}{\sqrt{N}} \iint \mathrm{d}x\, \mathrm{d}y\, |w_N(x-y)|\, |u_N(x)|\, \big|\langle \Phi_N, \mathcal{R}^{-1/2} [a_x^\dagger a_y^\dagger a_y, \mathcal{R}^{1/2}] \omega_3 \Phi_{N,M}\rangle\big| \\ &\le C_t(\mathcal{E}_{4,1} + \mathcal{E}_{4,2}),\end{aligned}\tag{5-72}$$

where

$$\mathcal{E}_{4,1} = \frac{1}{\sqrt{N}} \int_0^\infty \mathrm{d}s\, \sqrt{s} \iint \mathrm{d}x\, \mathrm{d}y\, |w_N(x-y)|^2 \left| \left\langle \Phi_N, \frac{\mathcal{R}^{-1/2}}{\mathcal{R}+s} a_x^\dagger a_y^\dagger a_y \frac{1}{\mathcal{R}+s} \omega_3 \Phi_{N,M} \right\rangle \right|, \tag{5-73}$$

$$\mathcal{E}_{4,2} = \frac{1}{\sqrt{N}} \int_0^\infty \mathrm{d}s\, \sqrt{s} \iiint \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, |w_N(x-y)|\, |w_N(x-z)| \times \left| \left\langle \Phi_N, \frac{\mathcal{R}^{-1/2}}{\mathcal{R}+s} a_x^\dagger a_y^\dagger a_z^\dagger a_z a_y \frac{1}{\mathcal{R}+s} \omega_3 \Phi_{N,M} \right\rangle \right|. \tag{5-74}$$

Estimate of $\mathcal{E}_{4,1}$. By the Cauchy–Schwarz inequality we have

$$\begin{aligned} \mathcal{E}_{4,1} &\le \frac{1}{\sqrt{N}} \int_0^\infty \mathrm{d}s\, \sqrt{s} \iint \mathrm{d}x\, \mathrm{d}y\, |w_N(x-y)|^2 \left\| a_x a_y \frac{\mathcal{R}^{-1/2}}{\mathcal{R}+s} \Phi_N \right\| \left\| a_y \frac{1}{\mathcal{R}+s} \omega_3 \Phi_{N,M} \right\| \\ &\le \frac{1}{\sqrt{N}} \int_0^\infty \mathrm{d}s\, \sqrt{s} \left(\iint \mathrm{d}x\, \mathrm{d}y\, |w_N(x-y)|^{2-\varepsilon} \left\| a_x a_y \frac{\mathcal{R}^{-1/2}}{\mathcal{R}+s} \Phi_N \right\|^2 \right)^{1/2} \\ &\qquad \times \left(\iint \mathrm{d}x\, \mathrm{d}y\, |w_N(x-y)|^{2+\varepsilon} \left\| a_y \frac{1}{\mathcal{R}+s} \omega_3 \Phi_{N,M} \right\|^2 \right)^{1/2}. \end{aligned} \tag{5-75}$$

The right-hand side can be simplified using (5-43) and the estimate

$$\begin{aligned} &\iint \mathrm{d}x\, \mathrm{d}y\, |w_N(x-y)|^{2+\varepsilon} \left\| a_y \frac{1}{\mathcal{R}+s} \omega_3 \Phi_{N,M} \right\|^2 \\ &\qquad = \big\| |w_N|^{2+\varepsilon} \big\|_{L^1} \left\langle \Phi_{N,M}, \frac{\mathcal{N} |\omega_3|^2}{(\mathcal{R}+s)^2} \Phi_{N,M} \right\rangle \le C_{t,\varepsilon} N^{(1+\varepsilon)2\beta} \frac{N^\varepsilon}{M^2 (1+s)^2}, \end{aligned} \tag{5-76}$$

which follows from (5-60), $\mathcal{R} \ge 1$, and the kinetic bound in Lemma 8. Altogether, this gives

$$\begin{aligned} \mathcal{E}_{4,1} &\le \frac{C_{t,\varepsilon}}{\sqrt{N}} \int_0^\infty \mathrm{d}s\, \sqrt{s} \sqrt{\frac{1}{(1+s)^{1+\varepsilon}}} \sqrt{N^{(1+\varepsilon)2\beta} \frac{N^\varepsilon}{M^2(1+s)^2}} \\ &\le C_{t,\varepsilon} \frac{N^{(1+\varepsilon)\beta+\varepsilon/2}}{\sqrt{N} M}. \end{aligned} \tag{5-77}$$

Estimate of $\mathcal{E}_{4,2}$. By the Cauchy–Schwarz inequality,

$$\begin{aligned} \mathcal{E}_{4,2} &= \frac{1}{\sqrt{N}} \int_0^\infty \mathrm{d}s\, \sqrt{s} \iiint \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, |w_N(x-y)|\, |w_N(x-z)| \\ &\qquad \times \left| \left\langle \Phi_N, \frac{\mathcal{R}^{-1/2} (\mathcal{N}+2)^{-1/2}}{\mathcal{R}+s} a_x^\dagger a_y^\dagger a_z^\dagger a_z a_y \frac{(\mathcal{N}+3)^{1/2}}{\mathcal{R}+s} \omega_3 \Phi_{N,M} \right\rangle \right| \\ &\le \frac{1}{\sqrt{N}} \int_0^\infty \mathrm{d}s\, \sqrt{s} \iiint \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, |w_N(x-y)|\, |w_N(x-z)| \\ &\qquad \times \left\| a_x a_y a_z \frac{\mathcal{R}^{-1/2} (\mathcal{N}+2)^{-1/2}}{\mathcal{R}+s} \Phi_N \right\| \left\| a_y a_z \frac{(\mathcal{N}+3)^{1/2}}{\mathcal{R}+s} \omega_3 \Phi_{N,M} \right\| \\ &\le \frac{1}{\sqrt{N}} \int_0^\infty \mathrm{d}s\, \sqrt{s} \left(\iiint \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, |w_N(x-y)|^{2-\varepsilon} \left\| a_x a_y a_z \frac{\mathcal{R}^{-1/2} (\mathcal{N}+2)^{-1/2}}{\mathcal{R}+s} \Phi_N \right\|^2 \right)^{1/2} \\ &\qquad \times \left(\iiint \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, |w_N(x-y)|^{\varepsilon} |w_N(x-z)|^2 \left\| a_y a_z \frac{(\mathcal{N}+3)^{1/2}}{\mathcal{R}+s} \omega_3 \Phi_{N,M} \right\|^2 \right)^{1/2}. \end{aligned} \tag{5-78}$$

We can bound

$$\iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,|w_N(x-y)|^{2-\varepsilon}\left\|a_x a_y a_z \frac{\mathcal{R}^{-1/2}(\mathcal{N}+2)^{-1/2}}{\mathcal{R}+s}\Phi_N\right\|^2 = \iint \mathrm{d}x\,\mathrm{d}y\,|w_N(x-y)|^{2-\varepsilon}\left\|a_x a_y \frac{\mathcal{R}^{-1/2}}{\mathcal{R}+s}\Phi_N\right\|^2 \le \frac{1}{(1+s)^{1+\varepsilon}} \tag{5-79}$$

as in (5-43). Since w is bounded and compactly supported, we have the pointwise estimate

$$\begin{aligned}|w_N(x-y)|^{\varepsilon}|w_N(x-z)|^2 &= |w_N(x-y)|^{\varepsilon}|w_N(x-z)|^2 \mathbb{1}_{\{|y-z|\le CN^{-\beta}\}}\\ &\le CN^{4\beta}|w_N(x-y)|^{\varepsilon}\mathbb{1}_{\{|y-z|\le CN^{-\beta}\}}.\end{aligned} \tag{5-80}$$

Moreover, the operators $\mathrm{d}\Gamma_2(\mathbb{1}_{\{|y-z|\le CN^{-\beta}\}})$, $\mathcal{R}$, $\mathcal{N}$ and ω_3 all commute. Consequently, using $\mathcal{R}\ge 1$ and (5-60), we can bound

$$\begin{aligned}\iint \mathrm{d}y\,\mathrm{d}z\,\mathbb{1}_{\{|y-z|\le CN^{-\beta}\}}\left\|a_y a_z \frac{(\mathcal{N}+3)^{1/2}}{\mathcal{R}+s}\omega_3\Phi_{N,M}\right\|^2 &= \left\langle \Phi_{N,M}, \mathrm{d}\Gamma_2(\mathbb{1}_{\{|y-z|\le CN^{-\beta}\}})\frac{\mathcal{N}+3}{(\mathcal{R}+s)^2}|\omega_3|^2\Phi_{N,M}\right\rangle\\ &\le \frac{C}{M(1+s)^2}\langle \Phi_{N,M}, \mathrm{d}\Gamma_2(\mathbb{1}_{\{|y-z|\le CN^{-\beta}\}})\Phi_{N,M}\rangle.\end{aligned} \tag{5-81}$$

Using Lemma 11 with $s=2\beta/(2\beta-\varepsilon)$, we obtain

$$\mathrm{d}\Gamma_2(\mathbb{1}_{\{|y-z|\le CN^{-\beta}\}}) \le C_\varepsilon N^{\varepsilon}N^{-2\beta}\mathcal{N}\,\mathrm{d}\Gamma_1(1-\Delta) \tag{5-82}$$

for every $\varepsilon>0$. Therefore, together with Lemma 8, we deduce that

$$\begin{aligned}\iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,|w_N(x-y)|^{\varepsilon}|w_N(x-z)|^2\left\|a_y a_z \frac{(\mathcal{N}+3)^{1/2}}{\mathcal{R}+s}\omega_3\Phi_{N,M}\right\|^2 &\le \frac{CN^{4\beta}}{M(1+s)^2}\big\||w_N|^{\varepsilon}\big\|_{L^1}\langle \Phi_{N,M}, \mathrm{d}\Gamma_2(\mathbb{1}_{\{|y-z|\le CN^{-\beta}\}})\Phi_{N,M}\rangle\\ &\le \frac{C_{t,\varepsilon}N^{(2\beta+2)\varepsilon}}{(1+s)^2}.\end{aligned} \tag{5-83}$$

Inserting (5-79) and (5-83) in (5-78) we find that

$$\mathcal{E}_{4,2} = \frac{C_{t,\varepsilon}}{\sqrt{N}}\int_0^\infty \mathrm{d}s\,\sqrt{s}\sqrt{\frac{1}{(1+s)^{1+\varepsilon}}}\sqrt{\frac{N^{(2\beta+2)\varepsilon}}{(1+s)^2}} \le \frac{C_{t,\varepsilon}N^{(\beta+1)\varepsilon}}{\sqrt{N}} \tag{5-84}$$

for every constant $\varepsilon>0$. From (5-77) and (5-84) we get

$$\mathcal{E}_4 \le C_{t,\varepsilon}\left(\frac{N^\beta}{\sqrt{N}M}+\frac{1}{\sqrt{N}}\right)N^{\varepsilon}. \tag{5-85}$$

Conclusion of (5-57). Given the decomposition (5-63), the desired bound (5-57) follows immediately from (5-69) and (5-85).

Step 4. It remains to prove (5-58). Similarly to (5-61), we can write

$$\langle \Phi_N, [\mathbb{G}_3^*, f_M^2]\Phi_{N,M}\rangle = \frac{1}{\sqrt{N}} \iint \mathrm{d}x\,\mathrm{d}y\, w_N(x-y)\overline{u_N(x)}\langle \Phi_N, a_y^\dagger a_x a_y \widetilde{\omega}_3 \Phi_{N,M}\rangle \tag{5-86}$$

with

$$\widetilde{\omega}_3 = \sqrt{1-\frac{\mathcal{N}}{N-1}}\left(f^2\left(\frac{\mathcal{N}-1}{M}\right) - f^2\left(\frac{\mathcal{N}}{M}\right)\right) \tag{5-87}$$

as an operator on $\mathcal{F}_\perp^{\leq N}$, which satisfies

$$|\widetilde{\omega}_3| \leq \frac{C}{M}\mathbb{1}^{\leq M}. \tag{5-88}$$

By the Cauchy–Schwarz inequality,

$$\begin{aligned}
&\big|\langle \Phi_N, [\mathbb{G}_3^*, f_M^2]\Phi_{N,M}\rangle\big| \\
&\quad= \frac{1}{\sqrt{N}}\left|\iint \mathrm{d}x\,\mathrm{d}y\, w_N(x-y)\overline{u_N(x)}\langle (\mathcal{N}+1)^{-1/2}\Phi_N, a_y^\dagger a_x a_y \mathcal{N}^{1/2}\widetilde{\omega}_3\Phi_{N,M}\rangle\right| \\
&\quad\leq \frac{\|u_N\|_{L^\infty}}{\sqrt{N}} \iint \mathrm{d}x\,\mathrm{d}y\, |w_N(x-y)|\,\|a_y(\mathcal{N}+1)^{-1/2}\Phi_N\|\,\|a_x a_y \mathcal{N}^{1/2}\widetilde{\omega}_3\Phi_{N,M}\| \\
&\quad\leq \frac{C_t}{\sqrt{N}}\left(\iint \mathrm{d}x\,\mathrm{d}y\, |w_N(x-y)|\,\|a_y(\mathcal{N}+1)^{-1/2}\Phi_N\|^2\right)^{1/2} \\
&\qquad\qquad\qquad\times\left(\iint \mathrm{d}x\,\mathrm{d}y\, |w_N(x-y)|\,\|a_x a_y\mathcal{N}^{1/2}\widetilde{\omega}_3\Phi_{N,M}\|^2\right)^{1/2} \\
&\quad= \frac{C_t}{\sqrt{N}}\langle \Phi_N, \|w_N\|_{L^1}\mathcal{N}(\mathcal{N}+1)^{-1}\Phi_N\rangle^{1/2}\big\langle \Phi_{N,M}, \mathrm{d}\Gamma_2(|w_N|)\mathcal{N}|\widetilde{\omega}_3|^2\Phi_{N,M}\big\rangle^{1/2} \\
&\quad\leq \frac{C_{t,\varepsilon}N^\varepsilon}{\sqrt{N}}\|\Phi_N\|\langle \Phi_{N,M}, \mathrm{d}\Gamma_1(1-\Delta)\mathcal{N}^2\mathbb{1}^{\leq M}M^{-2}\Phi_{N,M}\rangle^{1/2} \leq \frac{C_{t,\varepsilon}}{\sqrt{N}}N^{2\varepsilon},
\end{aligned} \tag{5-89}$$

where we used Lemma 11 and the kinetic bound in Lemma 8. This concludes the proof of (5-58) and thus of Lemma 15. □

5.4. ***Conclusion of Proposition 9.*** First, inserting the bounds from Lemmas 13, 14 and 15 in (5-1), and using $M \leq N$ to simplify some error terms, we find that the desired propagation bound (3-17) holds true, namely that

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}\langle \Phi_N(t), f_M^2\Phi_{N,M}(t)\rangle\right| \leq C_{t,\varepsilon}N^\varepsilon\left(\frac{1}{\sqrt{M}} + \frac{N^\beta}{M^{3/2}}\right).$$

Proof of Proposition 9. Define

$$\mathcal{B}(t) := 1 - \Re\langle \Phi_N(t), f_M^2\Phi_{N,M}(t)\rangle. \tag{5-90}$$

By (2-27) and by definition (3-16) of f_M, we obtain

$$\mathcal{B}(0) = \langle \Phi_0, (1-f_M^2)\Phi_0\rangle \leq \langle \Phi_0, \mathbb{1}^{>M/2}\Phi_0\rangle \leq \frac{2}{M}\langle \Phi_0, \mathcal{N}\Phi_0\rangle \leq \frac{C}{M}. \tag{5-91}$$

Combining this with (3-17), we can therefore bound

$$\mathcal{B}(t) \le C_{t,\varepsilon}\left(\frac{1}{\sqrt{M}} + \frac{N^{\beta}}{M^{3/2}}\right) \tag{5-92}$$

for all $t \in [0, T_{\max})$ and $\varepsilon > 0$.

To conclude Proposition 9, we prove that

$$\|\Phi_N(t) - \Phi_{N,M}(t)\|^2 \le 4\mathcal{B}(t). \tag{5-93}$$

Let us drop the time dependence from the notation for simplicity and write

$$\begin{aligned}\|\Phi_N - \Phi_{N,M}\|^2 &= \|\Phi_N\|^2 + \|\Phi_{N,M}\|^2 - 2\,\Re\langle\Phi_N, \Phi_{N,M}\rangle \\ &\le 2 - 2\,\Re\langle\Phi_N, f_M^2\Phi_{N,M}\rangle - 2\,\Re\langle\Phi_N, g_M^2\Phi_{N,M}\rangle.\end{aligned} \tag{5-94}$$

Here we defined $g_M^2 = 1 - f_M^2$ and used that $\|\Phi_N\| \le 1$, $\|\Phi_{N,M}\| \le 1$. Moreover, by the Cauchy–Schwarz inequality,

$$\begin{aligned}2\,|\langle\Phi_N, g_M^2\Phi_{N,M}\rangle| &\le \|g_M\Phi_N\|^2 + \|g_M\Phi_{N,M}\|^2 \\ &\le 2 - \|f_M\Phi_N\|^2 - \|f_M\Phi_{N,M}\|^2 \le 2 - 2\,|\langle\Phi_N, f_M^2\Phi_{N,M}\rangle|.\end{aligned} \tag{5-95}$$

Thus, (5-93) follows immediately. □

6. Conclusion of the main theorems

6.1. *Proof of Theorem 5.* Let $M = N^{1-\delta}$ with $\delta \in (0, 1)$. Recall that $\Phi_N(t)$ and $\Phi_{N,M}(t)$ are defined in (3-6) and (3-11), respectively. Since $U_N : \mathfrak{H}^N \to \mathcal{F}_\perp^{\le N}(t)$ is a unitary transformation, the desired norm approximation (2-29) is equivalent to

$$\|\Phi_N(t) - \Phi(t)\|^2 \le C_t N^{-\alpha_2}. \tag{6-1}$$

By Lemma 8 and Proposition 9, we can bound

$$\begin{aligned}\|\Phi_N(t) - \Phi(t)\|^2 &\le 2\,\|\Phi_N(t) - \Phi_{N,M}(t)\|^2 + 2\,\|\Phi_{N,M}(t) - \Phi(t)\|^2 \\ &\le C_{t,\varepsilon}N^{\varepsilon}\left(\frac{1}{\sqrt{M}} + \frac{N^{\beta}}{M^{3/2}} + \sqrt{\frac{M}{N}}\right) \\ &= C_{t,\varepsilon}N^{\varepsilon}(N^{(\delta-1)/2} + N^{3\delta/2+\beta-3/2} + N^{-\delta/2})\end{aligned} \tag{6-2}$$

for all $t \in [0, T_{\max})$ and $\varepsilon > 0$. Here we have put back $M = N^{1-\delta}$ at the end. The optimal choice for δ is

$$\delta = \begin{cases} \frac{1}{4}(3-2\beta) & \text{if } \beta \ge \frac{1}{2}, \\ \frac{1}{2} & \text{if } \beta \le \frac{1}{2}, \end{cases} \tag{6-3}$$

which implies (6-1) with every $0 < \alpha_2 < \min\left(\frac{1}{8}, \frac{1}{16}(3-2\beta)\right)$. □

6.2. ***Proof of Theorem 3.*** The implication of the convergence of density matrices from the norm convergence is well-known; see, e.g., [Lewin et al. 2015a, Corollary 2]. Here we recall a quick derivation for the reader's convenience. We will again drop the time dependence from the notation. Let $q = 1 - p = 1 - |u_N\rangle\langle u_N|$ as in (2-25). By using the rules (3-5) (see also Remark 6), Theorem 5 and Lemma 7, it follows that

$$N\,\mathrm{Tr}(q\gamma^{(1)}_{\Psi_N}q) = \|\sqrt{\mathcal{N}}\Phi_N\|^2 \le 2\,\|\sqrt{\mathcal{N}}\mathbb{1}^{\le N}(\Phi_N - \Phi)\|^2 + 2\,\|\sqrt{\mathcal{N}}\Phi\|^2 \le C_{t,\varepsilon}(N^{1-2\alpha_2} + N^{\varepsilon}).$$

Then by the triangle and Cauchy–Schwarz inequalities, we conclude that

$$\begin{aligned}\mathrm{Tr}\left|\gamma^{(1)}_{\Psi_N} - |\varphi\rangle\langle\varphi|\right| &\le \mathrm{Tr}\left|p - |\varphi\rangle\langle\varphi|\right| + \mathrm{Tr}\,|p(\gamma^{(1)}_{\Psi_1} - 1)p| + \mathrm{Tr}\,|q\gamma^{(1)}_{\Psi_1}q| + 2\,\mathrm{Tr}\,|p\gamma^{(1)}_{\Psi_1}q| \\ &\le 2\,\|u_N - \varphi\|_{L^2} + 2\,\mathrm{Tr}(q\gamma^{(1)}_{\Psi_1}q) + 2\sqrt{\mathrm{Tr}\,|q\gamma^{(1)}_{\Psi_1}q|}\sqrt{\mathrm{Tr}\,|p\gamma^{(1)}_{\Psi_1}p|} \\ &\le C_{t,\varepsilon}(N^{-\beta} + N^{-\alpha_2}N^{(\varepsilon-1)/2}).\end{aligned}$$

Here we used $\mathrm{Tr}(p) = \mathrm{Tr}\,\gamma^{(1)}_{\Psi_N} = 1$ and Lemma 10. Thus (2-6) holds for $\alpha_1 = \min(\beta, \alpha_2)$. □

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LOWER BOUNDS ON FIBERED YANG–MILLS FUNCTIONALS: GENERIC NEFNESS AND SEMISTABILITY OF DIRECT IMAGES

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The main goal of this paper is to generalize a part of the relationship between mean curvature and Harder–Narasimhan filtrations of holomorphic vector bundles to arbitrary polarized fibrations. More precisely, for a polarized family of complex projective manifolds, we establish lower bounds on a fibered version of Yang–Mills functionals in terms of the Harder–Narasimhan slopes of direct image sheaves associated with high tensor powers of the polarization. We discuss the optimality of these lower bounds and, as an application, provide an analytic characterisation of a fibered version of generic nefness. As another application, we refine the existent obstructions for finding metrics with constant horizontal mean curvature. The study of the semiclassical limit of Hermitian Yang–Mills functionals lies at the heart of our approach.

1. Introduction

Consider a holomorphic submersion $\pi : X \to B$ between compact complex manifolds X and B of dimensions $n+m$ and m, respectively, $n, m \in \mathbb{N}$. Let L be a holomorphic line bundle over X, which is relatively ample with respect to π. We fix a *Gauduchon Hermitian form* ω_B on B, i.e., a positive $(1,1)$-form, such that $\partial\bar{\partial}\omega_B^{m-1} = 0$; see [Gauduchon 1977]. The main goal of this paper is to study the relationship between the so-called horizontal mean curvature of the fibration, which is a certain differential-geometric invariant of the family defined using ω_B, and Harder–Narasimhan ω_B-slopes of direct images $E_k := R^0\pi_* L^k$, which are algebraic invariants.

More precisely, consider a Hermitian metric h^L on L, which is positive along the fibers of π. We denote by

$$\omega(h^L) := \frac{\sqrt{-1}}{2\pi} R^L$$

the first Chern form of (L, h^L), where R^L is the curvature of the Chern connection. When h^L is clear from the context, we omit it from the above notation.

As ω is positive along the fibers, it provides a (smooth) decomposition of the tangent space TX of X into the vertical component $T^V X$, corresponding to the tangent space of the fibers, and the horizontal component $T^H X$, corresponding to the orthogonal complement of $T^V X$ with respect to ω. The form ω then decomposes as $\omega = \omega_V + \omega_H$, $\omega_V \in \mathscr{C}^\infty\big(X, \bigwedge^{1,1} T^{V*}X\big)$, $\omega_H \in \mathscr{C}^\infty\big(X, \bigwedge^{1,1} T^{H*}X\big)$. Upon the natural identification of $T^H X$ with $\pi^* TB$, we may view ω_H as an element from $\mathscr{C}^\infty\big(X, \bigwedge^{1,1} \pi^* T^* B\big)$.

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The triple $(\pi, \omega, T^H X)$ then defines a *Kähler fibration* in the sense of [Bismut et al. 1988, Definition 1.4]. We define the *horizontal mean curvature*, $\bigwedge_{\omega_B} \omega_H(h^L) \in \mathscr{C}^\infty(X)$, as

$$\bigwedge_{\omega_B} \omega_H(h^L) := \frac{\omega_H(h^L) \wedge \omega_B^{m-1}}{\omega_B^m}. \tag{1-1}$$

We say that h^L is *fibered Einstein* if $\bigwedge_{\omega_B} \omega_H(h^L)$ is a constant. By decomposition into horizontal and vertical components, it is easy to see that this condition is equivalent to

$$\omega(h^L)^{n+1} \wedge \pi^* \omega_B^{m-1} = c \cdot \omega(h^L)^n \wedge \pi^* \omega_B^m, \tag{1-2}$$

where c is a constant. By integrating (1-2), we see that the constant c is independent of h^L, since ω_B is Gauduchon; see Section 4 for details. Remark the similarity of (1-2) with the J-equation if $m = 1$, and with optimal symplectic connection equation of Dervan and Sektnan [2021, Proposition 2.7] if the fibers are Fano. For families of manifolds given by projectivizations of vector bundles, the condition (1-2) was introduced by Kobayashi [1996], who called such metrics *Finsler–Einstein* metrics; then Feng, Liu, and Wan [Feng et al. 2019] generalized it for general Kähler submersions, and called such metrics *geodesic Einstein* metrics. If instead of a closed manifold B, one considers manifolds with boundary, equation (1-2) was studied extensively in the past: If B is a 1-dimensional annuli and $c = 0$, this is a geodesic equation in Mabuchi space [1987]; see [Semmes 1992] or [Donaldson 1999]. If B is a bounded smooth strongly pseudoconvex domain in $\mathbb{C}^n$, $c = 0$ and ω_B is the standard Kähler form, (1-2) was called Wess–Zumino–Witten equation in [Donaldson 1999] due to its connection with [Witten 1983].

Remark that in the important case when $X := \mathbb{P}(E^*)$ for some holomorphic vector bundle E over B, $L := \mathscr{O}(1)$, and h^L is induced by a Hermitian metric h^E on E, (L, h^L) is fibered Einstein if and only if (E, h^E) is Hermite–Einstein; see Remark 3.4 for details.

The first main observation of this paper is that the correspondence between fibered Einstein and Hermite Einstein equations is much tighter. Indeed, as we shall see, relying on the work of Ma and Zhang [2023], see Theorem 2.2, the fibered Einstein equation for L is *mutatis mutandis* the semiclassical limit (i.e., $k \to \infty$) of the Hermite–Einstein equation for $E_k := R^0\pi_* L^k$. Let us now explain the first manifestation of this correspondence.

Recall that a *slope* (or ω_B-slope) of a coherent sheaf $\mathscr{E}$ over B is defined as $\mu(\mathscr{E}) := \deg(\mathscr{E})/\mathrm{rk}(\mathscr{E})$, where the degree, $\deg(\mathscr{E})$, is given by $\deg(\mathscr{E}) := \int_B [c_1(\det \mathscr{E})] \cdot [\omega_B^{m-1}]$; here and after the intersection product is for Bott–Chern and Aeppli cohomology classes, ω_B^{m-1} represents an Aeppli cohomology class since ω_B is Gauduchon, see Section 4 for details, and $\det \mathscr{E}$ is the Knudsen–Mumford determinant of $\mathscr{E}$, see [Knudsen and Mumford 1976]. A torsion-free coherent sheaf $\mathscr{E}$ is called *semistable* or *ω_B-semistable* if for every coherent subsheaf $\mathcal{F}$ of $\mathscr{E}$, verifying $\mathrm{rk}(\mathcal{F}) > 0$, we have $\mu(\mathcal{F}) \leq \mu(\mathscr{E})$. When $\dim B = 1$, these notions clearly do not depend on ω_B.

Theorem 1.1. *Assume that L admits an approximate fibered Einstein metric*, i.e., *there is $c \in \mathbb{R}$ such that, for any $\epsilon > 0$, there is a relatively positive metric h_ϵ^L on L, verifying the bound*

$$\left| \bigwedge_{\omega_B} \omega_H(h_\epsilon^L) - c \right| < \epsilon. \tag{1-3}$$

Then the vector bundles $E_k := R^0\pi_* L^k$ are ***asymptotically semistable****, i.e., for any quotient sheaves $\mathcal{Q}_k$ of E_k, $\mathrm{rk}(\mathcal{Q}_k) > 0$, and any $\epsilon > 0$ for k big enough, we have $\mu(\mathcal{Q}_k) \geq \mu(E_k) - \epsilon k$.*

Remark 1.2. (a) It is likely that there is an even closer relationship between fibered Einstein metrics on L and Hermite Einstein metrics on E_k, paralleling the known correspondence between constant scalar curvature and balanced metrics; see [Donaldson 2001].

(b) We conjecture that the converse of Theorem 1.1 also holds. In fact, this will follow as a special case of a more general conjecture, which we discuss after Theorem 1.7.

When Theorem 1.1 is applied to $\pi : \mathbb{P}(E^*) \to B$ for some vector bundle E over B, and $L := \mathscr{O}(1)$, due to a precise relation between the slopes of $\mathrm{Sym}^k E = R^0\pi_* L^k$, $k \in \mathbb{N}$, and E, see [Chen 2011, §3.2], we recover the well-known fact, see [Kobayashi 2014, Theorem 6.10.13], that if E admits approximate Hermite–Einstein metrics, then E is semistable.

The asymptotic semistability condition from Theorem 1.1 seems rather difficult to verify at first sight. We will now discuss some numerical obstructions for it. More precisely, for an irreducible complex analytic subspace $Y \subset X$ of dimension $k+m$, $k \geq 0$, such that the restriction of π to Y, $\pi|_Y : Y \to B$, is a surjection, we define the ω_B-slope, $\mu(Y)$, as

$$\mu(Y) = \frac{1}{k+1} \cdot \frac{\int_Y [c_1(L)^{k+1}] \cdot [\omega_B^{m-1}]}{\int_Y [c_1(L)^k] \cdot [\omega_B^m]}. \tag{1-4}$$

By the Serre vanishing theorem, for $k \in \mathbb{N}^*$ big enough, the sheaf $\mathcal{Q}_k := R^0\pi|_{Y,*} L|_Y^k$ can be realized as a quotient of E_k through the restriction map; see the proof of Proposition 4.7 for details. By the asymptotic version of the Riemann–Roch–Grothendieck theorem, see Theorem 4.1, which we establish in our singular setting, we can calculate the asymptotics of the slopes of $\mathcal{Q}_k$ and E_k, as $k \to \infty$. By comparing the asymptotics of these slopes, we obtain in Section 4 the following result.

Theorem 1.3. *If the vector bundles E_k are asymptotically semistable, then X is* ***numerically semistable****, i.e., for any Y as above, we have $\mu(Y) \geq \mu(X)$. Moreover, if $\dim B = 1$, then asymptotic semistability of E_k is equivalent to numerical semistability of X.*

Remark 1.4. A combination of Theorems 1.1 and 1.3 shows that existence of approximate fibered Einstein metrics on L implies $\mu(Y) \geq \mu(X)$ for Y above. Feng, Liu, and Wan [Feng et al. 2019, Theorem 2.2], see also [Wan and Wang 2020], established this by different means under an assumption, requiring among others that the projection of the singular locus of Y to B has codimension at least 2.

As we explain later, Theorem 1.1 is a direct consequence of a more refined result concerning lower bounds on fibered Yang–Mills functionals. More precisely, for a relatively Kähler $(1,1)$-form ω on X and any $c \in \mathbb{R}$, $p \in [1, +\infty[$, we define the fibered Yang–Mills functional as

$$\begin{aligned} \mathrm{FYM}_{p,c}(\pi, \omega) &:= \int_X \big| \wedge_{\omega_B} \omega_H(x) - c \big|^p \omega^n \wedge \pi^* \omega_B^m(x), \\ \mathrm{FYM}_{+\infty,c}(\pi, \omega) &:= \sup_{x \in X} \big| \wedge_{\omega_B} \omega_H(x) - c \big|. \end{aligned} \tag{1-5}$$

We also let $\mathrm{FYM}_{p,c}(\pi, h^L) := \mathrm{FYM}_{p,c}(\pi, c_1(L, h^L))$ for a relatively positive metric h^L on L. We will now show that asymptotic Harder–Narasimhan slopes of E_k, as $k \to \infty$, yield lower bounds for these functionals. To readers familiar with Hermitian Yang–Mills theory, see [Atiyah and Bott 1983, Proposition 8.20; Donaldson 1985, Proposition 5; Daskalopoulos and Wentworth 2004, §§2.3, 2.4], this will sound very natural. Indeed, again from the work of Ma and Zhang [2023], one can view the horizontal mean curvature of L as the semiclassical limit (i.e., $k \to \infty$) of the mean curvature of E_k. From this, we establish the lower bounds on the fibered Yang–Mills functionals through the limits of the lower bounds on the Hermitian Yang–Mills functionals of E_k.

To explain this in detail, recall first that any torsion-free coherent sheaf $\mathscr{E}$ on $(B, [\omega_B])$ admits a unique filtration by subsheaves $\mathscr{E}_i$, $i = 1, \dots, s$, also called a *Harder–Narasimhan filtration*,

$$\mathscr{E} = \mathscr{E}_s \supset \mathscr{E}_{s-1} \supset \cdots \supset \mathscr{E}_1 \supset \mathscr{E}_0 = \{0\}, \tag{1-6}$$

such that, for any $1 \leq i \leq s-1$, the quotient sheaf $\mathscr{E}_i/\mathscr{E}_{i-1}$ is the maximal semistable (torsion-free coherent) subsheaf of $\mathscr{E}/\mathscr{E}_{i-1}$, i.e., for any subsheaf of $\mathcal{F}$ of a (torsion-free coherent) sheaf $\mathscr{E}/\mathscr{E}_{i-1}$, we have $\mu(\mathcal{F}) \leq \mu(\mathscr{E}_i/\mathscr{E}_{i-1})$ and $\mathrm{rk}(\mathcal{F}) \leq \mathrm{rk}(\mathscr{E}_i/\mathscr{E}_{i-1})$ if $\mu(\mathcal{F}) = \mu(\mathscr{E}_i/\mathscr{E}_{i-1})$. For the proof of this result in the setting of the Gauduchon form ω_B, see either [Bruasse 2001] or [Greb et al. 2016, Corollary 2.27]. We define the *Harder–Narasimhan slopes*, $\mu_1, \dots, \mu_{\mathrm{rk}(\mathscr{E})}$ of $\mathscr{E}$, such that $\mu(\mathscr{E}_i/\mathscr{E}_{i-1})$ appears among $\mu_1, \dots, \mu_{\mathrm{rk}(\mathscr{E})}$ exactly $\mathrm{rk}(\mathscr{E}_i/\mathscr{E}_{i-1})$ times, and the sequence $\mu_1, \dots, \mu_{\mathrm{rk}(\mathscr{E})}$ is nonincreasing. We let $\mu_{\min} := \mu_{\mathrm{rk}(\mathscr{E})}$, $\mu_{\max} := \mu_1$.

We let $N_k := \mathrm{rk}(E_k)$, and let $\mu_1^k, \dots, \mu_{N_k}^k$ be the Harder–Narasimhan slopes of E_k, and $\mu_{\min}^k$, $\mu_{\max}^k$ be the minimal and the maximal slopes. Define the probability measure η_k^{HN} on $\mathbb{R}$ as

$$\eta_k^{\mathrm{HN}} := \frac{1}{N_k} \sum_{i=1}^{N_k} \delta\left[\frac{\mu_i^k}{k}\right], \tag{1-7}$$

where $\delta[x]$ is the Dirac mass at $x \in \mathbb{R}$. Our lower bounds for the fibered Yang–Mills functionals will build upon the following result.

Theorem 1.5. *The sequence of measures η_k^{HN} converges weakly, as $k \to \infty$, to a probability measure η^{HN} on $\mathbb{R}$, and the limits below exist and relate with η^{HN} as follows*:

$$\eta_{\min}^{\mathrm{HN}} := \lim_{k\to\infty} \frac{\mu_{\min}^k}{k} \leq \operatorname{ess\,inf} \eta^{\mathrm{HN}}, \quad \eta_{\max}^{\mathrm{HN}} := \lim_{k\to\infty} \frac{\mu_{\max}^k}{k} = \operatorname{ess\,sup} \eta^{\mathrm{HN}}. \tag{1-8}$$

Remark 1.6. The proof of Theorem 1.5 follows the arguments from [Chen 2010; Finski 2024b, Theorem 1.1], establishing Theorem 1.5 in the projective setting for flat maps $\pi : X \to B$, for $\dim B = 1$ and $\dim B \geq 1$, respectively. The only difference is that due to the lack of algebraicity, the proofs from [Chen 2010; Finski 2024b] of the linear upper bound on $\mu_{\max}^k$ in $k \in \mathbb{N}^*$, crucial for Theorem 1.5, do not work. Here this bound is obtained by a differential-geometric argument; see Proposition 2.3.

We are finally ready to state our lower bounds for the fibered Yang–Mills functionals.

Theorem 1.7. *For any relatively positive metric h^L on L, we have*

$$\inf_{x \in X} \bigwedge_{\omega_B} \omega_H(x) \leq \eta^{\mathrm{HN}}_{\min}, \quad \sup_{x \in X} \bigwedge_{\omega_B} \omega_H(x) \geq \eta^{\mathrm{HN}}_{\max}. \tag{1-9}$$

If, moreover, ω_B is Kähler, then for any $c \in \mathbb{R}$, $p \in [1, +\infty[$, we have

$$\mathrm{FYM}_{p,c}(\pi, h^L) \geq \int_{\mathbb{R}} |x-c|^p d\eta^{\mathrm{HN}}(x) \cdot \int_X [\omega^n] \cdot \pi^*[\omega_B^m]. \tag{1-10}$$

Remark 1.8. (a) As we shall establish in Proposition 4.5, $\eta^{\mathrm{HN}}_{\min} = \eta^{\mathrm{HN}}_{\max}$ if and only if E_k, $k \in \mathbb{N}$, are asymptotically semistable. Hence, (1-9) refines Theorem 1.1.

(b) The left hand-side of (1-10) depends on h^L, but the right-hand side doesn't.

(c) When $X := \mathbb{P}(E^*)$ for some holomorphic vector bundle E over B, $L := \mathscr{O}(1)$, and h^L is induced by a Hermitian metric h^E on E, the result can be deduced from the lower bounds on the Hermitian Yang–Mills functionals due to Atiyah and Bott [1983] and Daskalopoulos and Wentworth [2004].

Note that similar lower bounds in the context of constant scalar curvature metrics were obtained by Donaldson [2005] for the Calabi functional. Here, as in [Donaldson 2005], we expect the bounds from Theorem 1.7 to be tight. In other words, it seems likely that the following conjecture holds.

Conjecture. *In the notation of Theorem 1.7, for any $p \in [1, +\infty[$, $c \in \mathbb{R}$, we have*

$$\begin{aligned} \inf_{h^L} \mathrm{FYM}_{p,c}(\pi, h^L) &= \int_{\mathbb{R}} \left|x-c\right|^p d\eta^{\mathrm{HN}}(x) \cdot \int_X [\omega^n] \cdot \pi^*[\omega_B^m], \\ \inf_{h^L} \mathrm{FYM}_{+\infty,c}(\pi, h^L) &= \max\{|\eta^{\mathrm{HN}}_{\min} - c|, |\eta^{\mathrm{HN}}_{\max} - c|\}, \end{aligned} \tag{1-11}$$

where the infimum is taken among all relatively positive metrics h^L on L.

Remark 1.9. In the recent paper [Finski 2024a], the author established the Conjecture for $p = 1$.

By Remark 1.8(a), if the Conjecture holds for $p = +\infty$, then the converse implication of Theorem 1.1 also follows, upon taking $c := \eta^{\mathrm{HN}}_{\min} = \eta^{\mathrm{HN}}_{\max}$.

For $\pi : \mathbb{P}(E^*) \to B$, $L = \mathscr{O}(1)$, where E is some holomorphic vector bundle over a complex compact manifold B, one can show that the Conjecture holds by the existence of the approximate critical hermitian structures on vector bundles, see [Daskalopoulos and Wentworth 2004, Definition 3.9], and the calculation of the asymptotic slopes of $\mathrm{Sym}^k E = R^0\pi_* L^k$, due to Chen [2011, Theorem 1.2]. The following result is another partial justification of the Conjecture.

Theorem 1.10. *The identity $\sup_{h^L} \inf_{x \in X} \bigwedge_{\omega_B} \omega_H(x) = \eta^{\mathrm{HN}}_{\min}$ holds, where the supremum is taken among all relatively positive metrics h^L on L.*

Remark 1.11. By [Li et al. 2022, Theorem 1.5], when $X := \mathbb{P}(E^*)$ for some holomorphic vector bundle E over B, and $L := \mathscr{O}(1)$, the above theorem remains valid even if one restricts attention to metrics h^L that are induced by a Hermitian metric h^E on E.

We assume now that B (and, hence, X) is projective. Recall that a line bundle L on X is called *nef* if for any irreducible curve C in X, $\int_C c_1(L) \geq 0$. It is well-known that this condition is equivalent to the existence of metrics with an arbitrarily small negative part of the curvature, as stated precisely in [Demailly 1992, Proposition 4.2]. One of the central concerns in complex geometry is the study of variations of this result, which provides a "dictionary" between the algebraic and analytic definitions of positivity. Let us now explain an application of Theorem 1.10 in this context.

We fix a very ample integral multipolarization $[\omega_{B,1}], \dots, [\omega_{B,m-1}]$ on B, which is a collection of very ample classes from $H^{1,1}(B, \mathbb{C}) \cap H^2(B, \mathbb{Z})$. We say that a $\mathbb{Q}$-line bundle L on X is $([\omega_{B,1}], \dots, [\omega_{B,m-1}])$-*generically fibered nef with respect to* π if there is $l_0 \in \mathbb{N}^*$ such that, for any regular curve $C = C(l) \subset B$, $l = (l_1, \dots, l_{m-1}) \in \mathbb{N}^{*(m-1)}$, $l_i \geq l_0$, $i = 1, \dots, m-1$, given by a complete intersection of *generic* divisors from classes $l_1[\omega_{B,1}], \dots, l_{m-1}[\omega_{B,m-1}]$, the restriction of $c_1(L)$ to $\pi^{-1}(C)$ is nef. When π is the projectivization of a vector bundle, an equivalent definition was given by Miyaoka [1987], see also [Peternell 2012]. The general case was introduced in [Finski 2024b]. We say L is *stably* $([\omega_{B,1}], \dots, [\omega_{B,m-1}])$-*generically fibered nef with respect to* π if for some (or any) ample line bundle L_0 on X, for any $\epsilon > 0$, $\epsilon \in \mathbb{Q}$, the $\mathbb{Q}$-line bundle $L \otimes L_0^{\epsilon}$ is $([\omega_{B,1}], \dots, [\omega_{B,m-1}])$-generically fibered nef with respect to π. Recall that L is called *relatively nef with respect to* π if its restriction to every fiber is nef. As we explain in Section 3, from the previously obtained algebraic description of $\eta^{\mathrm{HN}}_{\min}$ from [Finski 2024b, Corollary 1.4], Theorem 1.10 can be used to prove the following result.

Theorem 1.12. *Consider a holomorphic submersion* $\pi : X \to B$ *between projective manifolds* B, X. *A relatively nef line bundle* L *on* X *is stably* $([\omega_{B,1}], \dots, [\omega_{B,m-1}])$-*generically fibered nef if and only if for any* (*or some*) *Kähler forms* $\omega_{B,1}, \dots, \omega_{B,m-1}$ *on* B *in* $[\omega_{B,1}], \dots, [\omega_{B,m-1}]$, *and any* (*or some*) *Kähler form* ω_X *on* X, *for any* $\epsilon > 0$, *there is a Hermitian metric* h^L_ϵ *on* L, *such that*

$$\omega(h^L_\epsilon) \wedge \pi^*\omega_{B,1} \wedge \dots \wedge \pi^*\omega_{B,m-1} \geq -\epsilon \cdot \omega_X^m, \tag{1-12}$$

where by this we mean that the volume forms obtained by the restriction to every m-*dimensional complex hyperplane of each side of* (1-12) *compares as required in* (1-12); *see* [Demailly 2012, (III.1.6)].

Remark 1.13. Curiously, even though the forms $\omega_{B,1}, \dots, \omega_{B,m-1}$ are Kähler, if these forms are different, then in the proof of Theorem 1.12, we need to apply Theorem 1.10 for a non-Kähler Gauduchon form ω_B, constructed from $\omega_{B,1}, \dots, \omega_{B,m-1}$. This was our main motivation to write this article in the current generality. However, Theorem 1.12 is new even if the forms are equal.

In conclusion, it seems for us that a proof of the Conjecture might rely either on the techniques of geometric flows or continuity method as in [Donaldson 1985; Uhlenbeck and Yau 1986]. In this vein, the recent a priori bounds for Monge–Ampère and Hessian equations established by Guo, Phong, and Tong [2023] and Guo, Phong, Tong, and Wang [2021] will likely play an important role.

Note that for a Hermitian Yang–Mills functional, the analogous conjecture holds due to results of Atiyah and Bott [1983], Daskalopoulos and Wentworth [2004], Sibley [2015], Jacob [2016] and Li, Zhang, and Zhang [Li et al. 2022]; see Theorem 2.5 for a precise statement. We also mention the recent works of Xia [2021], Hisamoto [2023] and Dervan and Székelyhidi [2020], see also [Collins et al. 2022], proving versions of the Conjecture in the context of constant scalar curvature metrics.

In a different direction, when B is a bounded smooth strongly pseudoconvex domain in $\mathbb{C}^n$, $c = 0$ and ω_B is the standard Kähler form on $B \subset \mathbb{C}^n$, Donaldson [1992] and Coifman and Semmes [1993] established that Dirichlet problem associated with the Hermite–Einstein equation has solutions for any vector bundle over B (in particular for E_k, $k \in \mathbb{N}$). Wu [2023] showed that the Dirichlet problem associated with (1-2) always has weak solutions, and these solutions can be obtained as the semiclassical limit of the solutions of the Hermite–Einstein equations on E_k. See also [Phong and Sturm 2006; Rubinstein and Zelditch 2010; Song and Zelditch 2010] for earlier results in this direction. In other words, a phenomenon similar to Theorem 1.7 is present: there is a relation between the Hermite–Einstein and the Wess–Zumino–Witten equations. The major difference between these developments and our paper is that in our boundaryless setting, neither Hermite–Einstein equations nor fibered Einstein equations have solutions in general, and the methods of [Donaldson 1992; Coifman and Semmes 1993; Wu 2023] do not apply.

This article will be organized as follows. In Section 2, we will establish Theorems 1.5 and 1.7. We discuss how horizontal curvature behaves with respect to a restriction to a subfamily in Section 3, and using this, we establish Theorems 1.10 and 1.12. Finally, in Section 4, we establish a numerical obstruction for asymptotic semistability of direct images from Theorem 1.3.

2. Fibered Yang–Mills functionals through the semiclassical limit

The main goal of this section is to prove Theorems 1.5 and 1.7. The theory of Toeplitz operators and Hermitian Yang–Mills theory, which we recall below, will be particularly useful for that.

We begin by recalling some facts about Toeplitz operators. Let Y be a complex projective manifold of dimension n with an ample line bundle L. We fix a positive Hermitian metric h^L on L. We denote by ω its first Chern form, $c_1(L, h^L)$. For smooth sections f, f' of L^k, $k \in \mathbb{N}$, over Y, we define the L^2-scalar product using the pointwise scalar product $\langle \cdot, \cdot \rangle_{h^L}$ induced by h^L as

$$\langle f, f' \rangle_{L^2(Y)} := \int_Y \langle f(x), f'(x) \rangle_{h^{L^{\otimes k}}} \cdot \omega^n(x). \tag{2-1}$$

Recall that the *Bergman projector* B_k is given by the orthogonal projection (with respect to the scalar product (2-1)) from the space of L^2-sections of L^k to $H^0(Y, L^k)$. For any bounded function f on Y, we then define the Toeplitz operator, $T_k(f) : H^0(Y, L^k) \to H^0(Y, L^k)$, as

$$T_k(f)(s) = B_k(f \cdot s), \quad s \in H^0(Y, L^k). \tag{2-2}$$

Proposition 2.1. *For any bounded function $f : Y \to \mathbb{R}$, we have the inequalities*

$$\inf f \cdot \mathrm{Id}_{H^0(Y,L^k)} \le T_k(f) \le \sup f \cdot \mathrm{Id}_{H^0(Y,L^k)}, \tag{2-3}$$

where by $A \le B$ we mean that the difference $B - A$ is positive definite. Moreover, if f is smooth, then for any continuous function $\phi : \mathbb{R} \to \mathbb{R}$, we have

$$\begin{aligned} \lim_{k\to\infty} \frac{\mathrm{Tr}[\phi(T_k(f))]}{\dim H^0(Y, L^k)} &= \frac{\int_{x \in Y} \phi(f(x))\omega^n(x)}{\int_Y [\omega^n]}, \\ \lim_{k\to\infty} \|\phi(T_k(f))\| &= \max\{|\sup \phi(f)|, |\inf \phi(f)|\}, \end{aligned} \tag{2-4}$$

where $\|\cdot\|$ is the operator norm.

Proof. The statement (2-3) follows from the trivial fact that if f is a positive function, then the operator $T_k(f)$ is positive-definite. The statement (2-4) is a restatement of the weak convergence of spectral measures of Toeplitz operators due to Boutet de Monvel and Guillemin [1981, Theorem 13.13]. For an alternative proof through Bergman kernel expansion, see [Ma and Marinescu 2007, Theorem 7.4.1], [Barron et al. 2014, Theorem 3.8] or [Finski 2022, Appendix A]. See also [Ma and Marinescu 2012; 2013] for generalizations and more refined results. □

Now, the reason why Toeplitz operators are relevant to this paper is because they appear as the principal term in the asymptotic expansion of the curvature of L^2-metrics on direct images of a polarized fibrations. More precisely, consider a proper holomorphic submersion $\pi : X \to B$ between complex manifolds X and B of dimensions $n+m$ and m, respectively, $n, m \in \mathbb{N}$. Let L be a holomorphic line bundle over X, which is relatively ample with respect to π. Endow L with a relatively positive Hermitian metric h^L. Let $k \in \mathbb{N}$ be large enough that

$$E_k := R^0 \pi_* L^k \tag{2-5}$$

is locally free. The L^2-product (2-1) then defines a smooth Hermitian metric h^{E_k} on E_k. We denote by $R^{E_k} \in \mathscr{C}^\infty\big(B, \bigwedge^2 T^*B \otimes \operatorname{End}(E_k)\big)$ the curvature of its Chern connection.

Theorem 2.2 [Ma and Zhang 2023, Theorem 0.4]. *There are $C > 0$, $k_0 \in \mathbb{N}$, such that, for any $k \geq k_0$,*

$$\left\| \frac{\sqrt{-1}}{2\pi} R^{E_k} - k \cdot T_k(\omega_H) \right\| \leq C, \tag{2-6}$$

where $\|\cdot\|$ is the operator norm, and we naturally extended the definition of Toeplitz operators from functions to bounded sections of $\pi^* \bigwedge^2 T^*B$ as follows: for a decomposition $\omega_H = \sum f_{ij} dz_i d\bar{z}_j$, where $z_1, \dots, z_n$ are local coordinates on B, we let $T_k(\omega_H) := \sum T_k(f_{ij}) dz_i d\bar{z}_j$.

As we shall explain below, Theorem 2.2 is the crucial ingredient connecting fibered Yang–Mills functionals with Hermitian Yang–Mills functionals. But before this, let us mention another application of Theorem 2.2 to the study of Harder–Narasimhan slopes of direct images.

We fix now a *Gauduchon Hermitian form* ω_B on B. As before Theorem 1.5, we denote by $\mu^k_{\max}$ the maximal Harder–Narasimhan ω_B-slope of E_k.

Proposition 2.3. *There is $C > 0$, such that $\mu^k_{\max} \leq Ck$ for any $k \in \mathbb{N}^*$.*

Proof. For $p = 1, \dots, \operatorname{rk}(E_k)$, we denote by $R^{\bigwedge^p E_k}$ the curvature of the Chern connection on $\bigwedge^p E_k$, induced by the metric $h^{\bigwedge^p E_k}$ induced by h^{E_k}. By Theorem 2.2 and the very definition of $\bigwedge_{\omega_B}$ from (1-1), we conclude that there is $C > 0$ such that, for any $k \in \mathbb{N}^*$, we have

$$\frac{\sqrt{-1}}{2\pi} \textstyle\bigwedge_{\omega_B} R^{\bigwedge^p E_k} \leq Cpk \cdot \operatorname{Id}_{\bigwedge^p E_k}. \tag{2-7}$$

Let F be a line subbundle of $\bigwedge^p E_k$. We denote by h^F the Hermitian metric on F, induced by the metric h^{E_k}. By (2-7) and the well-known principle that curvature decreases in holomorphic subbundles, see [Demailly 2012, (V.14.6)], we deduce

$$\textstyle\bigwedge_{\omega_B} c_1(F, h^F) \leq Cpk. \tag{2-8}$$

However, it is classical, see [Kobayashi 2014, proofs of Lemma 5.7.16 and Theorem 5.8.3], that we have

$$\mu^k_{\max} \leq \max_{p=1,\dots,\mathrm{rk}(E_k)} \sup_{F \subset \bigwedge^p E_k} \frac{1}{p} \int_B c_1(F, h^F) \wedge \omega_B^{m-1}, \tag{2-9}$$

where the second supremum is taken over line subbundles F. We conclude by (2-8) and (2-9). □

Proof of Theorem 1.5. Taking into account the linear bound from Proposition 2.3, the proof of Theorem 1.5 is the same as in [Chen 2010; Finski 2024b, Theorem 1.1]. Let us briefly recall the main steps for completeness. We introduce the (nonincreasing) filtrations $\mathcal{F}_k(\lambda)$, $\lambda \in \mathbb{R}$, of E_k by coherent (torsion-free) subsheaves (defined over B), so that $\mathcal{F}_k(\lambda)$ is the maximal subsheaf of E_k such that all of its Harder–Narasimhan slopes are bigger than λ. The filtration $\mathcal{F}_k$ is just a "renaming" of the Harder–Narasimhan filtration of E_k. Now, for any $b \in B$, we denote by $\mathcal{F}_b$ the filtration induced by $\mathcal{F}_k(\lambda)$ on $R(X_b, L_b) = \bigoplus_{k=0}^{\infty} H^0(X_b, L_b^k)$ of the fiber $X_b = \pi^{-1}(b)$, $L_b = L|_{X_b}$, $b \in B$. It was established in [Chen 2010] for $\dim B = 1$ and in [Finski 2024b, Proposition 2.5] for any projective B, that for generic $b \in B$, the above filtration is submultiplicative, i.e., for any $t, s \in \mathbb{R}$, $k, l \in \mathbb{N}$, we have

$$\mathcal{F}_b^t H^0(X_b, L_b^k) \cdot \mathcal{F}_b^s H^0(X_b, L_b^l) \subset \mathcal{F}_b^{t+s} H^0(X_b, L_b^{k+l}). \tag{2-10}$$

Observe, however, that the projectivity assumption was never used in [Finski 2024b, Proposition 2.5], and so submultiplicativity holds for general complex manifolds B. Theorem 1.5 is then a formal consequence of the submultiplicativity and Proposition 2.3, saying that the above filtration is bounded in the terminology of [Boucksom and Chen 2011]. For the (different) proofs of this last result, see [Chen 2010, théorème 3.4.3; Boucksom and Chen 2011, Theorem A; Finski 2025, Theorem 1.9]. □

Let us now recall some crucial facts from Hermitian Yang–Mills theory, following the pioneering work of Atiyah and Bott [1983] and later developments by Donaldson [1985], Daskalopoulos and Wentworth [2004], and others. We fix a compact complex manifold B of dimension m with a Gauduchon Hermitian form ω_B on B. Let E be a holomorphic vector bundle of rank r over B. For a Hermitian metric h^E on E, we denote by R^E its curvature. For any $p \in [1, +\infty[$, $c \in \mathbb{R}$, we define the *Hermitian Yang–Mills functional* as

$$\begin{aligned} \mathrm{HYM}_{p,c}(E, h^E) &:= \int_B \mathrm{Tr}\left[\left|\frac{\sqrt{-1}}{2\pi} \Lambda_{\omega_B} R^E_x - c \cdot \mathrm{Id}_E\right|^p\right] \omega_B^m(x), \\ \mathrm{HYM}_{+\infty,c}(E, h^E) &:= \sup_{x \in X} \left\| \frac{\sqrt{-1}}{2\pi} \Lambda_{\omega_B} R^E_x - c \cdot \mathrm{Id}_E \right\|, \end{aligned} \tag{2-11}$$

where $\|\cdot\|$ means the operator norm, and $|A| := \sqrt{AA^*}$ for $A \in \mathrm{End}(V)$ on a Hermitian vector space (V, H).

As in (1-7), we denote the Harder–Narasimhan ω_B-slopes of E by $\mu_1, \dots, \mu_r$. Let $\mu_{\min} := \mu_r$, $\mu_{\max} := \mu_1$, be the minimal and the maximal slopes. We define the probability measure

$$\mu_E := \frac{1}{r} \sum_{i=1}^{r} \delta[\mu_i]. \tag{2-12}$$

The following result lies at the heart of this paper.

Theorem 2.4. *For any $c \in \mathbb{R}$ and a Hermitian metric h^E on E, we have*

$$\mathrm{HYM}_{+\infty,c}(E, h^E) \geq \max\{|\mu_{\min} - c|, |\mu_{\max} - c|\}. \tag{2-13}$$

If, moreover, ω_B is Kähler, then for any $p \in [1, +\infty[$, we have

$$\mathrm{HYM}_{p,c}(E, h^E) \geq r \cdot \int_{\mathbb{R}} |x - c|^p d\mu_E(x) \tag{2-14}$$

For the proof of Theorem 2.4 for $p \in [1, +\infty[$, see [Atiyah and Bott 1983, Proposition 8.20] if $\dim B = 1$, [Daskalopoulos and Wentworth 2004, Lemma 2.17, Corollary 2.22, Proposition 2.25] if B is Kähler of any dimension (even though the article [Daskalopoulos and Wentworth 2004] is written for surfaces, see [Sibley 2015, §3.1]). For the proof of the first part, consult [Li et al. 2022, Theorem 1.5]. It is remarkable that the bounds from Theorem 2.4 are actually tight. Although we will not use this result in what follows, we state it for the reader's convenience, as it clarifies our motivation for the Conjecture.

Theorem 2.5. *In the notation Theorem 2.4, assume that ω_B is Kähler. Then for any $c \in \mathbb{R}$, $p \in [1, +\infty[$, we have*

$$\inf_{h^E} \mathrm{HYM}_{p,c}(E, h^E) = r \cdot \int_{\mathbb{R}} |x - c|^p d\mu_E(x) \cdot \int_B [\omega_B^m]. \tag{2-15}$$

where the infimum is taken over all Hermitian metrics h^E on E.

For the proof of Theorem 2.5 for $p \in [1, +\infty[$, see [Atiyah and Bott 1983, Proposition 8.20] if $\dim B = 1$. For higher dimensions, this is a direct consequence of the existence of L^p-approximate critical hermitian structure on E, see [Daskalopoulos and Wentworth 2004, Definition 3.9] for the definition, and [Daskalopoulos and Wentworth 2004, Theorem 3.11; Sibley 2015, Theorem 1.3] for the proofs if B is Kähler of dimension 2 and any dimension, respectively. See also [Jacob 2016, Theorems 2, 3].

Proof of Theorem 1.7. Preserving the notation introduced in (1-7), we define the probability measure, $\eta^{\mathrm{HN}}_{k,0}$, $k \in \mathbb{N}$, on $\mathbb{R}$ as

$$\eta^{\mathrm{HN}}_{k,0} := \frac{1}{N_k} \sum_{i=1}^{N_k} \delta[\mu_i^k], \tag{2-16}$$

We apply Theorem 2.4 for (E_k, h^{E_k}), $k \in \mathbb{N}$, $c \in \mathbb{R}$, to get

$$\mathrm{HYM}_{+\infty,ck}(E_k, h^{E_k}) \geq \max\{|\mu^k_{\min} - ck|, |\mu^k_{\max} - ck|\}. \tag{2-17}$$

If, moreover, ω_B is Kähler, then for any $p \in [1, +\infty[$, we have

$$\mathrm{HYM}_{p,ck}(E_k, h^{E_k}) \geq N_k \cdot \int_{\mathbb{R}} |x - ck|^p d\eta^{\mathrm{HN}}_{k,0}(x) \cdot \int_B [\omega_B^m]. \tag{2-18}$$

Directly from Theorem 2.2 and Proposition 2.1, under the respective assumptions, for any $p \in [1, +\infty[$, $c \in \mathbb{R}$, we have

$$\begin{aligned} \lim_{k \to \infty} \frac{\mathrm{HYM}_{p,ck}(E_k, h^{E_k})}{k^p \cdot N_k} &= \frac{\mathrm{FYM}_{p,c}(\pi, h^L)}{\int_{X_b} [\omega^n]}, \\ \lim_{k \to \infty} \frac{\mathrm{HYM}_{+\infty,ck}(E_k, h^{E_k})}{k} &= \mathrm{FYM}_{+\infty,c}(\pi, h^L), \end{aligned} \tag{2-19}$$

where $b \in B$ is an arbitrary point, and X_b is the fiber of π at b.

We now divide both sides of the first inequality of (2-17) by $k^p \cdot N_k$, take the limit $k \to \infty$, and apply Theorem 1.5 and (2-19) to deduce

$$\mathrm{FYM}_{p,c}(\pi, h^L) \geq \int_{\mathbb{R}} |x-c|^p d\eta^{\mathrm{HN}}(x) \cdot \int_{X_b} [\omega^n] \cdot \int_B [\omega_B^m]. \tag{2-20}$$

This establishes Theorem 1.7 for $p \in [1, +\infty[$, as $\int_{X_b} [\omega^n] \cdot \int_B [\omega_B^m] = \int_X [\omega^n] \cdot \pi^* [\omega_B^m]$. To get Theorem 1.7 for $p = +\infty$, we divide both sides of the second inequality of (2-17) by k, take the limit $k \to \infty$, and apply Theorem 1.5 and (2-19). □

3. Horizontal curvature on subfamilies and generic fibered nefness

The main goal of this section is to establish Theorems 1.10 and 1.12. For this, we construct a sequence of metrics on the polarizing line bundle from a sequence of Hermitian metrics on direct images. To show that horizontal mean curvature behaves well under this procedure, we rely on a fibered analogue of the principle that "a curvature of a vector bundle increases under taking quotients".

More precisely, consider a holomorphic submersion $\pi : X \to B$ between compact complex manifolds X and B. We let $m := \dim B$. Consider an embedding $\iota : Y \hookrightarrow X$ of a smooth complex manifold Y, such that restriction of π, $\pi|_Y : Y \to B$, is a submersion. We fix a $(1,1)$-form ω_X on X, which is positive along the fibers of π, and let $\omega_Y := \iota^* \omega_X$. We fix a Hermitian $(1,1)$-form ω_B on B, and denote by $\bigwedge_{\omega_B} \omega_{Y,H} \in \mathscr{C}^\infty(Y)$, $\bigwedge_{\omega_B} \omega_{X,H} \in \mathscr{C}^\infty(X)$, the horizontal mean curvatures of ω_Y and ω_X, respectively.

Lemma 3.1. *For any $y \in Y$, we have $\bigwedge_{\omega_B} \omega_{Y,H}(y) \geq \bigwedge_{\omega_B} \omega_{X,H}(\iota(y))$.*

Remark 3.2. An equivalent result was established in [Feng et al. 2019, (2.2)] by a slightly different method.

Proof. Let us fix $y \in Y$, and denote by $b := \pi|_Y(y)$, $x := \iota(y)$, and by $e_1, \dots, e_m$ an orthonormal basis of $T_b^{1,0} B$ with respect to ω_B. We denote by $e_1^X, \dots, e_m^X \in T_x^{1,0} X$ the horizontal lifts of $e_1, \dots, e_m$, defined with respect to ω_X, i.e., $d\pi(e_i^X) = e_i$, $i = 1, \dots, m$ and $e_1^X, \dots, e_m^X$ are orthogonal (with respect to ω_X) to the tangent space of the fibers, $T^V X$, of π. Similarly, we denote by $e_1^Y, \dots, e_m^Y \in T_y^{1,0} Y$ the horizontal lifts of $e_1, \dots, e_m$, defined with respect to ω_Y. Clearly, using implicitly the embedding of $T_y Y$ in $T_x X$ through ι, we can write $e_i^Y = e_i^X + v_i$, where $v_i \in T_x^V X$. But then, since e_i^X and v_i are orthogonal with respect to ω_X, and ω_X is positive in the vertical directions, we obtain $\sqrt{-1}\omega_Y(e_i^Y, \bar{e}_i^Y) = \sqrt{-1}\omega_X(e_i^X, \bar{e}_i^X) + \sqrt{-1}\omega_X(v_i, \bar{v}_i) \geq \sqrt{-1}\omega_X(e_i^X, \bar{e}_i^X)$. By taking a sum of the above inequality over all $i = 1, \dots, m$, we establish the needed inequality. □

Another ingredient we need is the calculation of the horizontal mean curvature for projectivizations of vector bundles. More precisely, let (F, h^F) be a Hermitian vector bundle over B of rank r. Let $\mathcal{O}(1)$ be the hyperplane bundle over $\mathbb{P}(F^*)$, $\pi : \mathbb{P}(F^*) \to X$. We endow $\mathcal{O}(1)$ with the metric $h^{\mathcal{O}(1)}$ induced by h^F. We denote by R^F the curvature of the Chern connection on (F, h^F), by ω the first Chern class of $(\mathcal{O}(1), h^{\mathcal{O}(1)})$, and by ω_H its horizontal component.

Lemma 3.3. *In the above notation, for any $x \in X$, we have*

$$\inf_{y \in \mathbb{P}(F_x^*)} \Lambda_{\omega_B} \omega_H(y) = \inf_{\substack{f \in F_x \\ \|f\|_{h^F}=1}} \left\langle \frac{\sqrt{-1}}{2\pi} \Lambda_{\omega_B} R^F f, f \right\rangle_{h^F}. \tag{3-1}$$

Proof. We fix some local coordinates $z := (z_1, \dots, z_n)$ on B, centered at $x \in B$, and a local normal frame $f_1, \dots, f_r$ of F at x, defined in a neighborhood U of x. By a *normal frame* we mean a holomorphic frame satisfying $\langle f_i, f_j \rangle_{h^F} = \delta_{ij} - \sum_{\lambda\mu} d_{\lambda\mu ij} z_\lambda \bar{z}_\mu + O(|z|^3)$ for some constants $d_{\lambda\mu ij}$. We denote by $f_1^*, \dots, f_r^*$ the dual frame of F^*. The above data defines a trivialization of $U \times \mathbb{P}(\mathbb{C}^r) \to \mathbb{P}(F^*)$ near $\pi^{-1}(x)$ as follows. For $a := (a_1, \dots, a_r)$, where $a_i \in \mathbb{C}$, $1 \le i \le r$, and not all a_i are equal to zero, the trivialization is given by the map $(z, [a]) \to \left[\sum_{i=1}^r a_i f_i^*(z)\right] \in \mathbb{P}(F^*)$. Now we take $a_1 = 1$ and let $b_i := a_i$, $2 \le i \le r$, $b := (b_i)$. Then (z, b) gives a chart for $\mathbb{P}(F^*)$. The well-known formula, see [Demailly 2012, Formula (V.15.15)], shows that at the point $(x, [f_1^*]) \in \mathbb{P}(F^*)$, the curvature, $R^{\mathcal{O}(1)}$, of the hyperplane bundle $(\mathcal{O}(1), h^{\mathcal{O}(1)})$, equals

$$R^{\mathcal{O}(1)}_{(x,[f_1^*])} = \sum_{2 \le j \le r} db_j \wedge d\bar{b}_j + \langle R^F f_1, f_1 \rangle_{h^F}. \tag{3-2}$$

In particular, we see that the vertical part of the form $\omega = c_1(\mathcal{O}(1), h^{\mathcal{O}(1)})$ is the Fubini–Study form induced by h^F, and the horizontal part of ω, ω_H, evaluated at $(x, [f_1^*]) \in \mathbb{P}(E^*)$, coincides with $\sqrt{-1}/(2\pi) \langle R^F f_1, f_1 \rangle_{h^F}$. The result follows directly from this. □

Remark 3.4. From the proof of the above lemma, we see that $\Lambda_{\omega_B} \omega_H$ is constant if and only if $\Lambda_{\omega_B} R^F$ is the identity endomorphism up to a constant, which means that ω is fibered Einstein if and only if (F, h^F) is Hermite Einstein.

Recall also the following result.

Proposition 3.5 [Li et al. 2022, Theorem 1.5]. *For any $\epsilon > 0$, there is a Hermitian metric h^E_ϵ on E, such that the associated curvature, R^E_ϵ, for any $b \in B$, $e \in E_b$, verifies*

$$\frac{\sqrt{-1}}{2\pi} \Lambda_{\omega_B} R^E_\epsilon \ge (\mu_{\min} - \epsilon) \cdot \mathrm{Id}_E .$$

Proof of Theorem 1.10. First of all, for a given $\epsilon > 0$, let $k \in \mathbb{N}$ be such that $\mu^k_{\min}/k > \eta^{\mathrm{HN}}_{\min} - \frac{1}{2}\epsilon$. By Proposition 3.5, there is a metric h^ϵ_k on E_k such that, for the associated curvature, $R^{E_k}_\epsilon$, we have

$$\frac{\sqrt{-1}}{2\pi} \Lambda_{\omega_B} R^{E_k}_\epsilon \ge \left(\mu^k_{\min} - \tfrac{1}{2}\epsilon\right) \cdot \mathrm{Id}_{E_k} . \tag{3-3}$$

We denote by ω_k the $(1, 1)$-form on $\mathbb{P}(E_k^*)$, given by the first Chern class of the curvature of the hyperplane line bundle induced by the metric h^ϵ_k. We denote by $\omega_{H,k}$ the horizontal part of this curvature. From Lemma 3.3, the choice of $k \in \mathbb{N}$ and (3-3), we deduce

$$\inf_{x \in \mathbb{P}(E_k^*)} \Lambda_{\omega_B} \omega_{H,k}(x) \ge k \cdot (\eta^{\mathrm{HN}}_{\min} - \epsilon). \tag{3-4}$$

We will now assume that k was chosen big enough so that L^k is relatively ample. Consider now the Kodaira embedding $\iota_k : X \hookrightarrow \mathbb{P}(E_k^*)$. It is well-known that there is a canonical isomorphism between $\iota_k^* \mathscr{O}(1)$ and L^k. We denote by h_ϵ^L the metric induced on L by the pull-back; then $\omega(h_\epsilon^L) = \frac{1}{k} \iota_k^* \omega_{H,k}$. By Lemma 3.1 and (3-4), we conclude that $\inf_{x \in X} \bigwedge_{\omega_B} \omega_H(h_\epsilon^L) \geq \eta_{\min}^{\mathrm{HN}} - \epsilon$. Since $\epsilon > 0$ can be taken arbitrarily small, we deduce $\sup_{h^L} \inf_{x \in X} \bigwedge_{\omega_B} \omega_H(h^L) \geq \eta_{\min}^{\mathrm{HN}}$. In combination with the upper bound from (1-9), this finishes the proof. □

Now, let us establish Theorem 1.12. As in the statement of Theorem 1.12, we fix any Kähler forms $\omega_{B,1}, \dots, \omega_{B,m-1}, \omega_X$. Then the form $\omega_{B,1} \wedge \cdots \wedge \omega_{B,m-1}$ is positive in the sense of [Demailly 2012, (III.1.1)]. By [Michelsohn 1982, (4.8)], there is a Hermitian form ω_B on B, verifying

$$\omega_B^{m-1} = \omega_{B,1} \wedge \cdots \wedge \omega_{B,m-1}. \tag{3-5}$$

Note that ω_B is automatically Gauduchon, but not necessarily Kähler. Since the form ω_B is Gauduchon, it makes sense to define the ω_B-degree and study the Harder–Narasimhan ω_B-slopes, as we did before Theorem 1.1. We remark that due to a relation (3-5), this ω_B-degree coincides with the degree associated with a multipolarization $([\omega_{B,1}], \dots, [\omega_{B,m-1}])$, as defined in [Finski 2024b, before (1.1)]. Below, the invariant $\eta_{\min}^{\mathrm{HN}}$ and other quantities are calculated with respect to ω_B. The following result, together with Theorem 1.10, lie at the core of the proof of Theorem 1.12.

Proposition 3.6 [Finski 2024b, Proposition 5.2]. *A relatively ample line bundle L over X is stably $([\omega_{B,1}], \dots, [\omega_{B,m-1}])$-generically fibered nef with respect to π if and only if $\eta_{\min}^{\mathrm{HN}} \geq 0$.*

Proof of Theorem 1.12. Let us first establish Theorem 1.12 under an additional assumption that L is relatively ample. We assume first that L is stably $([\omega_{B,1}], \dots, [\omega_{B,m-1}])$-generically fibered nef with respect to π. By Theorem 1.10 and Proposition 3.6, we establish that for any $\epsilon > 0$, there is a relatively positive Hermitian metric h_ϵ^L on L, such that $\bigwedge_{\omega_B} \omega_H(h_\epsilon^L) > -\epsilon$. From the definition of $\bigwedge_{\omega_B}$ and the trivial fact that there is $C > 0$, such that $\omega_B^m < C \omega_X^m$, we establish

$$\omega_H(h_\epsilon^L) \wedge \pi^* \omega_{B,1} \wedge \cdots \wedge \pi^* \omega_{B,m-1} \geq -C\epsilon \cdot \omega_X^m. \tag{3-6}$$

But the form $\omega(h_\epsilon^L)$ is relatively positive, so (3-6) implies (1-12) for $\epsilon := C\epsilon$, which finishes the proof of one direction of Theorem 1.12 under an additional assumption that L is relatively ample.

To prove the opposite direction under the same additional assumption that L is relatively ample, assume that we have a sequence of metrics h_ϵ^L, verifying (1-12). We will now show that one can cook up a sequence of relatively positive metrics, $h_{\epsilon,0}^L$, verifying similar bounds. Indeed, let us fix an arbitrary relatively positive metric h_0^L on L. By (1-12), it is easy to see that there is $c > 0$ such that, for any $\epsilon > 0$, over the fibers, the following inequality is satisfied: $c_1(L, h_\epsilon^L) \geq -\epsilon c \cdot c_1(L, h_0^L)$. Then an easy calculation shows that the sequence of metrics $h_{\epsilon,0}^L := (h_\epsilon^L)^{1-2c\epsilon} \cdot (h_0^L)^{2c\epsilon}$ is positive along the fibers and verifies the inequality (1-12) with $C\epsilon$ in place of ϵ, for some $C > 0$. Then as in (3-6), there is $C > 0$ such that, for any $\epsilon > 0$, we have $\bigwedge_{\omega_B} \omega_H(h_{\epsilon,0}^L) > -C\epsilon$. By Theorem 1.10, we then conclude that $\eta_{\min}^{\mathrm{HN}} \geq 0$, which implies that L is stably $([\omega_{B,1}], \dots, [\omega_{B,m-1}])$-generically fibered nef by Proposition 3.6.

We now only assume that L is relatively nef. We assume first that L is stably $([\omega_{B,1}], \dots, [\omega_{B,m-1}])$-generically fibered nef with respect to π. Now, for any $\delta \in \mathbb{Q}$, $\delta > 0$, consider the $\mathbb{Q}$-line bundle $L_\delta := L \otimes L_0^\delta$, where L_0 is some ample line bundle on X. Clearly, L_δ is relatively ample, and it is also stably $([\omega_{B,1}], \dots, [\omega_{B,m-1}])$-generically fibered nef with respect to π. The already established relatively ample case of Theorem 1.12 says that L_δ is $([\omega_{B,1}], \dots, [\omega_{B,m-1}])$-generically fibered nef if and only if for any $\epsilon > 0$, there is a Hermitian metric $h_\epsilon^{L_\delta}$ on L_δ, such that the analogue of (1-12) holds. Let h_0^L be now an arbitrary positive metric on L_0. It is easy to see that if δ and ϵ are sufficiently small, then the metric h_ϵ^L on L, which is constructed as the only metric verifying $h_\epsilon^{L_\delta} = h_\epsilon^L \cdot (h_0^L)^\delta$, will satisfy the analogue of (1-12) (for $C\epsilon$ instead of ϵ for some $C > 0$). This shows one direction of Theorem 1.12.

Inversely, if for any $\epsilon > 0$ there is a metric h_ϵ^L as in (1-12), then the metrics $h_\epsilon^{L_\delta}$, defined by the above formula, will also satisfy a similar inequality. Hence, by the already established case of Theorem 1.12, L_δ is then stably $([\omega_{B,1}], \dots, [\omega_{B,m-1}])$-generically fibered nef for any $\delta \in \mathbb{Q}$, $\delta > 0$. In particular, for any $\delta \in \mathbb{Q}$, $\delta > 0$, the line bundle $L_{2\delta} = L_\delta \otimes L_0^\delta$ is $([\omega_{B,1}], \dots, [\omega_{B,m-1}])$-generically fibered nef for any $\delta \in \mathbb{Q}$, $\delta > 0$, which means that L is stably $([\omega_{B,1}], \dots, [\omega_{B,m-1}])$-generically fibered nef, as $L_{2\delta} = L \otimes L_0^{2\delta}$. This finishes the proof. □

4. Asymptotic Riemann–Roch–Grothendieck and semistability

The main goal of this section is to prove a numerical obstruction for asymptotic semistability of direct images from Theorem 1.3. This will be based on an asymptotic version of Riemann–Roch–Grothendieck theorem, which we establish here in the singular setting.

To begin, let us recall some basic facts about Bott–Chern and Aeppli cohomologies. Let Y be a compact complex manifold of dimension n. We denote by $\Omega^{(p,q)}(Y)$ the vector space of (p,q)-differential forms on Y, $p, q \in \mathbb{N}$, and define $\partial : \Omega^{(p,q)}(Y) \to \Omega^{(p+1,q)}(Y)$, $\bar\partial : \Omega^{(p,q)}(Y) \to \Omega^{(p,q+1)}(Y)$, as usual. Recall that Bott–Chern cohomology, $H_{BC}^{p,q}(Y)$, is defined as

$$H_{BC}^{p,q}(Y) := \frac{\big(\ker \partial : \Omega^{(p,q)}(Y) \to \Omega^{(p+1,q)}(Y)\big) \cap \big(\ker \bar\partial : \Omega^{(p,q)}(Y) \to \Omega^{(p,q+1)}(Y)\big)}{\operatorname{im} \partial\bar\partial : \Omega^{(p-1,q-1)}(Y) \to \Omega^{(p,q)}(Y)}. \tag{4-1}$$

Recall that Aeppli cohomology, $H_A^{p,q}(Y)$, is defined as

$$H_A^{p,q}(Y) := \frac{\ker \partial\bar\partial : \Omega^{(p,q)}(Y) \to \Omega^{(p+1,q+1)}(Y)}{\big(\operatorname{im} \partial : \Omega^{(p-1,q)}(Y) \to \Omega^{(p,q)}(Y)\big) + \big(\operatorname{im} \bar\partial : \Omega^{(p,q-1)}(Y) \to \Omega^{(p,q)}(Y)\big)}. \tag{4-2}$$

It is standard that for compact Kähler manifolds, the two cohomologies coincide. For $p, q = 0, \dots, n$, we have the natural pairing

$$\wedge : H_{BC}^{p,q}(Y) \times H_A^{n-p,n-q}(Y) \to \mathbb{C}, \tag{4-3}$$

given by the wedge product and integration. If $p : Y \to B$ is a holomorphic map between compact complex manifolds, then for $s := \dim Y - \dim B$, we have a natural map $p_* : H_{BC}^{p,q}(Y) \to H_{BC}^{p-s,q-s}(B)$, defined by the pairing (4-3) and the pull-back p^*.

The Bott–Chern cohomology can be generally defined for arbitrary complex analytic spaces Y in the sense of [Demailly 2012, Definition II.5.2], where one considers differential forms on Y obtained by pullbacks of smooth differential forms through local embeddings of the space into complex vector spaces. Due to a theorem of Lelong, see [Demailly 2012, Theorem III.2.7], the intersection pairing (4-3) can still be defined in this setting, and so the slope (1-4) is well-defined. By resolving the singularities, we can extend the definition of the pushforward for maps between a compact complex analytic spaces Y and a compact manifold B.

Now, let E be a holomorphic vector bundle over Y. Using Chern–Weil theory, one can construct for any Hermitian metric h^E on E a corresponding Chern character form, $\mathrm{ch}(E, h^E)$, which is a d-closed form in $\bigoplus_{p=0}^{+\infty} \Omega^{(p,p)}(Y)$. Bott and Chern [1965] showed that the resulting class in Bott–Chern cohomology doesn't depend on the choice of the metric. This gives a definition of the Chern character, $\mathrm{ch}(E)$ of a vector bundle E with values in Bott–Chern cohomology.

Bismut, Shu, and Wei [Bismut et al. 2023] generalized the definition of the Chern character with values in Bott–Chern cohomology for any coherent sheaf $\mathscr{E}$ on Y. If $\mathscr{E}$ has a finite locally free projective resolution (which is always the case if Y is projective), this construction corresponds to the one given by the alternating sum of Chern characters of the resolution. By [Bismut et al. 2023, §8.6], the (k, k)-component of the Chern character, $\mathrm{ch}_k(\mathscr{E})$, we have

$$\mathrm{ch}_0(\mathscr{E}) = \mathrm{rk}(\mathscr{E}), \quad \mathrm{ch}_1(\mathscr{E}) = c_1(\det \mathscr{E}), \tag{4-4}$$

where $\det \mathscr{E}$ is the Knudsen–Mumford determinant [1976]. Without entering into details of the construction, we mention that the absence of finite locally free projective resolutions of coherent sheaves for general complex manifolds is circumvented in [Bismut et al. 2023] by the use of so-called antiholomorphic superconnections; see [Bismut et al. 2023, Theorem 6.7].

Now, recall that for any proper holomorphic map $p : Y \to B$, and any coherent sheaf $\mathscr{E}$, the Grauert theorem tells that the direct image sheaves $R^q p_* \mathscr{E}$, $q \in \mathbb{N}$, are coherent. The main result of this section goes as follows.

Theorem 4.1. *Let Y be an irreducible compact complex analytic space, L an arbitrary line bundle on Y and $\mathscr{E}$ a coherent sheaf on Y. Let $p : Y \to B$ be a holomorphic map to a compact complex manifold B. Then for any $r \in \mathbb{N}$, and $s := \dim Y - \dim B + r$, in the Bott–Chern cohomology,*

$$\lim_{k\to\infty} \frac{1}{k^s} \sum_{t=0}^{\dim Y} (-1)^t \mathrm{ch}_r(R^t p_*(\mathscr{E} \otimes L^k)) = \frac{\mathrm{rk}(\mathscr{E})}{s!} \cdot p_*(c_1(L)^s). \tag{4-5}$$

Remark 4.2. Despite a huge amount of literature, we were not able to find the proof of this result under the stated hypotheses (even for projective Y, B). For flat maps p and relatively ample L, this result can be alternatively established using Knudsen–Mumford expansions; see [Knudsen and Mumford 1976; Phong et al. 2008, Theorem 3]. Note, however, that flatness doesn't pass through subfamilies, and there is no flatness assumption in Theorem 1.3.

The proof of this result relies on the recent result of [Bismut et al. 2023] establishing the Riemann–Roch–Grothendieck theorem in Bott–Chern cohomology for arbitrary holomorphic maps between (*smooth*!) complex manifolds. More precisely, the main result of [Bismut et al. 2023] says the following.

Theorem 4.3. *Let $p : Y \to B$ be a holomorphic map between compact complex manifolds. Then for any coherent sheaf $\mathscr{E}$ on Y, the identity*

$$\mathrm{Td}(TB) \cdot \sum_{t=0}^{\dim Y} (-1)^t \mathrm{ch}(R^t p_*(\mathscr{E})) = p_*(\mathrm{Td}(TY) \cdot \mathrm{ch}(\mathscr{E})) \tag{4-6}$$

holds in Bott–Chern cohomology, where $\mathrm{Td}(TB)$, $\mathrm{Td}(TY)$ *are the Todd classes.*

Proof of Theorem 4.1. Note first that for smooth manifolds Y, the result follows directly from Theorem 4.3 by (4-4) and the fact that the 0-degree part of the Todd class is identity. If $\dim Y = 0$, then Y is automatically smooth, and, hence, Theorem 4.1 holds as stated.

We will argue by induction on the dimension of Y. For this, we consider a resolution of singularities $f : \hat{Y} \to Y$ of Y. For any $q = 1, \dots, \dim Y$, we define the sheaves $\mathscr{Q}_q$ on Y as $\mathscr{Q}_q := R^q f_* f^* \mathscr{E}$, where $f^* \mathscr{E} := f^{-1} \mathscr{E} \otimes_{f^{-1} \mathscr{O}_Y} \mathscr{O}_{\hat{Y}}$. We define the sheaf $\mathscr{Q}_0$ on Y by the short exact sequence

$$0 \to \mathscr{E} \to R^0 f_* f^* \mathscr{E} \to \mathscr{Q}_0 \to 0. \tag{4-7}$$

By the Grauert theorem, the sheaves $\mathscr{Q}_q$, $q = 0, \dots, \dim Y$, are coherent. Since the resolution of singularities is biholomorphic away from a subset of singular points of Y, and over the locally free locus of $\mathscr{E}$, by the projection formula, see [Hartshorne 1977, Exercise II.5.1d)], we have $R^0 f_* f^* \mathscr{E} = \mathscr{E}$, the supports of the sheaves $\mathscr{Q}_q$, $q = 0, \dots, \dim Y$, are *proper* analytic subsets of Y, which, by irreducibility of Y, have strictly smaller dimension than Y; see [Demailly 2012, Proposition II.4.2.6]. By this and the usual *devissage* techniques (see [EGA III$_1$ 1961, théorème 3.1.2], cf. [Hartshorne 1977, Proposition I.7.4]), for any $q = 0, \dots, \dim Y$, there is $r(q) \in \mathbb{N}$, and complex analytic subspaces $\iota_{i,q} : Z_{i,q} \hookrightarrow Y$, with some ideal sheaves $\mathscr{J}_{i,q}$ on $Z_{i,q}$ and a filtration $\mathscr{F}_{i,q}$ of $\mathscr{Q}_q$, $i = 0, \dots, r(q)$, $\mathscr{F}_{0,q} = \{0\}$, $\mathscr{F}_{r(q),q} = \mathscr{Q}_q$, $\mathscr{F}_{i-1,q} \subset \mathscr{F}_{i,q}$, $i = 1, \dots, r_q$, such that, for any $i = 1, \dots, r(q)$, we have $\mathscr{F}_{i,q} / \mathscr{F}_{i-1,q} = \iota_{i,q,*}(\mathscr{J}_{i,q})$. We let $p_{i,q} := p \circ \iota_{i,q}$, $i = 1, \dots, r(q)$, $\hat{p} := p \circ f$. We argue that for any $k \in \mathbb{N}$, we have

$$\sum_{t=0}^{\dim Y} (-1)^t \mathrm{ch}(R^t p_*(\mathscr{E} \otimes L^k)) = \sum_{t=0}^{\dim Y} (-1)^t \mathrm{ch}(R^t \hat{p}_*(f^* \mathscr{E} \otimes f^* L^k)) - \sum_{t,u=0}^{\dim Y} (-1)^{t+u} \sum_{i=1}^{r(q)} \mathrm{ch}(R^t (p_{i,u})_*(\mathscr{J}_{i,u} \otimes \iota_{i,u}^* L^k)). \tag{4-8}$$

Once (4-8) is established, Theorem 4.1 would follow by induction, as the space $\hat{Y}$ is smooth, and so for the first summand on the right-hand side of (4-8), the smooth version of Theorem 4.1 applies, and the second summand doesn't contribute to the asymptotics by induction hypothesis, as all $Z_{i,q}$ have strictly smaller dimensions than Y.

Now, let us establish (4-8). First of all, since in the derived category, there is a canonical isomorphism between the functors $R\hat{p}_*$ and $Rp_* Rf_*$, see [Bismut et al. 2023, (3.13)], and the construction of Chern character, defined using derived category of coherent sheaves, factors through the K-theory of the derived category of coherent sheaves [Bismut et al. 2023, Theorem 8.11 and §8.9], we have

$$\sum_{t=0}^{\dim Y}(-1)^t \mathrm{ch}(R^t \hat{p}_*(f^*\mathscr{E}\otimes f^*L^k)) = \sum_{t,u=0}^{\dim Y}(-1)^{t+u}\mathrm{ch}\big(R^t p_*(R^u f_*(f^*\mathscr{E}\otimes f^*L^k))\big). \tag{4-9}$$

Now, from the exact sequence (4-7), using again the fact that the construction of the Chern character passes through the formation of K-theory, we obtain

$$\sum_{t=0}^{\dim Y}(-1)^t \mathrm{ch}\big(R^t p_*(R^0 f_*(f^*\mathscr{E}\otimes f^*L^k))\big) = \sum_{t=0}^{\dim Y}(-1)^t \mathrm{ch}(R^t p_*(\mathscr{E}\otimes L^k)) + \sum_{t=0}^{\dim Y}(-1)^t \mathrm{ch}(R^t p_*(\mathscr{Q}_0\otimes L^k)). \tag{4-10}$$

Similarly, for any $q=0,\dots,\dim Y$, we obtain

$$\sum_{t=0}^{\dim Y}(-1)^t \mathrm{ch}(R^t p_*(\mathscr{Q}_q\otimes L^k)) = \sum_{t=0}^{\dim Y}(-1)^t \sum_{i=0}^{r(q)}\mathrm{ch}\big(R^t p_*(\iota_{i,q,*}(\mathscr{J}_{i,q})\otimes L^k)\big). \tag{4-11}$$

Remark, however, that since $\iota_{i,q}$ is a closed embedding, $\iota_{i,q,*}$ is an exact functor, so we have $R^v\iota_{i,q,*}=0$ for $v=1,\dots,\dim Y$, and $R^0\iota_{i,q,*}=\iota_{i,q,*}$. Moreover, by the projection formula, see [Hartshorne 1977, Exercise II.5.1d)], we have $R^0\iota_{i,q,*}(\mathscr{J}_{i,q})\otimes L^k = R^0\iota_{i,q,*}(\mathscr{J}_{i,q}\otimes \iota_{i,q}^* L^k)$. In particular, for any $t,q=0,\dots,\dim Y,\ i=1,\dots,r(q)$, we can write

$$\mathrm{ch}(R^t p_*(\iota_{i,q,*}(\mathscr{J}_{i,q})\otimes L^k)) = \sum_{v=0}^{\dim Y}(-1)^v \mathrm{ch}\big(R^t p_*(R^v\iota_{i,q,*}(\mathscr{J}_{i,q}\otimes \iota_{i,q}^* L^k))\big). \tag{4-12}$$

But using the same argument as in (4-9), we have

$$\sum_{t,v=0}^{\dim Y}(-1)^{t+v}\mathrm{ch}\big(R^t p_*(R^v\iota_{i,q,*}(\mathscr{J}_{i,q}\otimes \iota_{i,q}^* L^k))\big) = \sum_{t=0}^{\dim Y}(-1)^t \mathrm{ch}\big(R^t (p_{i,q})_*(\mathscr{J}_{i,q}\otimes \iota_{i,q}^* L^k)\big). \tag{4-13}$$

Now, a combination of (4-9), (4-10), (4-11), (4-12) and (4-13), gives us (4-8). □

Now, let us finally establish an application of Theorem 4.1 towards the study of Harder–Narasimhan slopes of direct images. We fix an irreducible compact complex analytic space Y of dimension $k+m$, $k\geq 0$, with a surjective holomorphic map $\pi: Y\to B$. Let ω_B be a Gauduchon Hermitian form on B. Let L be a relatively ample line bundle on Y. Recall that in (1-4), we defined the slope of Y, and before Theorem 1.1, we defined the slopes of coherent sheaves.

Lemma 4.4. $$\mu(Y)\cdot\int_B[\omega_B^m] = \lim_{k\to\infty}\mu(R^0\pi_*L^k)/k.$$

Proof. By the Serre vanishing theorem, the higher direct images $R^v\pi_*L^k,\ v\geq 1$, vanish. By (4-4), we conclude that

$$\mu(R^0\pi_*L^k) = \frac{\int_Y[\mathrm{ch}_1(R^0\pi_*L^k)]\cdot[\omega_B^{m-1}]}{\mathrm{ch}_0(R^0\pi_*L^k)}. \tag{4-14}$$

The result now follows directly from Theorem 4.1. □

Proposition 4.5. *The vector bundles E_k are asymptotically semistable if and only if $\eta^{\mathrm{HN}}_{\min} = \eta^{\mathrm{HN}}_{\max}$. Moreover, if E_k are asymptotically semistable, then for any subsheaves $\mathcal{F}_k$ of E_k, $\mathrm{rk}(\mathcal{F}_k) > 0$, and any $\epsilon > 0$, for k big enough, we have $\mu(\mathcal{F}_k) \leq \mu(E_k) + \epsilon k$.*

Proof. The maximal and the minimal slopes satisfy

$$\begin{aligned} \mu^k_{\max} &= \sup\big\{\mu(\mathcal{F}_k) : \mathcal{F}_k \text{ is a subsheaf of } E_k\big\}, \\ \mu^k_{\min} &= \inf\big\{\mu(\mathcal{Q}_k) : \mathcal{Q}_k \text{ is a quotient sheaf of } E_k\big\}. \end{aligned} \tag{4-15}$$

Now, by Theorem 1.5, as $k \to \infty$, we have

$$\lim_{k\to\infty} \frac{\mu(E_k)}{k} = \int_{\mathbb{R}} x d\eta^{\mathrm{HN}}(x). \tag{4-16}$$

From (4-15) and (4-16), we see that E_k are asymptotically semistable if and only if $\eta^{\mathrm{HN}}_{\min} = \operatorname{ess\,sup} \eta^{\mathrm{HN}}$. However, by Theorem 1.5, $\operatorname{ess\,sup} \eta^{\mathrm{HN}}$ coincides with $\eta^{\mathrm{HN}}_{\max}$, which finishes the proof of the first part of the theorem. The proof of the second statement of Proposition 4.5 follows directly by (4-15) and the first part. □

Remark 4.6. From [Finski 2024b, Proposition 5.1], see also [Xu and Zhuang 2020], we know that if $\dim B = 1$, then $\operatorname{ess\,inf} \eta^{\mathrm{HN}}$ coincides with $\eta^{\mathrm{HN}}_{\min}$. The above proof shows that for $\dim B = 1$, the condition on the subsheaves from Proposition 4.5 is equivalent to asymptotic semistability.

Proof of Theorem 1.1. This follows immediately from Theorem 1.7 and Proposition 4.5. □

Proposition 4.7. *For any complex analytic subspace Y of X as in Theorem 1.3, the bound*

$$\mu(Y) \cdot \int_B [\omega_B^m] \geq \eta^{\mathrm{HN}}_{\min}$$

holds.

Proof. Consider the following short exact sequence of sheaves associated with Y

$$0 \to \mathscr{J}_Y \to \mathscr{O}_X \to \iota_* \mathscr{O}_Y \to 0, \tag{4-17}$$

where $\mathscr{J}_Y$ is the ideal sheaf of Y, consisting of local holomorphic functions on X, vanishing along Y, and $\mathscr{O}_Y$ is the structure sheaf of Y associated with the reduced scheme structure of Y, i.e., defined by (4-17). By considering a long exact sequence of direct images associated with (4-17) and the map π, and using the Serre vanishing theorem, we conclude that the restriction map $R^0\pi_* L^k \to R^0\pi|_{Y,*} L|_Y^k$ is surjective. Then, in the notation of (4-15), we have $\mu^k_{\min} \leq \mu(R^0\pi|_{Y,*} L|_Y^k)$. We deduce Proposition 4.7 from Lemma 4.4 by diving by k and passing to the limit $k \to \infty$. □

Proof of Theorem 1.3. First of all, by Lemma 4.4, we conclude that

$$\lim_{k\to\infty} \mu(E_k)/k = \mu(X) \cdot \int_B [\omega_B^m] \geq \eta^{\mathrm{HN}}_{\min}. \tag{4-18}$$

Moreover, since $\operatorname{ess\,sup} \eta^{\mathrm{HN}}$ coincides with $\eta^{\mathrm{HN}}_{\max}$ by [Finski 2024b, Theorem 1.1], by (4-16), we conclude that the equality in the above inequality holds if and only if $\eta^{\mathrm{HN}}_{\min} = \eta^{\mathrm{HN}}_{\max}$, i.e., when E_k is asymptotically semistable by Proposition 4.5. In particular, if E_k is asymptotically semistable, then by $\eta^{\mathrm{HN}}_{\min} = \eta^{\mathrm{HN}}_{\max}$, Proposition 4.7 and (4-18), we establish the first part of Theorem 1.3.

Let us now establish the second part. By a reformulation of the result of Xu and Zhuang [2020, Lemma 2.26 and Proposition 2.28] from [Finski 2024b, (1.5)], we have

$$\eta^{\mathrm{HN}}_{\min} = \inf_{C \subset X} \mu(C) \cdot \int_B [\omega_B^m], \tag{4-19}$$

where C runs over all irreducible curves in X, with project surjectively to B. In particular, from (4-19), we conclude that

$$\eta^{\mathrm{HN}}_{\min} \geq \inf_{Y \subset X} \mu(Y) \cdot \int_B [\omega_B^m], \tag{4-20}$$

where Y are as in Theorem 1.3. A combination of (4-18) and (4-20) shows that if $\inf_{Y \subset X} \mu(Y) = \mu(X)$, then both (4-18) and (4-20) are actually equalities. By the remark after (4-18), this implies that E_k is asymptotically semistable, which finishes the proof. □

Remark 4.8. It is interesting to know if the second part of Theorem 1.3 continues to hold for $\dim B > 1$. There are several potential pitfalls for that. First, since B is not necessarily projective, there might be very few analytic subspaces $Y \subset X$, projecting surjectively to B. Second, even for projective B, the main result of [Finski 2024b, Theorem 1.4] implies that the analogue of the bound (4-19) becomes tight if one considers among Y all subcurves in X projecting to generic curves over the base. But it seems that there are many more curves like that than analytic subspaces projecting surjectively to the base.

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HESSIAN ESTIMATES FOR SPECIAL LAGRANGIAN EQUATION BY DOUBLING

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New doubling proofs are given for the interior Hessian estimates of the special Lagrangian equation. These estimates were originally shown by Chen, Warren and Yuan in CPAM 2009 and Wang and Yuan in AJM 2014. This yields a higher codimension analogue of Korevaar's 1987 pointwise proof of the gradient estimate for minimal hypersurfaces, without using the Michael–Simon mean value inequality.

1. Introduction

The pointwise estimate for minimal surfaces. Korevaar [1987] gave a new pointwise proof of the gradient estimate for solutions of the minimal hypersurface PDE. The proof was modeled after Cheng and Yau's cutoff [1976] in the maximal surface context. Korevaar's pointwise proof was robust enough to give gradient estimates for fully nonlinear relatives, the sigma-k curvature equations.

The original proof by Bombieri, De Giorgi and Miranda [1969], and simplified by Trudinger [1972], uses two tools from minimal surface theory: the Michael–Simon mean value inequality for graphs with bounded mean curvature, and the Jacobi inequality $\Delta b \geq |\nabla b|^2$, a strong subharmonicity originating from Jacobi fields in the vertical direction. The Korevaar proof relies only on the Jacobi inequality. The two-dimensional surface proof of Gregori [1994] uses isothermal coordinates.

Although the Jacobi inequality can sometimes be found in other categories using ordinary differential calculus, the mean value inequality, and its cousin the monotonicity formula, is a delicate integral relation which is difficult to establish outside the minimal surface context.

Higher codimensions? Despite its versatility, an analogous Korevaar argument is missing for higher codimension minimal surfaces. Wang [2004] established a gradient estimate under the area decreasing condition using an integral method. More recently, Dimler [2023] found a pointwise proof under the area decreasing condition, using Savin's theory of viscosity solutions. However, the method requires an additional condition, that all but one component of the graph to be small.

Main result of this paper. We find a Korevaar-type proof of the gradient estimate for a class of high-codimension minimal surfaces. These surfaces can be described by a single potential function u, such that (x, Du) is a minimal surface. The potential solves a second-order, fully nonlinear, elliptic PDE (2-1) called the special Lagrangian equation, as shown by Harvey and Lawson [1982]. In this context, the gradient estimate for (x, Du) is a Hessian estimate for u.

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Despite its relative simplicity compared to general high-codimension surfaces, a Korevaar proof of the Hessian estimate for the special Lagrangian equation was elusive. Integral proofs under much weaker, and sharp by [Nadirashvili and Vlăduţ 2010; Wang and Yuan 2013; Mooney and Savin 2024] singular solutions, conditions were only established by Chen, Warren and Yuan [Chen et al. 2009], and Wang and Yuan [2014]. A pointwise proof was attempted in [Warren and Yuan 2008] but required a flatness condition on the gradient.

The main technical ingredient of our proof is a Korevaar-type pointwise calculation. The other ingredients are pure PDE techniques, described below. In particular, nowhere is the Michael–Simon mean value inequality used.

A doubling approach. Our approach to the Hessian estimate is based on Shankar and Yuan's resolution of the Hessian estimate for the sigma-2 equation in dimension four [2025]. The first step is to derive partial regularity by combining an Alexandrov (D^2u-existing-a.e.) theorem with Savin's ε-regularity [2007]: the singular set is closed and Lebesgue measure zero. The next step is to propagate this partial regularity to the entire domain using a doubling inequality for the Hessian. Partial regularity implies local boundedness of the Hessian inside the smooth set, so the doubling gives a global $C^{1,1}$ estimate and rules out the singular set.

The doubling inequality generally requires a Jacobi field type inequality $\Delta b \geq |\nabla b|^2$. Trudinger [1980] showed doubling in the uniformly elliptic Harnack inequality context. Using the Guan–Qiu test function [2019], Qiu [2024b] established doubling for the sigma-2 equation in dimension three, for which Jacobi is available. In fact, the sigma-2 equation is a special Lagrangian equation in dimension three only. Shankar and Yuan [2025] showed doubling for the sigma-2 equation in dimension four using an almost-Jacobi inequality with a degenerate coefficient. Shankar and Yuan [2024] found a geometric doubling inequality for the Monge–Ampère equation.

In the present paper, we use the Jacobi inequalities of [Chen et al. 2009; Wang and Yuan 2014] to discover doubling inequalities for the special Lagrangian equation in convex and critical/supercritical phase categories.

Another partial regularity propagation has been used for the minimal hypersurface equation. Caffarelli and Wang [1993] gave another proof of the $C^{1,\alpha}$ regularity of Lipschitz solutions. Starting with $C^{1,\alpha}$ partial regularity (page 155), they use a geometric Harnack inequality to propagate this flatness to the entire domain (page 156).

New ideas to establish the doubling inequality. We modify the Korevaar-type calculation to our high-codimension setting. This fails to give a Hessian estimate, but it yields a doubling inequality. Two modifications are needed to Korevaar to achieve this. We first mix Guan and Qiu's test function involving the radial derivative $x \cdot Du - u$ with the Korevaar cutoff to create a minimal surface version of Guan–Qiu. Secondly, for critical phases, the equation's ellipticity and concavity degenerate, and we need to add an additional increasing, concave term to the cutoff to compensate. Unfortunately, only Green's-type functions have strong enough concavity, and the cutoff becomes singular. Nevertheless, we only need to establish a doubling inequality, rather than a Hessian estimate. We are free to exclude a small sphere from our calculations. We can then place the singularity inside this inner sphere without analytic problems.

The Qiu cutoff [2024b] used for sigma-2 in three dimensions (i.e., critical phase sLag in 3D) does not seem to extend to the special Lagrangian equation in the convex or higher-dimensional critical phase settings. Either a modification of this cutoff or a singular cutoff of Korevaar/Guan–Qiu type seems important to obtain the doubling inequality.

Wang and Yuan [2014] established $n-1$ convexity of solutions. This slightly weaker version of convexity and the black box in [Chaudhuri and Trudinger 2005] allow us to establish Alexandrov regularity without any trouble. In other situations, Alexandrov regularity can be challenging.

2. Statement of results

This paper gives pointwise proofs of the Hessian estimates for the special Lagrangian equation:

$$\sum_{i=1}^{n} \arctan \lambda_i(D^2u) = \Theta = \text{constant} \in \left(-n\frac{\pi}{2}, n\frac{\pi}{2}\right). \tag{2-1}$$

Here, the λ_i are the eigenvalues of the Hessian D^2u of solution $u(x)$. The symmetric polynomial σ_k version of this equation is

$$\cos\Theta\,(\sigma_1-\sigma_3+\sigma_5-\cdots)-\sin\Theta\,(1-\sigma_2+\sigma_4-\cdots)=0.$$

Harvey and Lawson [1982] showed that Lagrangian graph $(x, Du(x)) \in (\mathbb{R}^n\times\mathbb{R}^n, dx^2+dy^2)$ is a volume minimizing submanifold. The phase is called critical or supercritical if $\Theta \geq (n-2)\pi/2$ [Yuan 2006]. In this case, Yuan showed that the PDE has convex level set.

The result of this paper is a new proof of the following two Hessian estimates. The first was shown in [Chen et al. 2009], with interior regularity in [Chen et al. 2023] and further developments for prescribed phase and mean curvature flows in [Warren 2008; Bhattacharya and Shankar 2023; 2024; Bhattacharya and Wall 2024]. The Chen–Warren–Yuan estimate is explicit, while our proof is by compactness.

Theorem 2.1 (convex solutions). *Let u be a smooth convex solution of* (2-1) *in $B_2(0)$. Then*

$$|D^2u(0)| \leq C(n, \|u\|_{C^{0,1}(B_1(0))}, \Theta).$$

Stronger forms of the next estimate were shown in [Warren and Yuan 2009b; 2010; Wang and Yuan 2014] for $n \geq 3$ and [Warren and Yuan 2009a] in dimension two. Further developments include inhomogeneous equations [Bhattacharya 2021; 2022; Lu 2023a; 2023b; Zhou 2025], curvature equations [Qiu 2024a; Qiu and Zhou 2024], and mean curvature flows [Bhattacharya and Wall 2025]. We also restrict to $n \geq 3$. The dimension-two case is either harmonic, or covered by the simple compactness method in [Li 2019]. These two-dimensional cases were first consequences of results by Heinz [1959] and Gregori [1994] using isothermal coordinates.

Theorem 2.2 (critical phase). *Let u be a smooth solution of* (2-1) *on $B_2(0)$ for phase Θ critical $\Theta=(n-2)\pi/2$ or supercritical $\Theta \in ((n-2)\pi/2, n\pi/2)$ for $n \geq 3$. Then*

$$|D^2u(0)| \leq C(n, \|u\|_{C^{0,1}(B_1(0))}, \Theta).$$

A byproduct is a removal of the flatness condition in the pointwise proof of [Warren and Yuan 2008], and a generalization of their condition required for the estimate. Given a smooth solution u of (2-1), we say that positive, proper, smooth function $a(D^2u)$ of the Hessian has a *Jacobi inequality* if $\Delta_g a \geq 2|\nabla_g a|^2/a$. We also recall that a semiconvex function has a Hessian lower bound $D^2u \geq -KI$ for some $K > 0$, and that a proper function a satisfies $a^{-1}(B)$ is bounded for any bounded set B.

Theorem 2.3 (semiconvex and Jacobi). *Let u be a smooth solution of* (2-1) *on $B_2(0)$ which is semiconvex and has a Jacobi inequality. Then*

$$|D^2u(0)| \leq C(n, \|u\|_{C^{0,1}(B_1(0))}, a, K, \Theta).$$

Remark 2.4. One consequence is a new proof of the following. The Hessian estimate was earlier shown in a pointwise proof of [Warren and Yuan 2008, Lemma 2.2] assuming the Hessian eigenvalue condition

$$3 + (1-\varepsilon)\lambda_i^2 + 2\lambda_i\lambda_j \geq 0, \quad 1 \leq i, j \leq n, \tag{2-2}$$

for some $\varepsilon > 0$, under an additional flatness condition $|Du(x)| \leq \delta(n)|x|$. A similar estimate for convex Lagrangian mean curvature flow appears in [Bhattacharya et al. 2025]. Later, this estimate was shown in [Ding 2023, Theorem 5.1] without flatness, for a slightly negative ε above, using the Michael–Simon mean value inequality. Theorem 2.3 shows how to remove the Warren–Yuan flatness condition on Du in the pointwise proof. Indeed, equation (4.52) and Lemma 4.1 in [Ding 2023] show that u is semiconvex under condition (2-2). The Jacobi inequality in [Warren and Yuan 2008, Lemma 2.1] then verifies that the assumptions for Theorem 2.3 are verified. It is likely that doubling proofs for the subcritical estimates in [Zhou 2022; Zhou 2023] are also possible.

Remark 2.5. In view of Mooney and Savin's [2024] recent semiconvex singular solution of (2-1), it is reasonable to expect that the Jacobi inequality required for Theorem 2.3 fails for such solutions. In fact, after a Legendre–Lewy transform, their solution satisfies $\det D^2\bar{u} = 0$ on a subdomain. This equation lacks ellipticity and concavity, which seems necessary to establish Jacobi inequalities.

3. Preliminaries

3.1. ***Notation.*** For a function $u(x)$, we define $u_i = \partial u/\partial x^i$ and $u_{ij} = \partial^2 u/\partial x^i \partial x^j$. On the other hand, eigenvalues λ_i of the Hessian and subharmonic quantities $b_m = m^{-1}\big(\ln\sqrt{1+\lambda_1^2} + \cdots + \ln\sqrt{1+\lambda_m^2}\big)$ do not denote partial derivatives. Moreover, $C(n)$ denotes various dimensional constants.

3.2. ***Differential operators.*** For $g = dx^2 + dy^2|_{y=Du}$, or $g = I + D^2uD^2u$, the Laplace–Beltrami operator is

$$\Delta_g = \frac{1}{\sqrt{\det g}}\partial_i\big(\sqrt{\det g}\, g^{ij}\partial_j\big). \tag{3-1}$$

In fact, the mean curvature is $H = \Delta_g(x, Du(x))$. By [Harvey and Lawson 1982], it follows that $H = 0$ on solutions of (2-1). Since this implies x^i are harmonic coordinates where $\Delta_g x = 0$, the Laplace operator simplifies to the linearized operator of (2-1),

$$\Delta_g = g^{ij}\partial_{ij} \overset{p}{=} \frac{1}{1+\lambda_i^2}\partial_{ii} \tag{3-2}$$

at any diagonal point $\lambda_i = u_{ii}$ of the Hessian, such as after composition with a rotation. Here, we assume summation over repeated indices, unless the index ranges are stated. The gradient and inner product with respect to the metric are

$$\nabla_g v = (g^{1i}v_i, \dots, g^{n1}v_i), \quad \langle \nabla_g v, \nabla_g w\rangle_g = g^{ij}v_i w_j \overset{p}{=} g^{ii}v_i w_i, \quad |\nabla_g v|^2 = \langle \nabla_g v, \nabla_g v\rangle_g \overset{p}{=} g^{ii}v_i^2, \tag{3-3}$$

where $v_i = \partial_i v$ for a function v.

3.3. *Jacobi inequality*: *convex*. We recall the Jacobi inequality for smooth convex solutions of (2-1). Given a volume form $dV_g = \sqrt{\det g}\,dx$, we define

$$V = \sqrt{\det g} = \sqrt{\det(I + (D^2u)^2)} = \prod_{i=1}^{n} \sqrt{1+\lambda_i^2}. \tag{3-4}$$

Then the Jacobi inequality is established by directly taking derivatives and using algebra.

Proposition 3.1 [Chen et al. 2009, Proposition 2.1]. *Let u be a smooth **convex** solution of* (2-1) *on $B_R(0) \subset \mathbb{R}^n$. Then*

$$\Delta_g \ln V \geq \frac{1}{n}|\nabla_g \ln V|^2, \tag{3-5}$$

or equivalently, for $a = V^{1/n}$,

$$\Delta_g a \geq 2\frac{|\nabla_g a|^2}{a}. \tag{3-6}$$

3.4. *Jacobi inequality*: *critical or supercritical phase*. We order the eigenvalues of the Hessian by $\lambda_1 \geq \cdots \geq \lambda_n$.

Proposition 3.2 [Wang and Yuan 2014, Lemma 2.3]. *Let u be a smooth solution of* (2-1) *with $\Theta \geq (n-2)\pi/2$. Suppose u is smooth near $x = p$ and that at $x = p$, $\lambda_1 = \cdots = \lambda_m > \lambda_{m+1}$. Then the function $b_m = m^{-1}\sum_1^m \ln\sqrt{1+\lambda_m^2}$ is smooth near $x = p$, and satisfies*

$$\Delta_g b_m \geq M|\nabla_g b_m|^2, \quad M := \left(1 - \frac{4}{\sqrt{4n+1}+1}\right), \tag{3-7}$$

or equivalently, for $a_m = \exp(M b_m)$,

$$\Delta_g a_m \geq 2\frac{|\nabla_g a_m|^2}{a_m}. \tag{3-8}$$

Note that b_m is symmetric in the degenerate eigenvalues. See [Andrews 2007, Theorem 5.1] for the second derivative calculation of symmetric eigenvalue functions. One can take a degenerate limit in this calculation if b_m is symmetric.

3.5. ***The $n-1$ convexity for critical or supercritical phases.*** We recall the following eigenvalue pinching obtained from (2-1) for large phases using trigonometric identities.

Lemma 3.3 [Wang and Yuan 2014, Lemma 2.1]. *Suppose the ordered numbers $\lambda_1 \geq \cdots \geq \lambda_n$ solve* (2-1) *with $\Theta \geq (n-2)\pi/2$ and $n \geq 2$. Then*

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} > 0 \quad \textit{and} \quad \lambda_{n-1} \geq |\lambda_n|, \tag{3-9}$$

$$\lambda_1 + n\lambda_n \geq 0, \tag{3-10}$$

$$\sigma_k(\lambda_1, \dots, \lambda_n) \geq 0 \quad \textit{for all} \ \ 1 \leq k \leq n-1. \tag{3-11}$$

Condition (3-11) is called $n-1$ *convexity*. More generally, we say u is k-convex if $\sigma_\ell \geq 0$ for $1 \leq \ell \leq k$. It is interpreted in the viscosity sense for nonsmooth u. Condition (3-9) is related to the convexity of the PDE level set $F^{-1}\{0\}$, since derivative $1/(1+\lambda_i^2)$ is increasing with i; see [Yuan 2006] for a proof of this fact.

3.6. ***Closedness of viscosity subsolutions.*** We say that u is a viscosity subsolution of a fully nonlinear elliptic PDE $F(D^2u) = 0$, i.e., locally uniformly continuous F satisfies $F(M+N) > F(M)$ for any $N > 0$ at each matrix M in a convex cone of symmetric matrices containing the positive definite ones, if $F(D^2Q) \geq 0$ for each quadratic Q touching u from above near a point, or $Q(x_0) = u(x_0)$ with $Q \geq u$ near $x_0 \in \Omega$; see [Caffarelli and Cabré 1995, Proposition 2.4]. A smooth viscosity subsolution satisfies $F(D^2u) \geq 0$ pointwise. A supersolution satisfies the reverse inequality, and a solution is both a subsolution and a supersolution.

Special Lagrangian equation (2-1) is elliptic, and σ_k is elliptic on the cone of k-convex matrices, or the M satisfying $\sigma_\ell(M) \geq 0$ for $1 \leq \ell \leq k$; see [Trudinger and Wang 1999, equation (2.3)] for this and similar basics of k-convexity.

We will use the standard fact that the uniform limit of a sequence of viscosity solutions of an elliptic equation is also viscosity. This is stated in [Caffarelli and Cabré 1995], and this basic proof is written down in, for example, [Shankar and Yuan 2025, Appendix]. Since the domain of the special Lagrangian equation is entire, this is clear. For k-convexity, we repeat the proof verbatim to show the known fact that a uniform limit of k-convex solutions is also k-convex.

Lemma 3.4 [Caffarelli and Cabré 1995]. *Let $u_k \in C(\Omega)$ be a sequence of k-convex functions converging uniformly to $u \in C(\Omega)$. Then u is k-convex.*

3.7. ***Alexandrov theorem on bounded domains.*** The condition of k-convexity leads to an Alexandrov theorem, which is standard for convex, i.e., n-convex functions. Let us verify the standard fact that the "black box" still works on bounded domains.

Proposition 3.5 [Chaudhuri and Trudinger 2005, Theorem 1.1]. *Let $u \in C(\Omega)$ for a domain $\Omega \subset \mathbb{R}^n$ with $n \geq 2$. Suppose u is k-convex for $k > n/2$. Then u is twice differentiable almost everywhere in Ω. More precisely, for almost every $x_0 \in \Omega$, there is a quadratic Q such that $u(x) - Q(x) = o(|x-x_0|^2)$.*

Proof. Theorem 1.1 in [Chaudhuri and Trudinger 2005] works if $\Omega = \mathbb{R}^n$, so it suffices to extend u to a k-convex function $\mathbb{R}^n$ outside a small neighborhood of any point $x_0 \in \mathbb{R}^n$. Since u is continuous, we can choose a tall enough convex polynomial P such that $P(x_0) < 0$ but $P(x) > u(x)$ on some $\partial B_r(x_0) \Subset \Omega$. Since P is convex, it is k-convex, so if we define $\bar{u} := \max(P, u)$ on $B_r(x_0)$ and $\bar{u} = P$ outside $B_r(x_0)$, this is a viscosity subsolution of $\sigma_\ell \geq 0$, hence k-convex. By Alexandrov theorem [Chaudhuri and Trudinger 2005, Theorem 1.1], we conclude $\bar{u}$ is second-order differentiable almost everywhere, hence u is also Alexandrov on a neighborhood of x_0. Varying $x_0 \in \Omega$, we conclude the proof. □

3.8. ***Savin small perturbation theorem.*** We restate [Savin 2007, Theorem 1.3] for equations $F(M)$ only depending on the Hessian, defined on $\mathrm{Sym}(n; \mathbb{R})$

Proposition 3.6 [Savin 2007, Theorem 1.3]. *Let $F(D^2u)$ satisfy the following hypotheses*:

(i) $F \in C^2$.

(ii) *F is locally uniformly elliptic*, $F'(M) > 0$.

(iii) $F(0) = 0$.

Then there exists c_1 small enough depending on n, F such that if a viscosity solution u of $F(D^2u) = 0$ satisfies flatness $\|u\|_{L^\infty(B_1(0))} \leq c_1$, then $u \in C^{2,\alpha}(B_{1/2})$ with $\|u\|_{C^{2,\alpha}(B_{1/2})} \leq 1$.

3.9. ***Partial regularity.*** Suppose u is a viscosity solution of (2-1) with Alexandrov, or D^2u exists a.e. Then by combining with Savin, we deduce the singular set of u is closed and measure zero (partial regularity). Indeed, if $u - Q = o(|x|^2)$, then one can apply Savin (Proposition 3.6) to

$$v_r(x) = \frac{u(rx) - Q(rx)}{r^2} = \frac{o(r^2)}{r^2}.$$

This function is flat and solves $G(D^2v) = F(D^2Q + D^2v) = 0$ with $G(0) = 0$, so Savin gives $C^{2,\alpha}$ regularity nearby the Alexandrov point. This shows the set of second-order differentiable points is open, full measure, and contained in the C^∞ set. In particular, we have partial regularity for (2-1) in the cases of convex solutions and critical or supercritical phases.

4. Doubling for convex or semiconvex solutions

This section establishes a doubling inequality for the Hessian. First we consider the convex solution case, with Jacobi inequality (3-6). Recall that a proper function f satisfies $f^{-1}(B)$ bounded for bounded set B.

Proposition 4.1. *Let $u \in C^\infty$ solve* (2-1) *on $B_2(0)$ with u convex. Then for any $y \in B_{1/2}(0)$, there exists $R(n, \|u\|_{C^{0,1}(B_1(0))}) > 0$ small enough such that, for any $r \leq R$,*

$$\sup_{B_R(y)} a(D^2u) \leq C(r, n, \|u\|_{C^{0,1}(B_1(0))}) \sup_{B_r(y)} a(D^2u). \tag{4-1}$$

By the properness of $a = V^{1/n}$, we obtain

$$\sup_{B_R(y)} |D^2u| \leq C(r, n, \|u\|_{C^{0,1}(B_1(0))}, \sup_{B_r(y)} |D^2u|). \tag{4-2}$$

Next we consider the semiconvex solution with a Jacobi inequality case.

Proposition 4.2. *Let $u \in C^\infty$ solve* (2-1) *on $B_2(0)$ with u semiconvex $D^2u \ge -KI$ with a Jacobi inequality $\Delta_g a \ge 2|\nabla_g a|^2/a$. Then for any $y \in B_{1/2}(0)$ and $0 < r \le \frac{1}{4}$, there exists $R(n, K, \|u\|_{C^{0,1}(B_1(0))}) > 0$ small enough such that*

$$\sup_{B_R(y)} a(D^2u) \le C(r, K, n, \|u\|_{C^{0,1}(B_1(0))}) \sup_{B_r(y)} a(D^2u). \tag{4-3}$$

By the properness of a, we obtain

$$\sup_{B_R(y)} |D^2u| \le C(r, K, n, \|u\|_{C^{0,1}(B_1(0))}, a, \sup_{B_r(y)} |D^2u|). \tag{4-4}$$

We prove this in two separate cases of the same calculation.

Proof. Letting $h \ll 1$ and $t \gg 1$ with $y \in B_{1/2}(0)$, we define a Korevaar [1987] exponential cutoff using a Guan–Qiu [2019] type radial derivative for the phase:

$$\eta = (e^{(1-\varphi)/h} - 1)_+, \quad \varphi = (x-y)\cdot Du - u + u(y) + \tfrac{1}{2}t|x-y|^2. \tag{4-5}$$

We make sure $t \ge C(\|u\|_{C^{0,1}(B_1)})$ is large enough for $\varphi > 1$ on $\partial B_{1/2}(y)$. Then $\operatorname{supp}(\eta) \Subset B_1(0)$. Also $B_r(y) \Subset \operatorname{supp}(\eta)$ for $r \le R(t, \|u\|_{C^{0,1}(B_1)})$ small enough. Note that we continuously extend $\eta = 0$ outside the connected component of $B_1(0)$ containing $x = y$. We also note that the cutoff is rotationally invariant about the point $x = y$.

We now start with a standard calculation. At the max point of ηa, we know

$$\nabla_g \eta = -\frac{\eta \nabla_g a}{a}, \tag{4-6}$$

so the Jacobi implies

$$\begin{aligned} 0 &\ge a\Delta_g\eta + 2\langle\nabla_g\eta, \nabla_g a\rangle + \eta\Delta_g a \\ &= a\Delta_g\eta + \eta\left(\Delta_g a - \frac{2|\nabla_g a|^2}{a}\right) \\ &\ge a\Delta_g\eta. \end{aligned} \tag{4-7}$$

Therefore,

$$|\nabla_g\varphi|^2 \le h\Delta_g\varphi. \tag{4-8}$$

The right-hand side at a diagonal point $u_{ii} = \lambda_i$ with $\lambda_1 \ge \lambda_n$ (omitting sums) is

$$\Delta_g\varphi = \frac{2\lambda_i + t}{1+\lambda_i^2} \le Ct. \tag{4-9}$$

The left-hand side is

$$|\nabla_g\varphi|^2 = (x_i - y_i)^2\frac{(\lambda_i + t)^2}{1+\lambda_i^2}. \tag{4-10}$$

(i) Suppose *u* is convex. Since $\lambda_i \ge 0$, $t > 1$, we get

$$(x_i - y_i)^2\frac{t^2 + 2t\lambda_i + \lambda_i^2}{1+\lambda_i^2} \ge |x-y|^2. \tag{4-11}$$

We obtain

$$|x-y|^2 \le Cht \le r^2 \tag{4-12}$$

if $h = r^2/Ct$.

Therefore, the maximum value occurs in $\overline{B_r(y)}$ or on the boundary of $B_1(0)$. Since $\eta = 0$ on $\partial B_1(0)$, it occurs in $\overline{B_r(y)}$. Using $\eta > 0$ on $B_R(y)$, we obtain the doubling inequality

$$\sup_{B_R(y)} a \le C \sup_{B_R(y)} \eta a \le C \sup_{B_1(0)} \eta a \le C \sup_{B_r(y)} \eta a \le C \sup_{B_r(y)} a. \tag{4-13}$$

Here, $C = C(r, n, \|u\|_{C^{0,1}(B_1(0))})$.

(ii) Suppose u is semiconvex, $\lambda_i \ge -K$. We first ensure $t \ge 2K$. Suppose $|x_i - y_i| \ge |x - y|/\sqrt{n}$ for some $1 \le i \le n$.

Subcase $\lambda_i \le 3K$. Then by

$$(\lambda_i + t)^2 = ((\lambda_i + K) + (t - K))^2 \ge (t - K)^2 \ge K^2,$$

we get

$$(x_i - y_i)^2 \frac{(\lambda_i + t)^2}{1 + \lambda_i^2} \ge (x_i - y_i)^2 \frac{K^2}{1 + 9K^2} \ge c\,|x - y|^2. \tag{4-14}$$

Subcase $\lambda_i > 3K$. Supposing also $t > 1$, then as in the convex case,

$$(x_i - y_i)^2 \frac{t^2 + 2t\lambda_i + \lambda_i^2}{1 + \lambda_i^2} \ge \frac{|x - y|^2}{n}. \tag{4-15}$$

Overall, we obtain from (4-8)

$$|x - y|^2 \le C(n, K)ht \le r^2, \tag{4-16}$$

if $h \le C(n, K, t)r^2$. As in case (i) above, we obtain the doubling inequality, noting the dependence $t = t(n, K, \|u\|_{C^{0,1}(B_1(0))})$. □

5. Doubling for critical special Lagrangian equation by singular cutoff

We establish the doubling inequality for critical phases $\Theta \ge (n-2)\pi/2$. Recall (3-8).

Proposition 5.1. *Let $u \in C^\infty$ solve* (2-1) *on $B_2(0)$ with $\Theta \ge (n-2)\pi/2$. Then for any $y \in B_{1/2}(0)$ and $r < \frac{1}{4}$,*

$$\sup_{B_{1/4}(y)} a_1(D^2 u) \le C(r, n, \|u\|_{C^{0,1}(B_1(0))}) \sup_{B_r(y)} a_1(D^2 u). \tag{5-1}$$

By the pinching (3-9), *we obtain properness, and conclude*

$$\sup_{B_{1/4}(y)} |D^2 u| \le C(r, n, \|u\|_{C^{0,1}(B_1(0))}, \sup_{B_r(y)} |D^2 u|). \tag{5-2}$$

In order to establish a doubling inequality, we are free to sacrifice all control inside a small ball. Therefore, we can add a singularity to our cutoff inside this ball.

Proof. **Step 1: cutoff.** Let $\alpha, h^{-1} \gg 1$. We form the *singular cutoff* on $B_1(0) \setminus \{y\}$ of Korevaar exponential type,

$$\eta = (e^{(S-\varphi)/h} - 1)_+, \tag{5-3}$$

where, for $y \in B_{1/2}(0)$, we add an increasing concave term to Guan and Qiu's radial derivative:

$$\varphi = (x-y)\cdot Du - u + u(y) - \frac{\alpha^{-1}2^{\alpha}}{|x-y|^{2\alpha}},$$
$$S = -1 - \|(x-y)\cdot Du - u + u(y)\|_{L^\infty(B_{1/2}(y))} - \alpha^{-1}2^{3\alpha}. \tag{5-4}$$

Then $S-\varphi < 0$ on $\partial B_{1/2}(y)$ and $S-\varphi > 0$ on $B_{1/4}(y)$ for α large enough. In general,

$$B_{1/4}(y)\setminus\{y\} \Subset \operatorname{supp}(\eta) \Subset B_{1/2}(y) \subset B_1(0).$$

We extend $\eta = 0$ outside the connected component of $\{\eta > 0\}$ in $B_1 \setminus \{y\}$ containing the hole at $x = y$.

Step 2: test function. We next consider the maximum point p of ηa_1 on $B_{1/2}(y)\setminus B_r(y)$. If p is in the interior, then suppose that $\lambda_1 = \cdots = \lambda_m > \lambda_{m+1}$ at $x = p$. It follows that a_m in Proposition 3.2 is smooth near $x = p$ and attains its maximum at $x = p$. As in the Jacobi calculation (4-7), we obtain at p

$$|\nabla_g \varphi|^2 \le h\Delta_g \varphi. \tag{5-5}$$

After a rotation about y, we suppose D^2u is diagonalized at p with $\lambda_i = u_{ii}$ and $\lambda_1 \ge \cdots \ge \lambda_n$. We also define $z_i = x_i - y_i$. Then the increasing term increases the left-hand side:

$$|\nabla_g \varphi|^2 = \sum_i z_i^2 \frac{(\lambda_i + Z^{-\alpha-1})^2}{1+\lambda_i^2}, \qquad Z := \tfrac{1}{2}|z|^2. \tag{5-6}$$

The right-hand side has an extra negative term from the concave cutoff:

$$\Delta_g \varphi = \sum_i \frac{2\lambda_i + Z^{-\alpha-1}}{1+\lambda_i^2} - (\alpha+1)Z^{-\alpha-2}\sum_i \frac{z_i^2}{1+\lambda_i^2}. \tag{5-7}$$

We emphasize that the correct signs in these equations require the extra term to be singular. This is usually a fatal problem, but restricting to $|x-y| \ge r$, we encounter no issues.

Case 1: $|z_n| \ge |z|/\sqrt{n}$. Using $|\lambda_n| \le \lambda_i$ for $i < n$ from (3-9), inequality (5-5) becomes

$$Z\frac{(\lambda_n + Z^{-\alpha-1})^2}{1+\lambda_n^2} \le C(n)h\left(\frac{|\lambda_n| + Z^{-\alpha-1}}{1+\lambda_n^2} - \frac{c(n)(\alpha+1)Z^{-\alpha-1}}{1+\lambda_n^2}\right). \tag{5-8}$$

To derive the first term on the right-hand side, we consider the function

$$f(x) := \frac{x}{1+x^2}, \qquad f'(x) = \frac{1-x^2}{(1+x^2)^2} \le 0 \quad \text{if } |x| \ge 1.$$

If $|\lambda_n| \ge 1$, then $f(\lambda_i) \le f(|\lambda_n|)$, and it works. Consider now the case $|\lambda_n| < 1$. In $B_{1/2}(y)\setminus B_r(y)$, we have $Z^{-\alpha-1} > 8$. Moreover, $1/(1+\lambda_n^2) > \frac{1}{2}$. So in this case, we obtain the bound

$$\sum_i \frac{2\lambda_i}{1+\lambda_i^2} \le n \le n\cdot\frac{1}{4}\cdot\frac{Z^{-\alpha-1}}{1+\lambda_n^2}.$$

So for small enough $c(n)$ and large enough $C(n)$, we obtain (5-8).

Hard subcase: $|\lambda_n + Z^{-\alpha-1}| \le 4Z^{-\alpha-1}$. This means $|\lambda_n| \le 5Z^{-\alpha-1}$. Using the last negative term,

$$\alpha + 1 \le C(n). \tag{5-9}$$

This is a contradiction for fixed $\alpha = \alpha(n, \|u\|_{C^{0,1}(B_1(0))})$ large enough. This case is hard because $h \ll 1$ is unavailable.

Easy subcase: $|\lambda_n + Z^{-\alpha-1}| > 4Z^{-\alpha-1}$. This means $|\lambda_n| \ge 3Z^{-\alpha-1}$. If $\lambda_n < 0$,

$$C(n)h|\lambda_n| \ge Z(-\lambda_n - Z^{-\alpha-1})^2 \ge cZ\lambda_n^2 \ge cZ|\lambda_n|Z^{-\alpha-1}. \tag{5-10}$$

The $\lambda_n \ge 0$ case gives the same result. In fact, in $B_{1/2}(y) \setminus B_r(y)$, we have $Z \le \frac{1}{8}$, so we obtain

$$h \ge \frac{1}{C(n)}. \tag{5-11}$$

This is a contradiction for $h = h(n, \|u\|_{C^{0,1}(B_2)})$ small enough.

Case 2: $|z_i| \ge |z|/\sqrt{n}$ for $i < n$. Since $Z^{-\alpha-1} > 1$ on $B_{1/2}(y) \setminus B_r(y)$, and $\lambda_i \ge |\lambda_n| \ge 0$ by (3-9), the left-hand side (5-6) becomes

$$|\nabla_g \varphi|^2 \ge c(n)Z\frac{\lambda_i^2 + 2\lambda_i Z^{-\alpha-1} + Z^{-2(\alpha+1)}}{1+\lambda_i^2} > c(n)Z \ge c(n)r^2. \tag{5-12}$$

Then (5-5) becomes

$$\tfrac{1}{2}r^2 \le C(n)h(1 + Z^{-(\alpha+1)}) \le C(n)hr^{-2(\alpha+1)}. \tag{5-13}$$

This is a contradiction for $h(r, \alpha, n) = h(r, n, \|u\|_{C^{0,1}(B_2)})$ small enough.

Conclusion of Step 2. The max must occur on the boundary. Since $\eta = 0$ on $\partial B_{1/2}(y)$,

$$\sup_{B_{1/2}(y)\setminus B_r(y)} \eta b = \sup_{\partial B_r(y)} \eta b \le C(r, n, \|u\|_{C^{0,1}(B_1)(0)}) \sup_{B_r(y)} b. \tag{5-14}$$

Step 3: doubling inequality. For $r < \frac{1}{4}$, the above conclusion gives

$$\sup_{B_{1/4}(y)} b \le \sup_{B_{1/4}\setminus B_r(y)} b + \sup_{B_r(y)} b \le C \sup_{B_{1/4}(y)\setminus B_r(y)} \eta b + \sup_{B_r(y)} b \le C \sup_{B_r(y)} b. \tag{5-15}$$

Here, $C = C(r, n, \|u\|_{C^{0,1}(B_1(0))})$. □

6. Proof of the theorems

Let $u_k \in C^\infty$ solve (2-1) on $B_2(0)$ with $\|u_k\|_{C^{0,1}(B_1(0))} \le A$ but blowup $|D^2u_k(0)| \to \infty$. We choose a uniformly convergent subsequence in $B_1(0)$ to viscosity solution $u \in C^0(\overline{B_1(0)})$ of (2-1).

Step 1: partial regularity of the limit. There are two cases, and we claim Alexandrov is valid in both:

(i) Suppose u_k are convex solutions or semiconvex with a Jacobi inequality. It follows that u is also convex, and Alexandrov's theorem shows that D^2u exists a.e. in $B_1(0)$.

(ii) Suppose $\Theta \ge (n-2)\pi/2$. Then u_k is $n-1$ convex by (3-11), so by Lemma 3.4, u is also $n-1$ convex in the viscosity sense. Then Proposition 3.5 shows that Alexandrov's theorem is true for $n \ge 3$.

Using Alexandrov, we choose $y \in B_{1/2}(0)$ such that $|y| \le R(n, K, A)/2$ is sufficiently close to $x = 0$ as in Propositions 4.1, 4.2, and 5.1. Letting $Q(x)$ be the Taylor polynomial of u at $x = y$, we have $|u(x) - Q(x)| \le \sigma(|x - y|)$ for some modulus $\sigma(r) = o(r^2)/r^2$ as $r \to 0$. This implies Q solves (2-1), using quadratic comparison functions.

Step 2: flattening the error. We follow [Shankar and Yuan 2025, page 17]. We let error v_k equal $u_k - Q$, then rescale

$$\bar{v}_k(\bar{x}) = r^{-2} v_k(y + r\bar{x}), \quad \bar{x} \in B_1(0). \tag{6-1}$$

Then

$$\begin{aligned} \|\bar{v}_k\|_{L^\infty(B_1(0))} &\le r^{-2} \|u_k(y + r\bar{x}) - u(y + r\bar{x})\|_{L^\infty(B_1(0))} + \left\| \frac{u(y + r\bar{x}) - Q(y + r\bar{x})}{r^2} \right\|_{L^\infty(B_1(0))} \\ &\le r^{-2} \frac{o(k)}{k} + \sigma(r). \end{aligned} \tag{6-2}$$

The last inequality comes from uniform convergence and Alexandrov.

Step 3: Savin stability of partial regularity. Since Q is a solution of (2-1), observe that $\bar{v}_k$ solves the fully nonlinear elliptic PDE on $B_1(0)$

$$G(D^2 \bar{v}_k) = \sum_{i=1}^{n} (\arctan \lambda_i (D^2 Q + D^2 \bar{v}_k) - \arctan \lambda_i (D^2 Q)) = 0. \tag{6-3}$$

We see that $G(0) = 0$, and Savin's conditions are satisfied. We use Proposition 3.6 to find c_1. In (6-2), we can choose $r = r(\sigma) \ll 1$, then all $k \ge k(r(\sigma)) \gg 1$, such that $\|\bar{v}_k\|_{L^\infty(B_1(0))} \le c_1$. By Savin (Proposition 3.6), we deduce that $\|\bar{v}_k\|_{C^{2,\alpha}(B_{1/2}(0))} \le 1$. Equivalently, if we relabel $r/2$ as $r = r(\sigma)$,

$$\|u_k\|_{C^{2,\alpha}(B_r(y))} \le C(n, Q, \sigma). \tag{6-4}$$

Step 4: doubling to propagate the partial regularity. By Propositions 4.1, 4.2, or 5.1, we use (6-4) to obtain for smooth solutions u_k

$$\begin{aligned} \sup_{B_R(y)} |D^2 u_k| &\le C(r, n, K, A, a, \underline{\overline{\sup_{B_r(y)} |D^2 u_k|}}) \\ &\le C(r, n, K, A, a, \underline{C(n, Q, \sigma)}). \end{aligned} \tag{6-5}$$

Since $B_{R/2}(0) \subset B_R(y)$ and $r = r(\sigma)$, we obtain overall

$$|D^2 u_k(0)| \le \sup_{B_{R/2}(y)} |D^2 u| \le C(\sigma, n, K, A, Q, a). \tag{6-6}$$

This contradicts the blowup assumption. We conclude the proof.

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REGULARITY FOR NONLOCAL EQUATIONS WITH LOCAL NEUMANN BOUNDARY CONDITIONS

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We establish fine results on the boundary behavior of solutions to nonlocal equations in $C^{k,\gamma}$ domains which satisfy local Neumann conditions on the boundary. Such solutions typically blow up at the boundary like $v \asymp \mathrm{dist}^{s-1}$ and are sometimes called large solutions. In this setup we prove optimal regularity results for the quotients v/dist^{s-1}, depending on the regularity of the domain and on the data of the problem. The results of this article will be important in a forthcoming work on nonlocal free boundary problems.

1. Introduction

The study of nonlocal operators of the form

$$Lv(x) = \mathrm{p.v.}\int_{\mathbb{R}^n} (v(x) - v(x+h))K(h)\,\mathrm{d}h, \tag{1-1}$$

where $K : \mathbb{R}^n \to [0, \infty]$ is a kernel satisfying for some $s \in (0, 1)$

$$K(h) = \frac{K(h/|h|)}{|h|^{n+2s}}, \quad 0 < \lambda \le K(\theta) \le \Lambda \text{ for all } \theta \in \mathbb{S}^{n-1}, \quad K(h) = K(-h) \tag{1-2}$$

has been an important area of research in analysis and probability for the past 30 years. Operators L of the type (1-1)–(1-2) arise naturally as generators of $2s$-stable Lévy processes, and are used to model different kinds of real-world phenomena involving long range interactions, e.g., in mathematical finance and in physics. From a PDE perspective, it is of particular interest to study the effect of the nonlocality of L on the regularity of solutions to nonlocal equations. By now, the question of *interior* regularity of solutions

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is fairly well-understood, and there are several important works in this context, such as [Caffarelli and Silvestre 2009; 2011a; 2011b; Silvestre 2006; Bass and Levin 2002; Kassmann 2009; Di Castro et al. 2014; 2016; Barrios et al. 2014; Ros-Oton and Serra 2016b].

A much more delicate question is the one of *boundary* regularity of solutions to nonlocal problems. Previous works have mostly focused on nonlocal Poisson problems, given as

$$\begin{cases} Lv = f & \text{in } \Omega, \\ v = 0 & \text{in } \mathbb{R}^n \setminus \Omega. \end{cases} \tag{1-3}$$

The nonlocal Poisson problem (1-3) arises naturally as the Euler–Lagrange equation of a nonlocal energy minimization problem and can therefore be studied via variational methods, but also via nonvariational methods. For (1-3) it was proved (see [Ros-Oton and Serra 2014; Grubb 2015]) that weak solutions satisfy $v \in C^s(\overline{\Omega})$, once $\partial\Omega \in C^{1,\gamma}$ and $f \in L^\infty(\Omega)$. The C^s regularity of solutions is optimal, as one can see from the explicit example (see [Getoor 1961; Landkof 1972; Dyda 2012])

$$(-\Delta)^s (1-|x|^2)_+^s = c_{n,s} > 0 \quad \text{in } B_1, \tag{1-4}$$

which also remains valid for L satisfying (1-1)–(1-2) (see [Ros-Oton 2016]). However, it turns out that once the domain, the kernel, and the data are regular enough, also the quotient v/d^s will be regular, yielding a fine description of the behavior of the solution v at the boundary. The best known result in the literature, establishing optimal boundary regularity of weak solutions of (1-3) in terms of the regularity of the domain and the data was shown in [Ros-Oton and Serra 2017; Abatangelo and Ros-Oton 2020; Grubb 2015] (see also [Ros-Oton and Serra 2016a; 2016b; Abels and Grubb 2023]) and reads as

$$\partial\Omega \in C^{k+1,\gamma}, \quad f \in C^{k+\gamma-s}(\overline{\Omega}) \quad \Longrightarrow \quad \frac{v}{d^s} \in C^{k,\gamma}(\overline{\Omega}) \quad \text{for all } k \in \mathbb{N}\cup\{0\},\ \gamma \in (0,1). \tag{1-5}$$

All the previously mentioned results on the nonlocal Poisson problem (1-3) address weak solutions for which one can prove that they must remain bounded in $\overline{\Omega}$ (see [Servadei and Valdinoci 2014; Korvenpää et al. 2016]). However, explicit computations reveal that there also exist pointwise solutions of (1-3), which explode at the boundary of the domain behaving asymptotically like d^{s-1}. The following most prominent example goes back to a work by Hmissi [1994] (see also [Bogdan 1999, Example 1, p. 239; Bogdan et al. 2009, Example 3.3; Dyda 2012]):

$$(-\Delta)^s (1-|x|^2)_+^{s-1} = 0 \quad \text{in } B_1. \tag{1-6}$$

The example (1-6) has initiated the conceptual study of boundary blow-up for solutions to nonlocal equations (see [Grubb 2014; 2015; 2018; 2023; Abatangelo 2015; 2017; Abatangelo et al. 2023; Chan et al. 2021]). In this theory, solutions such as (1-6) are sometimes called "large solutions". Due to the explosion at the boundary, the above function cannot be a weak solution, and clearly violates (1-5).

In order to have a unified framework which also allows for singular behavior at the boundary, it is necessary to keep track of the boundary behavior of the solution, or more precisely to prescribe somehow the behavior of the quotient v/d^{s-1}. In this spirit, the following Neumann problem, which was introduced in [Grubb 2014] (see also [Grubb 2018; 2023]), can be seen as a generalization of (1-3)

$$\begin{cases} Lv = f & \text{in } \Omega, \\ v = 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ \partial_\nu\left(\dfrac{v}{d^{s-1}}\right) = g & \text{on } \partial\Omega, \end{cases} \tag{1-7}$$

where $\nu(x_0) \in \mathbb{S}^{n-1}$ denotes the inner unit normal at $x_0 \in \partial\Omega$. The problem (1-7) is a natural *nonlocal Neumann problem* with inhomogeneous Neumann data g, and one can show that the problem is well-posed in suitable function spaces, at least if the domain is C^∞ (see [Grubb 2014]). Moreover, the solutions blow up at every boundary point where v/d^{s-1} does not vanish.

Remark 1.1. The functions in (1-4) and (1-6), are both solutions to (1-7), with $g \equiv 1$ and $f = c_{n,s}$ and with $g \equiv (s-1)2^{s-2}$ and $f = 0$, respectively, in case $\Omega = B_1$.

The Neumann condition in (1-7) is purely local in nature in the sense that it is imposed only on the topological boundary $\partial\Omega$. Therefore, (1-7) is conceptually completely different from the nonlocal Neumann problem introduced in [Du et al. 2012; Dipierro et al. 2017] (see also [Alves and Torres Ledesma 2020; Vondraček 2021; Audrito et al. 2023; Foghem and Kassmann 2024; Grube and Hensiek 2024]). It is also of entirely different nature than [Barles et al. 2014a; 2014b; Bogdan et al. 2003; Chen and Kim 2002], where local boundary conditions are imposed, but instead the operator is changed, depending on the domain.

Main result. The aforementioned regularity results (1-5) from [Ros-Oton and Serra 2017; Abatangelo and Ros-Oton 2020] do not apply to (1-7) since solutions are in general not continuous and might even explode at the boundary. However, it is natural to expect fine regularity results for the quotients v/d^{s-1} depending on the regularity of the domain and the data.

When Ω is C^∞ and $K|_{\mathbb{S}^{n-1}}$ is C^∞, the regularity theory for (1-7) was developed by Grubb [2014] using an approach via pseudodifferential operators.

Our goal in this work is twofold: to establish sharp boundary regularity estimates for (1-7) in $C^{k,\gamma}$ domains, and at the same time to prove them for the first time as localized estimates in $\Omega \cap B_2$. This is new even for C^∞ domains, and it is crucial for our application to free boundary problems.

Our main result is the following:

Theorem 1.2. *Let L, K, s, λ, Λ be as in* (1-1)–(1-2). *Let $k \in \mathbb{N}$, $\gamma \in (0,1)$ with $\gamma \neq s$, and $\Omega \subset \mathbb{R}^n$ be a $C^{k+1,\gamma}$ domain, and $K \in C^{2k+2\gamma+3}(\mathbb{S}^{n-1})$. Let $v \in L^1_{2s}(\mathbb{R}^n)$ with $v/d^{s-1} \in C(\overline{\Omega})$ be a viscosity solution to*

$$\begin{cases} Lv = f & \text{in } \Omega \cap B_2, \\ v = 0 & \text{in } B_2 \setminus \Omega, \\ \partial_\nu\left(\dfrac{v}{d^{s-1}}\right) = g & \text{on } \partial\Omega \cap B_2, \end{cases}$$

where $\nu : \partial\Omega \to \mathbb{S}^{n-1}$ is the normal vector of Ω, and $f \in C(\Omega) \cap \mathcal{X}(\Omega \cap B_2)$, $g \in C^{k-1+\gamma}(\partial\Omega \cap B_2)$,

$$\mathcal{X}(\Omega \cap B_2) = \begin{cases} d^{s-\gamma} L^\infty(\Omega \cap B_2) & \text{if } k+\gamma \le 2s, \\ C^{k-2s+\gamma}(\Omega \cap B_2) & \text{if } k+\gamma > 2s. \end{cases} \tag{1-8}$$

Then, it holds that $v/d^{s-1} \in C^{k+\gamma}_{\mathrm{loc}}(\overline{\Omega} \cap B_2)$ *and*

$$\left\| \frac{v}{d^{s-1}} \right\|_{C^{k,\gamma}(\overline{\Omega}\cap B_1)} \leq c\left(\left\| \frac{v}{d^{s-1}} \right\|_{L^\infty(\Omega\cap B_2)} + \|v\|_{L^1_{2s}(\mathbb{R}^n\setminus B_2)} + \|f\|_{\mathcal{X}(\Omega\cap B_2)} + \|g\|_{C^{k-1+\gamma}(\partial\Omega\cap B_2)} \right),$$

for some $c > 0$, *which only depends on* $n, s, \lambda, \Lambda, k, \gamma, \Omega$, *and* $\|K\|_{C^{2k+2\gamma+3}(\mathbb{S}^{n-1})}$.

For the definition of $L^1_{2s}(\mathbb{R}^n)$ and the notion of viscosity solutions, we refer to Section 2.

The regularity we obtain for v/d^{s-1} depending on the regularity of the domain Ω and the data f, g is expected to be optimal. For f and g, this is an immediate consequence of interior Schauder theory (see [Ros-Oton and Serra 2016b]), and the order of the equation. For the regularity of the domain, we observe that our results align with the ones in [Abatangelo and Ros-Oton 2020] once $v \in C(\overline{\Omega} \cap B_2)$. We obtain results with regularity assumptions on K that are expected to be optimal in case Ω is a half-space (see Theorem 1.7). As in [Grubb 2014], we rule out the case $\gamma = s$. The result is expected to be false in this case. It corresponds to proving Schauder-type regularity estimates of integer order.

Another key advantage of our approach is that it allows for localized results in $\Omega \cap B_2$. Nonetheless, if $\Omega \subset B_2$, and v is a solution to (1-7), by application of the maximum principle (see Lemma 3.4) to the estimate in Theorem 1.2 we can obtain the following bound which is purely in terms of f and g:

$$\left\| \frac{v}{d^{s-1}} \right\|_{C^{k,\gamma}(\overline{\Omega})} \leq c(\|f\|_{\mathcal{X}(\Omega)} + \|g\|_{C^{k-1+\gamma}(\partial\Omega)}).$$

Thus, we have the following generalization of (1-5) to solutions of (1-7):

$$\partial\Omega \in C^{k+1,\gamma}, \quad f \in C^{k-2s+\gamma}(\overline{\Omega}), \quad g \in C^{k-1+\gamma}(\partial\Omega) \qquad \Longrightarrow \qquad \frac{v}{d^{s-1}} \in C^{k,\gamma}(\overline{\Omega}) \quad \text{for all } k \in \mathbb{N},\ \gamma \in (0,1). \tag{1-9}$$

A weak maximum principle and nonlocal problems with local Dirichlet conditions. The example (1-6) of a nontrivial s-harmonic function that vanishes outside B_1 implies that the Poisson problem (1-3) for the fractional Laplacian is ill-posed even in the homogeneous case. Therefore, maximum principles are usually established under an additional assumption on the boundary behavior of the solution, ruling out "large" solutions such as (1-6) (see [Silvestre 2007; Servadei and Valdinoci 2014; Felsinger et al. 2015; Jarohs and Weth 2019; Feulefack and Jarohs 2023; Fernández-Real and Ros-Oton 2024a]). Note that a similar phenomenon occurs for local equations, where any constant function is a pointwise solution inside the solution domain.

In this paper, we prove the following nonlocal weak maximum principle, which allows for solutions that blow up at the boundary.

Proposition 1.3. *Let* $L, K, s, \lambda, \Lambda$ *be as in* (1-1)–(1-2). *Let* $\gamma > 0$ *and* $\Omega \subset \mathbb{R}^n$ *be a* $C^{1,\gamma}$ *domain. Let* $v \in L^1_{2s}(\mathbb{R}^n)$ *with* $v/d^{s-1} \in C(\overline{\Omega})$ *be a viscosity solution to*

$$\begin{cases} Lv \geq 0 & \text{in } \Omega, \\ v \geq 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ \frac{v}{d^{s-1}} \geq 0 & \text{on } \partial\Omega. \end{cases}$$

Then, $v \geq 0$.

The condition $v/d^{s-1} \geq 0$ in Proposition 1.3 includes solutions that blow up at the boundary, such as (1-6). Previously, maximum principles including large solutions have been established in [Abatangelo 2015; Grube and Hensiek 2023; Liu and Zhuo 2025; Li and Liu 2023]. Proposition 1.3 extends these results to general $2s$-stable integrodifferential operators, and to $C^{1,\gamma}$ domains, respectively.

Recall that a natural way to make the nonlocal Poisson problem (1-3) well-posed is to impose Neumann boundary conditions as in (1-7). Another way would be to prescribe the limit of the quotient v/d^{s-1} directly, which leads to the following nonlocal problem with local Dirichlet data, which was introduced independently in [Grubb 2014; Abatangelo 2015]:

$$\begin{cases} Lv = f & \text{in } \Omega, \\ v = 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ \dfrac{v}{d^{s-1}} = h & \text{on } \partial\Omega. \end{cases} \tag{1-10}$$

The weak maximum principle in Proposition 1.3 implies that the problems (1-10) and (1-3) are equivalent, when $h \equiv 0$. Thus, (1-10) can be seen as an inhomogeneous nonlocal Dirichlet problem.

Another contribution of this article is the following Schauder-type boundary regularity estimate for solutions to nonlocal equations with local Dirichlet data:

Theorem 1.4. *Let $L, K, s, \lambda, \Lambda$ be as in* (1-1)–(1-2). *Let $k \in \mathbb{N}$, $\gamma \in (0,1)$ with $\gamma \neq s$, and $\Omega \subset \mathbb{R}^n$ be a $C^{k+1,\gamma}$ domain, and $K \in C^{2k+2\gamma+3}(\mathbb{S}^{n-1})$. Let $v \in L^1_{2s}(\mathbb{R}^n)$ with $v/d^{s-1} \in C(\overline{\Omega})$ be a viscosity solution to* (1-10) *with $f \in C(\Omega) \cap \mathcal{X}(\Omega)$ and $h \in C^{k+\gamma}(\partial\Omega)$, where $\mathcal{X}$ is as in* (1-8).

Then, it holds that $v/d^{s-1} \in C^{1+\gamma}_{\mathrm{loc}}(\overline{\Omega})$, and

$$\left\| \frac{v}{d^{s-1}} \right\|_{C^{k,\gamma}(\overline{\Omega})} \leq c(\|f\|_{\mathcal{X}(\Omega)} + \|h\|_{C^{k+\gamma}(\partial\Omega)})$$

for some $c > 0$, which only depends on $n, s, \lambda, \Lambda, k, \gamma, \Omega$, and $\|K\|_{C^{2k+2\gamma+3}(\mathbb{S}^{n-1})}$.

We refer to [Grubb 2015; 2023] for similar results in the framework of pseudodifferential operators.

Note that (1-10) can always be reduced to the homogeneous problem (1-3). In fact, if Ω and h are regular enough, one can extend h to a smooth function in $\overline{\Omega}$ and consider $w := v - d^{s-1}h$. Then, w solves the homogeneous problem (1-3) with a new right-hand side $\tilde{f} = f - L(d^{s-1}h)$. Since $L(d^{s-1}h)$ has good regularity properties (see Corollary 2.5), we can prove Theorem 1.4, by application of the results in [Ros-Oton and Serra 2017; Abatangelo and Ros-Oton 2020].

Strategy of the proof: regularity for nonlocal problems with local Neumann data. Since the nonlocal problem with inhomogeneous local Dirichlet data (1-10) can always be reduced to the homogeneous problem (1-3) for which the boundary regularity theory was already established (see [Ros-Oton and Serra 2017; Abatangelo and Ros-Oton 2020]), the proof of Theorem 1.4 is rather simple.

In sharp contrast to that, for the Neumann problem (1-7) there is no cheap way to obtain the boundary regularity results in Theorem 1.2 from the existing theory. In fact, it is already highly nontrivial to establish Hölder continuity of the quotient v/d^{s-1} up to the boundary (see Theorem 1.6 below).

Our proof of Theorem 1.6 goes in *three main steps*.

First, we establish a weak maximum principle for solutions to the Neumann problem (1-7).

Proposition 1.5. *Let L, K, s, λ, Λ be as in* (1-1)–(1-2). *Let $\gamma > 0$, $\Omega \subset \mathbb{R}^n$ be a $C^{2,\gamma}$ domain, and $K \in C^{5+2\gamma}(\mathbb{S}^{n-1})$. Let $v \in L^1_{2s}(\mathbb{R}^n)$ with $v/d^{s-1} \in C(\overline{\Omega})$ be a viscosity solution to*

$$\begin{cases} Lv \geq 0 & \text{in } \Omega, \\ v \geq 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ \partial_\nu\left(\dfrac{v}{b_\Omega}\right) \leq 0 & \text{on } \partial\Omega, \end{cases}$$

where b_Ω is defined in (3-2). *Then $v \geq 0$.*

This result seems to be the first maximum principle for nonlocal problems with local Neumann boundary conditions in the literature. We believe it to be of independent interest and refer to Lemma 3.4 for a corresponding L^∞ bound in the case of inhomogeneous data. The function b can be thought of as a special regularized distance function taken to the power $s-1$. We stress that the result is no longer true if the function b is replaced by $\tilde{d}^{s-1}$, where $\tilde{d}$ is another regularized distance function. In fact, Proposition 1.5 holds true for the function in (1-6) if $b = (1-|\cdot|)_+^{s-1}$, but fails if we replace b by the regularized distance $\tilde{d} = (1-|\cdot|^4)$.

The proof of Proposition 1.5 follows from a nonlocal Hopf-type lemma for solutions to the inhomogeneous Dirichlet problem (1-10) (see Lemma 3.3), which in turn follows from the weak maximum principle in Proposition 1.3. All of these results rely heavily on explicit barriers for (1-10) in $C^{1,\gamma}$ domains that are adapted to the geometry of the domain and blow up at the boundary like d^{s-1}. These barriers can be seen as perturbations of (1-6), or rather of 1D solutions such as

$$L(x_n)_+^{s-1} = 0 \quad \text{in } \{x_n > 0\}. \tag{1-11}$$

Note that (1-11) follows simply by differentiating the equation

$$L(x_n)_+^{s} = 0 \quad \text{in } \{x_n > 0\}.$$

The previous identity is a classical fact for nonlocal operators (1-1)–(1-2) (see [Fernández-Real and Ros-Oton 2024a, Lemma 2.6.2]).

The *second* main step in the proof of Theorem 1.6 is to establish Hölder continuity of order α, for $\alpha \in (0,1)$ small enough, up to the boundary of v/d^{s-1} for solutions to (1-7) in $C^{1,\gamma}$ domains.

Theorem 1.6. *Let L, K, s, λ, Λ be as in* (1-1)–(1-2). *Let $\gamma \in (0,1)$, $\Omega \subset \mathbb{R}^n$ be a $C^{2,\gamma}$ domain, and $K \in C^{5+2\gamma}(\mathbb{S}^{n-1})$. Let $v \in L^1_{2s}(\mathbb{R}^n)$ with $v/d^{s-1} \in C(\overline{\Omega})$ be a viscosity solution to*

$$\begin{cases} Lv = f & \text{in } \Omega \cap B_2, \\ v = 0 & \text{in } B_2 \setminus \Omega, \\ \partial_\nu\left(\dfrac{v}{d^{s-1}}\right) = g & \text{on } \partial\Omega \cap B_2, \end{cases}$$

with $f \in C(\Omega \cap B_2)$ and $g \in C(\partial\Omega \cap B_2)$. Then, there exists $\alpha_0 > 0$, such that when $d^{s-\alpha} f \in L^\infty(\Omega \cap B_2)$ for some $\alpha \in (0, \alpha_0]$, and it holds that $v/d^{s-1} \in C^\alpha_{\mathrm{loc}}(\overline{\Omega} \cap B_2)$, and

$$\left\| \frac{v}{d^{s-1}} \right\|_{C^\alpha(\overline{\Omega} \cap B_1)} \leq c\left(\left\| \frac{v}{d^{s-1}} \right\|_{L^\infty(\Omega \cap B_2)} + \|v\|_{L^1_{2s}(\mathbb{R}^n \setminus B_2)} + \|d^{s-\alpha} f\|_{L^\infty(\Omega \cap B_2)} + \|g\|_{L^\infty(\partial\Omega \cap B_2)} \right),$$

where $c > 0$ and α_0 depend only on n, s, λ, Λ, γ, and the $C^{2,\gamma}$ radius of Ω.

The proof of Theorem 1.6 uses the weak maximum principle in Proposition 1.5 and the interior weak Harnack inequality, to establish a weak Harnack inequality for v/d^{s-1} at the boundary (see Lemma 4.1). This allows us to deduce a so called "growth lemma" for v/d^{s-1}, stating that v/d^{s-1} must be large pointwise in a ball centered at the boundary, if v/d^{s-1} was large in a measure-theoretic sense in a ball away from the boundary. Such growth lemma allows to establish oscillation decay for v/d^{s-1} at the boundary, and to deduce the Hölder estimate in Theorem 1.6. A similar proof for the classical Laplacian can be found in [Lian and Zhang 2023].

Once the boundary Hölder estimate is shown, we can establish the higher order boundary regularity in Theorem 1.2 via a blow-up argument. This is the *third*, and last step of the proof. Theorem 1.6 is crucial in order to deduce uniform convergence of the blow-up sequence.

The blow-up argument follows the scheme in [Abatangelo and Ros-Oton 2020] and relies on a Liouville theorem in the half-space with local Neumann data (see Theorem 5.1). However, major modifications have to be made in most of the steps due to the boundary blow-up of solutions. For instance, we need to show the following new result (see Corollary 2.5):

$$\partial\Omega \in C^{k+1,\gamma} \quad \Longrightarrow \quad L(d^{s-1}) \in C^{k-1+\gamma-s}(\overline{\Omega}) \quad \text{if } k+\gamma > 1+s.$$

Moreover, the presence of a Neumann boundary condition complicates some of the arguments, such as the proof of a stability result for viscosity solutions (see Lemma 2.13). Finally, as in [Abatangelo and Ros-Oton 2020] we need to make use of a suitable notion of nonlocal equations up to a polynomial (see [Dipierro et al. 2019; 2022]) in order to account for solutions that grow too fast at infinity (see Definition 2.8).

Applications to free-boundary problems. We end the discussion of the main results of this article by shedding some light on a, perhaps unexpected, connection between nonlocal problems with local Neumann boundary data and free boundary problems. This connection is a main motivation for us to study (1-7). Let us explain this phenomenon in the particular case of the fractional Laplacian.

The nonlocal one-phase free boundary problem, which was introduced in [Caffarelli et al. 2010] (see also [Ros-Oton and Weidner 2024]), deals with the minimization of the functional

$$\mathcal{I}(w) := \iint_{(B_1^c \times B_1^c)^c} (w(x)-w(y))^2 \frac{\mathrm{d}y\,\mathrm{d}x}{|x-y|^{n+2s}} + M|\{w>0\}\cap B_1| \tag{1-12}$$

for some $M > 0$ and with prescribed values of w in $\mathbb{R}^n \setminus B_1$. One can show (see [Caffarelli et al. 2010; Fernández-Real and Ros-Oton 2024b]) that local minimizers of (1-12) are $C^s(B_1)$ and that they are viscosity solutions to

$$\begin{cases} (-\Delta)^s w = 0 & \text{in } \Omega\cap B_1, \\ w = 0 & \text{in } B_1\setminus\Omega, \\ \dfrac{w}{d^s} = c_{n,s}M & \text{on } \partial\Omega\cap B_1, \end{cases} \tag{1-13}$$

where $c_{n,s} > 0$ is a constant and $\Omega := \{w > 0\}$. An important question in the theory is to determine the regularity of the free boundary $\partial\Omega$ near so called "regular points". These are the points $x_0 \in \partial\Omega \cap B_1$ for which blow-ups of w are half-space solutions, i.e., (up to rotations and multiplicative constants)

$$\frac{w(x_0+rx)}{r^s} \to w_0(x) := (x_n)_+^s \quad \text{locally uniformly.}$$

One can show using the extension for $(-\Delta)^s$ (see [De Silva and Roquejoffre 2012; De Silva and Savin 2012; De Silva et al. 2014]) that once a sequence (w_ε) of viscosity solutions (1-13) is "ε-close" to the half-space solution w_0 in the sense that

$$(x_n-\varepsilon)_+^s \le w_\varepsilon(x) \le (x_n+\varepsilon)_+^s,$$

then it holds, as $\varepsilon \searrow 0$, that

$$\frac{w_\varepsilon(x)-(x_n)_+^s}{\varepsilon} \to (x_n)_+^{s-1}u(x),$$

where u solves the so called "linearized problem"

$$\begin{cases} (-\Delta)^s((x_n)_+^{s-1}u) = 0 & \text{in } \{x_n > 0\} \cap B_1, \\ \partial_n u = 0 & \text{on } \{x_n = 0\} \cap B_1. \end{cases} \tag{1-14}$$

Hence, $(x_n)_+^{s-1}u$ is a solution to a nonlocal problem with local Neumann data (1-7) in the half-space, and it explodes at the boundary $\{x_n = 0\} \cap B_1$.

In order to establish regularity results for the free boundary $\Omega = \{w > 0\}$ near regular points, it is an important step to establish boundary regularity results for the solution to the linearized problem. For (1-14) this was done in [De Silva and Roquejoffre 2012; De Silva and Savin 2012; De Silva et al. 2014], using the Caffarelli–Silvestre extension.

In the light of this connection, our main result Theorem 1.2 also makes a contribution to the theory of the nonlocal one-phase problem (1-12), and provides a completely new proof of the regularity for (1-14), even in the case of the fractional Laplacian.

We end this discussion by stating a variant of Theorem 1.2 in the special case $\Omega = \{x_n > 0\}$. This result holds true under assumptions on the regularity of K which are expected to be optimal, and it will be helpful in the study of the nonlocal one-phase free boundary problem (1-13) with respect to general nonlocal operators (1-1)–(1-2), which we plan to investigate in a future work (see [Ros-Oton and Weidner 2025]).

Theorem 1.7. *Let $L, K, s, \lambda, \Lambda$ be as in* (1-1)–(1-2). *Let $k \in \mathbb{N}$, $\gamma \in (0,1)$ with $\gamma \neq s$. Let*

$$u \in C(\{x_n \ge 0\} \cap B_2) \quad \text{with } (x_n)_+^{s-1}u \in L^1_{2s}(\mathbb{R}^n)$$

be a viscosity solution to

$$\begin{cases} L((x_n)_+^{s-1}u) = f & \text{in } \{x_n > 0\} \cap B_2, \\ \partial_n u = g & \text{on } \partial\{x_n = 0\} \cap B_2. \end{cases}$$

with $f \in C(\{x_n > 0\} \cap B_2) \cap \mathcal{X}(\{x_n > 0\} \cap B_2)$, $g \in C^{k-1+\gamma}(\{x_n = 0\} \cap B_2)$, and $K \in C^{k-2s+\gamma}(\mathbb{S}^{n-1})$ if $k+\gamma > 2s$, where $\mathcal{X}$ is as in (1-8). *Then, it holds that*

$$\|u\|_{C^{k,\gamma}(\{x_n\ge 0\}\cap B_1)} \le c\big(\|u\|_{L^\infty(\{x_n>0\}\cap B_2)} + \|(x_n)_+^{s-1}u\|_{L^1_{2s}(\mathbb{R}^n\setminus B_2)} + \|f\|_{\mathcal{X}(\{x_n>0\}\cap B_2)} + \|g\|_{C^{k-1+\gamma}(\{x_n=0\}\cap B_2)}\big)$$

for some $c > 0$, which only depends on $n, s, \lambda, \Lambda, k, \gamma$, and (if $k+\gamma > 2s$) also on $\|K\|_{C^{k-2s+\gamma}(\mathbb{S}^{n-1})}$.

Finally, we make the following remark.

Remark 1.8. The following two problems are equivalent if $v \in C(\overline{\Omega} \cap B_2)$, i.e., if solutions do not blow up on $\partial\Omega \cap B_2$:

$$\begin{cases} Lv = f & \text{in } \Omega \cap B_2, \\ v = 0 & \text{in } B_2 \setminus \Omega, \\ \partial_\nu\Big(\dfrac{v}{d^{s-1}}\Big) = g & \text{on } \partial\Omega \cap B_2, \end{cases} \quad \leftrightarrow \quad \begin{cases} Lv = f & \text{in } \Omega \cap B_2, \\ v = 0 & \text{in } B_2 \setminus \Omega, \\ \dfrac{v}{d^s} = g & \text{on } \partial\Omega \cap B_2. \end{cases}$$

Indeed, since $v \equiv 0$ in $B_2 \setminus \Omega$, it holds for any $x_0 \in \partial\Omega \cap B_2$ that

$$\partial_\nu\Big(\frac{v}{d^{s-1}}\Big) = \lim_{x \to x_0} \frac{\frac{v}{d^{s-1}}(x) - \lim_{z \to x_0} \frac{v}{d^{s-1}}(z)}{d(x)} = \lim_{x \to x_0} \frac{v}{d^s}(x).$$

Recall that the second problem is satisfied by minimizers to the nonlocal one-phase problem (1-13). Moreover, the above problem is the nonlocal counterpart of the over-determined Serrin's problem whenever $\Omega \subset B_2$ (see for instance [Fall and Jarohs 2015; Soave and Valdinoci 2019; Biswas and Jarohs 2020; Dipierro et al. 2023]).

Organization of the paper. In Section 2 we introduce the notion of viscosity solutions to (1-7) and give some preliminary lemmas. Among them are already several new results of independent interest, such as the construction of explicit barriers exploding at the boundary (see Section 2.3), an analysis of the regularity of $L(d^{s-1})$ in terms of the regularity of the domain (see Corollary 2.5), and a stability result for viscosity solutions (see Lemma 2.13). In Section 3 we prove maximum principles for solutions to nonlocal problems with local Dirichlet and Neumann data (see Propositions 1.3 and 1.5). Section 4 is devoted to the proof of the Hölder estimate up to the boundary (see Theorem 1.6). In Section 5 we prove a Liouville theorem in the half-space (see Theorem 5.1), and in Section 6 we carry out a blow-up argument to prove our main result, Theorem 1.2. Finally, Section 7 contains the proof of the regularity for the inhomogeneous Dirichlet problem (see Theorem 1.4).

2. Preliminaries

In this section, we give several important definitions, such as the definitions of viscosity solutions to (1-7). In Section 2.2 we establish the regularity of $L(d^{s-1})$ depending on the regularity of the domain and in Section 2.3 we use these results to construct barrier functions. In Section 2.4, we introduce the notion of nonlocal equations satisfied up to a polynomial, and in Section 2.5 we establish stability of viscosity solutions and prove that the sum of two viscosity solutions is again a viscosity solution.

From now on, we denote by $\mathcal{L}_s^{\text{hom}}(\lambda, \Lambda)$ the class of operators (1-1) with kernels satisfying (1-2). Moreover, whenever we say $K \in C^\alpha(\mathbb{S}^{n-1})$ for some $\alpha > 0$, we mean that $\|K\|_{C^\alpha(\mathbb{S}^{n-1})} \le \Lambda$. Sometimes, we denote the class of operators (1-1) satisfying (1-2) and $K \in C^\alpha(\mathbb{S}^{n-1})$ by $\mathcal{L}_s^{\text{hom}}(\lambda, \Lambda, \alpha)$.

Moreover, given an open, bounded domain $\Omega \subset \mathbb{R}^n$ with $\partial\Omega \in C^\beta$ for some $\beta > 1$, $d := d_\Omega : \mathbb{R}^n \to [0, \infty)$ will denote the regularized distance which satisfies $d \in C^\infty(\Omega) \cap C^\beta(\overline{\Omega})$ and $d \equiv 0$ in $\mathbb{R}^n \setminus \Omega$. Crucially, we have $\operatorname{dist}(\,\cdot\,, \Omega) \le d \le C \operatorname{dist}(\,\cdot\,, \Omega)$ in $\mathbb{R}^n$, i.e., the topological distance and the regularized distance are pointwise comparable. We will often use the fact that $|D^k d| \le c d^{\beta-k}$ (see [Fernández-Real and Ros-Oton 2024a, Definition 2.7.5]). Throughout this article, we will define $d^{s-1} \equiv 0$ in $\mathbb{R}^n \setminus \Omega$.

In the following, whenever $x_0 \in \partial\Omega$, we write $v/d^{s-1}(x_0) := \lim_{\Omega \ni x \to x_0} v/d_{\Omega}^{s-1}(x)$.

2.1. ***Function spaces and solution concepts.*** Let us introduce the following function space:

$$L^1_\alpha(\mathbb{R}^n) := \left\{ u : \|u\|_{L^1_\alpha(\mathbb{R}^n)} := \int_{\mathbb{R}^n} |u(y)|(1+|y|)^{-n-\alpha}\, dy < \infty \right\}, \quad \alpha > 0.$$

Typically, we will use the previous definition with $\alpha = 2s$. We are now in a position to give the notion of viscosity solution to (1-7).

Definition 2.1 (viscosity solution). Let $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $\partial\Omega \in C^{1,\gamma}$. By $\nu \in \mathbb{S}^{n-1}$, we denote the inner normal vector to $\partial\Omega$.

(i) We say that $v \in C(\Omega) \cap L^1_{2s}(\mathbb{R}^n)$ is a viscosity subsolution to

$$Lv = f \quad \text{in } \Omega \cap B_1, \tag{2-1}$$

where $f \in C(\Omega \cap B_1)$, if for any $x \in \Omega \cap B_1$ and any neighborhood $N_x \subset \Omega$ of x it holds that

$$L\phi(x) \le f(x) \quad \text{for all } \phi \in C^2(N_x) \cap L^1_{2s}(\mathbb{R}^n) \quad \text{such that } v(x) = \phi(x), \quad \phi \ge v. \tag{2-2}$$

We say that v is a viscosity supersolution to (2-2) if (2-2) holds true for $-v$ and $-f$ instead of v and f. Moreover, v is a viscosity solution to (2-2), if it is a viscosity subsolution and a viscosity supersolution.

(ii) For any function $b \in L^1_{2s}(\mathbb{R}^n)$ with $b/d^{s-1} \in C^1(\overline{\Omega})$ we say that $v \in L^1_{2s}(\mathbb{R}^n)$ with $v/d^{s-1} \in C(\overline{\Omega})$ is a viscosity subsolution to

$$\partial_\nu(v/b) = g \quad \text{on } \partial\Omega \cap B_1,$$

where $g \in C(\partial\Omega \cap B_1)$, if for any $x \in \partial\Omega \cap B_1$ and any neighborhood $N_x \subset \overline{\Omega} \cap B_1$ of x it holds that

$$\partial_\nu \phi(x) \le g(x) \quad \text{for all } \phi \in C^2(N_x) \cap L^\infty(\overline{\Omega}) \quad \text{such that } v/b(x) = \phi(x), \quad \phi \le v/b. \tag{2-3}$$

We say that v is a viscosity supersolution to (2-3) if (2-3) holds true for $-v$ and $-g$ instead of v and g. Moreover, v is a viscosity solution to (2-3), if it is a viscosity subsolution and a viscosity supersolution.

Clearly, if in (i) $Lv(x)$, or if in (ii) $\partial_\nu(v/d^{s-1})(x) = \lim_{\Omega \ni y \to x}(v/d^{s-1})(y)$ exists in the strong sense, then the notions of viscosity solutions coincide with the ones for strong solutions (see [Fernández-Real and Ros-Oton 2024a, Lemma 3.4.13]).

2.2. ***Nonlocal operators and the distance function.*** The goal of this subsection is to establish several lemmas on the regularity of $L(d^{s-1})$ depending on the regularity of Ω. Lemma 2.3 will help us to establish barriers in $C^{1,\gamma}$ domains and Corollary 2.5 is crucial for domains that are more regular.

The following lemma is a slight modification of [Fernández-Real and Ros-Oton 2024a, Lemma B.2.4].

Lemma 2.2. *Let $L \in \mathcal{L}_s^{\mathrm{hom}}(\lambda, \Lambda)$. Let $\Omega \subset \mathbb{R}^n$ be a bounded Lipschitz domain with Lipschitz constant L and $C^{0,1}$ radius $\rho_0 > 0$. Let $x_0 \in \Omega$ with $\rho := d_\Omega(x_0)$, $\gamma > -1$ and $\gamma < \beta$. Then,*

$$\int_{\Omega \setminus B_{\rho/2}} d_\Omega^\gamma(x_0 + y)|y|^{-n-\beta}\,\mathrm{d}y \le C(1 + \rho^{\gamma-\beta})$$

for some constant $C > 0$, depending only on n, γ, β, ρ_0, L, and, if $\gamma > 0$ or $\beta \le 0$ also on $\mathrm{diam}(\Omega)$.

Proof. We assume that $x_0 = 0$. By [Fernández-Real and Ros-Oton 2024a, Lemma B.2.4], there exists $\kappa > 0$ such that for any $t \in (0, \kappa)$,

$$\mathcal{H}^{n-1}\big(\{d = t\} \cap (B_{2^{j+1}\rho} \setminus B_{2^j\rho})\big) \le C(2^j\rho)^{n-1}. \tag{2-4}$$

Note that

$$\int_{(\Omega \setminus B_{\rho/2}) \cap \{d \ge \kappa\}} d^\gamma(y)|y|^{-n-\beta}\,\mathrm{d}y \le (\mathrm{diam}(\Omega)^\gamma \mathbb{1}_{\{\gamma > 0\}} + \kappa^\gamma \mathbb{1}_{\{\gamma \le 0\}}) \int_{(\Omega \setminus B_{\rho/2}) \cap \{d \ge \kappa\}} |y|^{-n-\beta}\,\mathrm{d}y \le c$$

for some constant $c > 0$ depending on κ and, if $\gamma > 0$ or $\beta \le 0$ also on $\mathrm{diam}(\Omega)$, independent of ρ. The independence of ρ is trivial if $\kappa \le 2\rho$ since then $\Omega \setminus B_{\rho/2} \subset \Omega \setminus B_{\kappa/4}$, and otherwise, it follows from the fact that $B_r \cap \{d \ge \kappa\} = \varnothing$ once $r \le \kappa/2 \le \kappa - \rho$ (recall that $d(0) = \rho$), so also in this case, we can replace the domain of integration by $\Omega \setminus B_{\kappa/2}$. Moreover, using (2-4) and the coarea formula,

$$\begin{aligned}
\int_{(\Omega \setminus B_{\rho/2}) \cap \{d \le \kappa\}} d^\gamma(y)|y|^{-n-\beta}\,\mathrm{d}y &\le c\sum_{j \ge 1}\bigg((2^j\rho)^{-n-\beta}\int_{(B_{2^{j+1}\rho} \setminus B_{3^j\rho}) \cap \{d \le \kappa\}} d^\gamma(y)|\nabla d(y)|\,\mathrm{d}y\bigg) \\
&\le c\sum_{j \ge 1}\bigg((2^j\rho)^{-n-\beta}\int_0^{\min\{2^j\rho, \kappa\}} t^\gamma\bigg[\int_{(B_{2^{j+1}\rho} \setminus B_{2^j\rho}) \cap \{d = t\}} \mathrm{d}\mathcal{H}^{n-1}(y)\bigg]\mathrm{d}t\bigg) \\
&\le c\sum_{j \ge 1}((2^j\rho)^{-\beta+\gamma}) \le c\rho^{\gamma-\beta}
\end{aligned}$$

for some $c > 0$, where we used that $\gamma - \beta < 0$. □

The following lemma will be of central importance for the proof of Lemmas 2.6 and 2.7.

Lemma 2.3. *Let $L \in \mathcal{L}_s^{\mathrm{hom}}(\lambda, \Lambda)$. Let $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $\partial\Omega \in C^{1,\gamma}$ for some $\gamma > 0$. Then, for any $\delta \in (0, s)$, there exists $c_1 > 0$, depending only on n, s, λ, Λ, Ω, γ, δ, and the $C^{1,\gamma}$ radius of Ω, such that*

$$|L(d^{s-1})| \le c_1 d^{\delta\gamma - s - 1} \quad \text{in } \Omega.$$

Moreover, for any $\varepsilon \in (0, s)$, there exist $c_2, c_3 > 0$ depending only on n, s, λ, Λ, γ, ε, and the $C^{1,\gamma}$ radius of Ω, such that

$$-L(d^{s-1+\varepsilon}) \le -c_2 d^{\varepsilon - s - 1} + c_3 \quad \text{in } \Omega.$$

The first claim follows in a similar way as [Fernández-Real and Ros-Oton 2024a, Proposition B.2.1].

Proof. We let $x_0 \in \Omega$ and write $\rho = d(x_0)$. Then, we let

$$l(x) = (d(x_0) + \nabla d(x_0) \cdot (x - x_0))_+$$

and observe that

$$L(l^{s-1}) = 0 \quad \text{in } \{l > 0\},$$

as a consequence of $L(l^s) = 0$ and $\nabla l^s = s l^{s-1} \nabla l = s \nabla d(x_0) l^{s-1}$. Next, we claim that

$$|d^{s-1} - l^{s-1}|(x_0 + y) \le \begin{cases} C\rho^{s+\gamma-3}|y|^2 & \text{in } B_{\rho/2}, \\ C|y|^{(1+\gamma)\delta}|d^{s-1-\delta}(x_0+y) + l^{s-1-\delta}(x_0+y)| & \text{in } \mathbb{R}^n \setminus B_{\rho/2}. \end{cases} \tag{2-5}$$

From here, we can compute

$$\begin{aligned} |L(d^{s-1})(x_0)| &= |L(d^{s-1} - l^{s-1})(x_0)| \\ &\le C\rho^{s+\gamma-3} \int_{B_{\rho/2}} |y|^{2-n-2s} \, \mathrm{d}y \\ &\qquad + C \int_{(x_0+\Omega)\setminus B_{\rho/2}} |y|^{-n-2s+(1+\gamma)\delta} |d^{s-1-\delta}(x_0+y) + l^{s-1-\delta}(x_0+y)| \, \mathrm{d}y \\ &\le C(1 + \rho^{\gamma-s-1} + \rho^{\gamma\delta-s-1}), \end{aligned}$$

where we applied Lemma 2.2 to d and to l with $s-1-\delta =: \gamma < \beta := 2s - (1+\gamma)\delta$ (choosing $\gamma \in (0, s)$ so small that $\beta > 0$), in order to estimate the third integral. Since this estimate implies the first result, it remains to verify the claim (2-5). In case $x \in B_{\rho/2}(x_0)$, we estimate

$$|d^{s-1} - l^{s-1}|(x) \le |d-l|(x) \|d^{s-2} + l^{s-2}\|_{L^\infty(B_{\rho/2}(x_0))} \le c\|D^2 d\|_{L^\infty(B_{\rho/2}(x_0))} |x_0 - x|^2 \rho^{s-2} \le C\rho^{s+\gamma-3}|y|^2.$$

Here, we used that $|D^2 d| \le C d^{-1+\gamma}$ by [Fernández-Real and Ros-Oton 2024a, Lemma B.0.1] and that $l \ge c\rho$ in $B_{\rho/2}(x_0)$. The latter statement follows since by the $C^{1,\gamma}$ regularity of d, it must be

$$\left| d(x) - d(x_0) - \nabla d(x_0) \cdot (x - x_0) \right| \le C\rho^{1+\gamma} \quad \text{for all } x \in B_{\rho/2}(x_0),$$

due to Taylor's formula, and therefore $d(x)$ and ρ are comparable in $B_{\rho/2}(x_0)$, which yields for small enough ρ for some $c > 0$,

$$l(x) \ge d(x_0) + \nabla d(x_0) \cdot (x - x_0) \ge d(x) - C\rho^{1+\gamma} \ge c\rho > 0 \quad \text{for all } x \in B_{\rho/2}(x_0).$$

We can always assume that $\rho > 0$ is small, since otherwise, the result follows by the regularity of d^{s-1} away from the boundary of Ω.

Next, for $x \in \mathbb{R}^n \setminus B_{\rho/2}(x_0)$, we make use of the following algebraic inequality, which follows from the C^δ regularity of the function $t \mapsto t^{s-1-\delta}$ in $[\min\{a, b\}, \max\{a, b\}]$,

$$|a^{s-1} - b^{s-1}| \le c|a-b|^\delta |a^{s-1-\delta} + b^{s-1-\delta}| \quad \text{for all } a, b > 0,$$

for any $\delta \in (0, s)$ and some $c > 0$, depending only on s, δ, which allows us to estimate

$$\begin{aligned} |d^{s-1}(x) - l^{s-1}(x)| &\le c|d(x) - l(x)|^\delta |d^{s-1-\delta}(x) + l^{s-1-\delta}(x)| \\ &\le c|x_0 - x|^{(1+\gamma)\delta} |d^{s-1-\delta}(x) + l^{s-1-\delta}(x)|, \end{aligned}$$

where we used that by [Fernández-Real and Ros-Oton 2024a, Lemma B.2.2] it holds

$$|d(x) - l(x)| \le C|x_0 - x|^{1+\gamma}.$$

This proves the first claim.

Now, we turn to the proof of the second result. First, we observe that by similar arguments as in the first part of the proof, we obtain

$$|d^{\varepsilon+s-1}-l^{\varepsilon+s-1}|(x_0+y) \le \begin{cases} C\rho^{\varepsilon+s+\gamma-3}|y|^2 & \text{in } B_{\rho/2}, \\ C|y|^{(1+\gamma)\delta}||d^{\varepsilon+s-1-\delta}(x_0+y)+l^{\varepsilon+s-1-\delta}(x_0+y)| & \text{in } \mathbb{R}^n \setminus B_{\rho/2}, \end{cases}$$

and therefore

$$|L(d^{\varepsilon+s-1}-l^{\varepsilon+s-1})(x_0)| \le C(1+\rho^{\varepsilon+\gamma-s-1}+\rho^{\varepsilon+\gamma\delta-s-1}).$$

We claim that for any $e \in \mathbb{S}^{n-1}$ it holds that

$$\begin{cases} L((x\cdot e)_+^{\varepsilon+s-1}) = c_e(x\cdot e)_+^{\varepsilon-s-1} & \text{in } \{x\cdot e>0\}, \\ (x\cdot e)_+^{s-1+\varepsilon}=0 & \text{in } \{x\cdot e \le 0\} \end{cases} \tag{2-6}$$

for some $c_e \in [c_-, c_+]$, where $c_+ > c_- > 0$ depend only on n, s, λ, Λ. Once we have shown the claim (2-6), we can conclude the proof, since it implies

$$\begin{aligned} -L(d^{\varepsilon+s-1})(x_0) &\le -L(l^{\varepsilon+s-1})(x_0) + |L(d^{\varepsilon+s-1}-l^{\varepsilon+s-1})(x_0)| \\ &\le -c\rho^{\varepsilon-s-1} + C(1+\rho^{\varepsilon+\gamma-s-1}+\rho^{\varepsilon+\gamma\delta-s-1}) \le -c\rho^{\varepsilon-s-1}+C. \end{aligned}$$

Hence, it remains to prove (2-6). By the $2s$-homogeneity of L we can apply [Fernández-Real and Ros-Oton 2024a, Lemmas B.1.5 and 1.10.3(iii)] and deduce

$$L((x\cdot e)_+^{\varepsilon+s-1}) = c_1(-\Delta)^s_{\mathbb{R}}(x\cdot e)_+^{\varepsilon+s-1} = c_1c_2(x\cdot e)_+^{\varepsilon-s-1}$$

for some constant $c_1 > 0$ and where c_2 is given by, see [Fall and Ros-Oton 2022, Lemma 2.4],

$$c_2 = (-\Delta)^s_{\mathbb{R}}(t_+^{\varepsilon+s-1})(1) = \frac{\Gamma(s+\varepsilon)}{\Gamma(-s+\varepsilon)}\frac{\sin(\pi(-1+\varepsilon))}{\sin(\pi(-1-s+\varepsilon))} > 0.$$

This concludes the proof. □

The following lemma is crucial in the proofs of Lemma 2.13, and in Section 6. It follows by differentiating the corresponding results in [Abatangelo and Ros-Oton 2020].

Lemma 2.4. *Let $L \in \mathcal{L}_s^{\text{hom}}(\lambda, \Lambda)$. Let $k \in \mathbb{N}$, and $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $\partial\Omega \in C^{k+1,\gamma}$ for some $\gamma \in (0,1)$ with $\gamma \neq s$, and $0 \in \partial\Omega$. Assume that $K \in C^{2k+2\gamma+3}(\mathbb{S}^{n-1})$. Let*

$$\eta \in C^{k,\gamma}(\overline{\Omega \cap B_1}) \cap C^\infty(\Omega \cap B_1).$$

Then, there exists $c > 0$, depending only on $n, s, \lambda, \Lambda, \Omega, \gamma, k$, such that the following holds true:

(i) *If $k = 1$ and $\gamma < s$, then*

$$|L(d^{s-1}(\nabla d)\eta)| \le c(|\cdot|+|\eta(0)|+|\nabla\eta(0)|)d^{\gamma-s} \quad \text{in } \overline{\Omega}\cap B_{1/2}.$$

(ii) *If $k \ge 2$ or $\gamma > s$, then*

$$[L(d^{s-1}(\nabla d)\eta)]_{C^{k-1-s+\gamma}(\overline{\Omega}\cap B_{1/2})} \le c(|\cdot|+|\eta(0)|+|\nabla\eta(0)|).$$

(iii) *If $k+\gamma > 2s$, then we have for any $x_0 \in \Omega \cap B_{1/2}$*

$$[L(d^{s-1}(\nabla d)\eta)]_{C^{k+\gamma-2s}(B_{d(x_0)/2}(x_0))} \le c(|\cdot|+|\eta(0)|+|\nabla\eta(0)|)d^{s-1}(x_0).$$

Proof. By [Abatangelo and Ros-Oton 2020, Corollary 2.3] (see also [Kukuljan 2021, Corollary 3.9] for $i > k+1$), we deduce that

$$|D^i L(d^s \eta)| \leq c(|\cdot| + |\eta(0)|) d^{k+\gamma-s-i} \quad \text{in } \overline{\Omega} \cap B_{1/2} \quad \text{for all } i \in \mathbb{N}. \tag{2-7}$$

By [Abatangelo and Ros-Oton 2020, Theorem 2.2] and the choice of ψ in the proof of [Abatangelo and Ros-Oton 2020, Corollary 2.3], it follows that the assumption $\eta \in C^{k,\gamma}(\overline{\Omega \cap B_1}) \cap C^\infty(\Omega \cap B_1)$ is sufficient for (2-7) to hold true. Let us now prove (i) and assume that $k = 1$ and $\gamma < s$. Then, since $D^i \eta \in C^\infty(\mathbb{R}^n)$, another application of [Abatangelo and Ros-Oton 2020, Corollary 2.3] yields

$$\|L(d^s D^i \eta)\|_{C^{1+\gamma-s}(\overline{\Omega} \cap B_{1/2})} \leq C \quad \text{for } i \in \{1, 2\}.$$

Since $\nabla(d^s \eta) = s d^{s-1} (\nabla d) \eta + d^s \nabla \eta$, a combination of the previous two estimates with $i = 1$ implies

$$|L(d^{s-1}(\nabla d)\eta)| \leq s^{-1} |\nabla L(d^s \eta)| + s^{-1} |L(d^s \nabla \eta)| \leq c(|\cdot| + |\eta(0)| + |\nabla \eta(0)|) d^{\gamma-s} \quad \text{in } \overline{\Omega} \cap B_{1/2},$$

which yields the result in (i).

To see (ii) and (iii), we observe first that by application of (2-7), we have for any $i \in \mathbb{N}$

$$|D^i L(d^s(\nabla \eta))| \leq c(|\cdot| + |\nabla \eta(0)|) d^{k+\gamma-s-i} \quad \text{in } \overline{\Omega} \cap B_{1/2}.$$

Next, by differentiation, we obtain

$$D^{i+1}(d^s \eta) = s D^i (d^{s-1}(\nabla d)\eta) + D^i (d^s \nabla \eta).$$

Thus, altogether for every $i \in \mathbb{N}$

$$\begin{aligned} |D^i(L(d^{s-1}(\nabla d)\eta))| &\leq s^{-1} |D^{i+1} L(d^s \eta)| + s^{-1} |D^i L(d^s(\nabla \eta))| \\ &\leq c(|\cdot| + |\eta(0)|) d^{k+\gamma-s-(i+1)} + c(|\cdot| + |\nabla \eta(0)|) d^{k+\gamma-s-i} \\ &\leq c(|\cdot| + |\eta(0)| + |\nabla \eta(0)|) d^{k+\gamma-s-i-1} \quad \text{in } \overline{\Omega} \cap B_{1/2}. \end{aligned} \tag{2-8}$$

To conclude the proof of (ii), let $x_0 \in \Omega \cap B_{1/2}$, and note that if $k \geq 2$ or $\gamma > s$, then (2-8) applied with $i = k - 1 + \lceil \gamma - s \rceil$ implies

$$\begin{aligned} [L(d^{s-1}(\nabla d)\eta)]_{C^{k-1-s+\gamma}(B_{d(x_0)/2}(x_0))} &\leq \sup_{x,y \in B_{d_{x_0}/2}(x_0)} \frac{\|D^{k-1+\lceil \gamma-s \rceil}(L(d^{s-1}(\nabla d)\eta))\|_{L^\infty(B_{d(x_0)/2}(x_0))}}{|x-y|^{\gamma-s-\lceil \gamma-s \rceil}} \\ &\leq c(|\cdot| + |\eta(0)| + |\nabla \eta(0)|) d^{\gamma-s-\lceil \gamma-s \rceil}(x_0) d^{s-\gamma+\lceil \gamma-s \rceil}(x_0) \\ &\leq c(|\cdot| + |\eta(0)| + |\nabla \eta(0)|), \end{aligned}$$

where we used that $\gamma < 1$. From here, a covering argument (see [Fernández-Real and Ros-Oton 2024a, Lemma A.1.4]) yields the desired regularity estimate in $\overline{\Omega} \cap B_{1/2}$.

To prove (iii), note that if $k+\gamma > 2s$, then (2-8) applied with $i = k + \lceil \gamma - s \rceil$ implies

$$
\begin{aligned}
[L(d^{s-1}(\nabla d)\eta)]_{C^{k+\gamma-2s}(B_{d(x_0)/2}(x_0))} &\le \sup_{x,y\in B_{d(x_0)/2}(x_0))} \frac{\|D^{k+\lceil\gamma-s\rceil}(L(d^{s-1}(\nabla d)\eta))\|_{L^\infty(B_{d(x_0)/2}(x_0))}}{|x-y|^{\gamma-2s-\lceil\gamma-s\rceil}} \\
&\le c(|\cdot| + |\eta(0)| + |\nabla\eta(0)|)d^{\gamma-s-1-\lceil\gamma-s\rceil}(x_0)d^{2s-\gamma+\lceil\gamma-s\rceil}(x_0) \\
&\le c(|\cdot| + |\eta(0)| + |\nabla\eta(0)|)d^{s-1}(x_0),
\end{aligned}
$$

where we used that $\gamma < 1$. This implies (iii), and we conclude the proof. □

As a corollary, we obtain the following result:

Corollary 2.5. *Let $L \in \mathcal{L}_s^{\mathrm{hom}}(\lambda, \Lambda)$. Let $k \in \mathbb{N}$, and $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $\partial\Omega \in C^{k+1,\gamma}$ for some $\gamma \in (0, 1)$ with $\gamma \ne s$, and $0 \in \partial\Omega$. Assume that $K \in C^{2k+2\gamma+3}(\mathbb{S}^{n-1})$. Let*

$$\eta \in C^{k,\gamma}(\overline{\Omega \cap B_1}) \cap C^\infty(\Omega \cap B_1).$$

Then, there exists $c > 0$, depending only on $n, s, \lambda, \Lambda, \Omega, \gamma, k$, such that the following holds true:

(i) *If $k = 1$ and $\gamma < s$, then*

$$|L(d^{s-1}\eta)| \le c\|\eta\|_{C^1(\overline{\Omega\cap B_{1/2}})} d^{\gamma-s} \quad \text{in } \overline{\Omega} \cap B_{1/2}.$$

(ii) *If $k \ge 2$ or $\gamma > s$, then*

$$[L(d^{s-1}\eta)]_{C^{k-1-s+\gamma}(\overline{\Omega}\cap B_{1/2})} \le c\big(\|\eta\|_{C^1(\overline{\Omega\cap B_{1/2}})} + \|\eta\|_{C^{k-1+s+\gamma}(\Omega\cap B_1)}\big).$$

(iii) *If $k+\gamma > 2s$, then we have for any $x_0 \in \Omega \cap B_{1/2}$*

$$[L(d^{s-1}\eta)]_{C^{k+\gamma-2s}(B_{d(x_0)/2}(x_0))} \le c\big(\|\eta\|_{C^1(\overline{\Omega\cap B_{1/2}})} + \|\eta\|_{C^{k+\gamma}(\Omega\cap B_1)}\big) d^{s-1}(x_0).$$

Proof. There exist $N \in \mathbb{N}$ and $\delta > 0$, $\nu_i \in \mathbb{S}^{n-1}$, $x_i \in \partial\Omega \cap B_1$, depending only on Ω, such that $\partial_{\nu_i} d \ge \frac{1}{2}$ in $\overline{\Omega \cap B_\delta(x_i)}$, for $i \in \{1, \dots, N\}$, and such that

$$\{x \in \overline{\Omega} \cap B_{1/2} : d(x) \le \delta/2\} \subset \bigcup_{i=1}^N B_\delta(x_i).$$

Then, by application of Lemma 2.4(i) to $\eta := (\partial_{\nu_i} d)^{-1}\eta \in C^{k,\gamma}(\overline{\Omega \cap B_\delta(x_i)}) \cap C^\infty(\Omega \cap B_\delta(x_i))$, we deduce that for any $i \in \{1, \dots, N\}$

$$|L(d^{s-1}\eta)| \le c(|\cdot| + |\eta(x_i)| + |\nabla\eta(x_i)|)d^{\gamma-s} \quad \text{in } \overline{\Omega} \cap B_{\delta/2}(x_i).$$

Thus, we have proved (i) in $\overline{\Omega} \cap B_{1/2} \cap \{d(x) \le \delta/2\}$. The result in $\overline{\Omega} \cap B_{1/2} \cap \{d(x) > \delta/2\}$ is immediate from the regularity of K (see [Fernández-Real and Ros-Oton 2024a, Lemma 2.2.6]).

The proofs of (ii) and (iii) follow from Lemma 2.4 in an analogous way. □

2.3. ***Barriers with boundary blow-up.*** Let us construct barrier functions that are suitable for establishing maximum principles for solutions that blow up at the boundary. We establish a subsolution and a supersolution in the following two lemmas.

Lemma 2.6. *Let $L \in \mathcal{L}_s^{\mathrm{hom}}(\lambda, \Lambda)$. Let $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $\partial\Omega \in C^{1,\gamma}$ for some $\gamma > 0$. Then, for any $l \in \mathbb{R}$, $\varepsilon \in (0, \min\{s, 1-s\})$, and $M > 0$ there exists $\phi_l \in C^\infty(\Omega)$ such that*

$$\begin{cases} L\phi_l \le -d^{\varepsilon-s-1} - M & \text{in } \Omega, \\ \phi_l = 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ \phi_l / d^{s-1} = l & \text{on } \partial\Omega. \end{cases}$$

Moreover, if $l \ge 0$, then there exists $\delta \in (0,1)$, depending only on $n, s, \lambda, \Lambda, \mathrm{diam}(\Omega), \varepsilon, M$, such that $\phi_l \ge 0$ in $\Omega \cap \{d \le \delta\}$. And if $l < 0$, then for M large enough, depending on $n, s, \lambda, \Lambda, \mathrm{diam}(\Omega), \varepsilon$, it holds that $\phi_l \le 0$ in Ω.

Proof. Let $\varepsilon \in (0, s)$ and $N > 1$ to be chosen small and large, respectively, later. We set

$$\phi_l(x) := l d^{s-1}(x) - d^{s-1+\varepsilon}(x) - N \mathbb{1}_\Omega(x).$$

Then, by Lemma 2.3,

$$L\phi_l \le c_1 l d^{\delta\gamma - s - 1} - c_2 d^{\varepsilon - s - 1} + c_3 - N L \mathbb{1}_\Omega.$$

Since $L\mathbb{1}_\Omega \ge 0$, by taking any $\delta \in (0, s)$ and then $\varepsilon < \delta\gamma$, we see that there exists $\eta > 0$, depending on $s, l, \varepsilon, M, \delta, \gamma$, such that

$$L\phi_l \le -d^{\varepsilon-s-1} - M \quad \text{in } \Omega \cap \{d < \eta\}.$$

Moreover, there exists $c_4 > 0$, depending on $\mathrm{diam}(\Omega)$, such that $L\mathbb{1}_\Omega \ge c_4$ in $\Omega \cap \{d \ge \eta\}$. Thus, choosing $N = M c_4^{-1}$, we deduce that

$$L\phi_l \le -d^{\varepsilon-s-1} - M \quad \text{in } \Omega,$$

as desired. The remaining properties of ϕ_l follow immediately from its construction. □

Lemma 2.7. *Let $L \in \mathcal{L}_s^{\mathrm{hom}}(\lambda, \Lambda)$. Let $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $\partial\Omega \in C^{1,\gamma}$ for some $\gamma > 0$. Then, there is $c_1 > 0$, depending only on n, s, λ, Λ, such that for any $l \in \mathbb{R}$, $\varepsilon \in (0, \min\{s\gamma, 1-s\})$, and $M > 0$ there exists $\psi_l \in C^\infty(\Omega)$ such that*

$$\begin{cases} L\psi_l \ge c_1 d^{\varepsilon-s-1} + M & \text{in } \Omega, \\ \psi_l = 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ \psi_l / d^{s-1} = l & \text{on } \partial\Omega. \end{cases}$$

Moreover, for any $M > 0$, if $l > 0$ is large enough, depending only on $n, s, \lambda, \Lambda, \mathrm{diam}(\Omega), \varepsilon$, it holds that $\psi_l \ge 0$ in Ω.

Moreover, for any $\varepsilon \in (0, s)$, there is $\widetilde{\psi} \in C^s(\overline{\Omega})$ such that for some $c_2 > 0$

$$\begin{cases} L\widetilde{\psi} \ge d^{\varepsilon-s} & \text{in } \Omega, \\ \widetilde{\psi} = 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ \widetilde{\psi} / d^{s-1} = 0 & \text{on } \partial\Omega, \\ \partial_\nu(\widetilde{\psi} / d^{s-1}) \le c_2 & \text{on } \partial\Omega. \end{cases}$$

Proof. Let $l \in \mathbb{R}$ and $\varepsilon \in (0, \min\{s\gamma, 1-s\})$. The proof is similar to the one of Lemma 2.6. We set

$$\psi_l(x) = l d^{s-1}(x) + d^{s-1+\varepsilon}(x) + C_2 \mathbb{1}_{\overline{\Omega}}(x)$$

and since $\varepsilon < s\gamma$, we can choose $\delta \in (0, s)$ such that $\varepsilon < \delta\gamma$ and take $C_2 > 0$ to be chosen later. By Lemma 2.3,

$$L\psi_l \geq -c_1 l d^{\delta\gamma - s - 1} + c_2 d^{\varepsilon - s - 1} - c_3 + c_4 C_2 \quad \text{in } \Omega,$$

for some constants $c_1, c_2, c_3, c_4 > 0$, depending only on $n, s, \lambda, \Lambda, \delta$, and the $C^{1,\gamma}$ radius of Ω. Thus, if we choose $C_2 > 0$ large enough, depending on $M, l, c_1, c_2, c_3, c_4, \varepsilon, \operatorname{diam}(\Omega)$, then we deduce

$$L\psi_l \geq c d^{\varepsilon - s - 1} + M \quad \text{in } \Omega.$$

Finally, we observe that upon choosing $l > 0$ large enough, depending only on $\varepsilon, \operatorname{diam}(\Omega)$, we have

$$\psi_l \geq l d^{s-1} + d^{s-1+\varepsilon} \geq 0 \quad \text{in } \Omega.$$

For the second claim, we recall from [Fernández-Real and Ros-Oton 2024a, Lemma B.2.6] that for any $\varepsilon \in (0, s)$, there exist $N > 0$ and $c_1 > 0$ such that

$$L(-N d^{s+\varepsilon}) \geq d^{\varepsilon - s} - c_1 \quad \text{in } \Omega.$$

Let $\widetilde{\psi}_2 \in L^\infty(\Omega)$ be the solution to the Dirichlet problem

$$\begin{cases} L\widetilde{\psi}_2 = c_1 & \text{in } \Omega, \\ \widetilde{\psi}_2 = 0 & \text{in } \mathbb{R}^n \setminus \Omega, \end{cases}$$

and observe that by the boundary regularity theory from [Fernández-Real and Ros-Oton 2024a], it holds that $\widetilde{\psi}_2 \in C^s(\overline{\Omega})$, and hence for $\widetilde{\psi} := -N d^{s+\varepsilon} - \widetilde{\psi}_2$, we obtain

$$\frac{\widetilde{\psi}}{d^{s-1}} = 0 \quad \text{on } \partial\Omega.$$

Therefore, for some $c_2 > 0$,

$$|\partial_\nu(\widetilde{\psi}/d^{s-1})| = (1-s)|\widetilde{\psi}/d^s| \leq c_2 \quad \text{on } \partial\Omega,$$

as desired. □

2.4. ***Nonlocal equations up to a polynomial.*** We will need the following definition of nonlocal equations that hold true up to a polynomial. It was introduced in [Dipierro et al. 2019] for the fractional Laplacian and the theory was extended in [Dipierro et al. 2022] to general nonlocal operators (see also [Abatangelo and Ros-Oton 2020]).

Definition 2.8. For $k \in \mathbb{N}$, a bounded domain $\Omega \subset \mathbb{R}^n$, $f \in C(\Omega)$, and $K \in C^{k-1+\delta}(\mathbb{S}^{n-1})$ for some $\delta > 0$, we say that a function $u \in C(\Omega) \cap L^1_{2s+k}(\mathbb{R}^n)$ solves in the viscosity sense

$$Lu \overset{k}{=} f \quad \text{in } \Omega,$$

if there exist polynomials $(p_R)_{R>1} \in \mathcal{P}_{k-1}$ of degree $k-1$, and functions $(f_R)_{R>1}$ such that

$$L(u\mathbb{1}_{B_R}) = f_R + p_R \quad \text{in } \Omega \quad \text{for all } R > \operatorname{diam}(\Omega),$$
$$\|f_R - f\|_{L^\infty(\Omega)} \to 0 \quad \text{as } R \to \infty.$$

Remark 2.9. • In case $k=0$, we set $\mathcal{P}_{0-1} = \mathcal{P}_{-1} = \{0\}$. Then, $Lu \overset{0}{=} f$ is equivalent to $Lu = f$ (see [Dipierro et al. 2022, Corollary 2.13]).

• Instead of $K \in C^k(\mathbb{S}^{n-1})$, here we only assume $K \in C^{k-1+\delta}(\mathbb{S}^{n-1})$ for some $\delta > 0$. It is easy to see that all the arguments in [Dipierro et al. 2022] remain valid under this weaker assumption. We decided to make this change in order to have optimal assumptions on K in Theorem 1.7.

• As in [Abatangelo and Ros-Oton 2020], we assume uniform convergence $f_R \to f$. This is slightly different from [Dipierro et al. 2019], where pointwise convergence was assumed.

The following lemma is a slight improvement of [Abatangelo and Ros-Oton 2020, Lemma 3.6] (see also [Ros-Oton et al. 2025, Lemma 8.1]) in the sense that the estimate involves a weighted L^1 norm instead of a weighted L^∞ norm.

Lemma 2.10. *Let $L \in \mathcal{L}_s^{\text{hom}}(\lambda, \Lambda)$. Let $u \in C(B_1)$ be a viscosity solution to*

$$Lu = f \quad \text{in } B_1.$$

Then, the following hold true:

(i) *Let $\beta \in (0, 2s]$ if $s \neq \frac{1}{2}$ and $\beta \in (0,1)$ if $s = \frac{1}{2}$. If $f \in C(B_1)$ and $u \in L^1_{2s}(\mathbb{R}^n)$, then it holds that $u \in C^\beta_{\text{loc}}(B_1)$ and*

$$\|u\|_{C^\beta(B_{1/2})} \le c\left(\|u\|_{L^\infty(B_1)} + \int_{\mathbb{R}^n \setminus B_1} \frac{|u(y)|}{|y|^{n+2s}} \, dy + \|f\|_{L^\infty(B_1)} \right)$$

for some $c > 0$, depending only on $n, s, \lambda, \Lambda, \beta$.

(ii) *If $f \in C^\alpha(B_1)$ for some $\alpha > 0$ such that $2s + \alpha \notin \mathbb{N}$, $K \in C^\alpha(\mathbb{S}^{n-1})$, and $u \in L^1_{2s+\alpha}(\mathbb{R}^n)$, then $u \in C^{2s+\alpha}_{\text{loc}}(B_1)$ and*

$$\|u\|_{C^{2s+\alpha}(B_{1/2})} \le c\left(\|u\|_{L^\infty(B_1)} + \int_{\mathbb{R}^n \setminus B_1} \frac{|u(y)|}{|y|^{n+2s+\alpha}} \, dy + [f]_{C^\alpha(B_1)} \right)$$

for some $c > 0$, depending only on $n, s, \lambda, \Lambda, \alpha$.

Remark 2.11. From the proof it is apparent, that Lemma 2.10(ii) remains true if $Lu \overset{k}{=} f$ for $k < \alpha$.

Proof. Let us first show (ii) in case $\alpha < 1$. Let us define $v = u\mathbb{1}_{B_1}$. We claim that v solves $Lv = \tilde{f}$ in $B_{3/4}$ for some $\tilde{f} \in C^{2s+\alpha}(B_{3/4})$ with

$$\|\tilde{f}\|_{C^\alpha(B_{3/4})} \le C\left(\|u\|_{L^\infty(B_1)} + \int_{\mathbb{R}^n \setminus B_1} \frac{|u(y)|}{|y|^{n+2s+\alpha}} \, dy + [f]_{C^\alpha(B_{3/4})} \right). \tag{2-9}$$

To prove it, first, we observe that for any $h \in B_{3/4}$ and $x \in B_{3/4-|h|}$, using that $K \in C^\alpha(\mathbb{S}^{n-1})$,

$$|L(u\mathbb{1}_{\mathbb{R}^n\setminus B_1})(x) - L(u\mathbb{1}_{\mathbb{R}^n\setminus B_1})(x+h)| \le |h|^\alpha \int_{\mathbb{R}^n\setminus B_1} |u(y)| \frac{|K(x-y) - K(x+h-y)|}{|h|^\alpha}\,\mathrm{d}y$$
$$\le c|h|^\alpha \int_{\mathbb{R}^n\setminus B_1} \frac{|u(y)|}{|y|^{n+2s+\alpha}}\,\mathrm{d}y.$$

Therefore, since we can add and subtract constants to $\tilde{f}$ without affecting the left-hand side of the next estimate, for any $h \in B_{3/4}$ it holds that

$$\|\tilde{f} - \tilde{f}(\,\cdot\,+h)\|_{L^\infty(B_{3/4-|h|})} \le C\biggl(\operatorname*{osc}_{B_{3/4}} f + |h|^\alpha \int_{\mathbb{R}^n\setminus B_1} \frac{|u(y)|}{|y|^{n+2s+\alpha}}\,\mathrm{d}y\biggr). \tag{2-10}$$

From here, we deduce that there exist $g \in L^\infty(B_{3/4})$ and a constant p such that $\tilde{f} = g + p$. By construction we have

$$\|\tilde{g}\|_{L^\infty(B_{3/4})} \le C\biggl(\|u\|_{L^\infty(B_1)} + \int_{\mathbb{R}^n\setminus B_1} \frac{|u(y)|}{|y|^{n+2s+\alpha}}\,\mathrm{d}y + \operatorname*{osc}_{B_{3/4}} f\biggr).$$

We split $v = v_1 + v_2$, where v_1 and v_2 are solutions to

$$\begin{cases} Lv_1 = \tilde{g} & \text{in } B_{3/4}, \\ v_1 = v & \text{in } \mathbb{R}^n \setminus B_{3/4}, \end{cases} \qquad \begin{cases} Lv_2 = p & \text{in } B_{3/4}, \\ v_2 = 0 & \text{in } \mathbb{R}^n \setminus B_{3/4}, \end{cases}$$

and note that the existence of v_1, v_2 follows from [Fernández-Real and Ros-Oton 2024a, Theorem 3.2.27]). Then, by the maximum principle (see [Fernández-Real and Ros-Oton 2024a, Corollary 3.2.22]) we deduce that

$$\|v_1\|_{L^\infty(B_{3/4})} \le C\Bigl(\|v\|_{L^\infty(\mathbb{R}^n\setminus B_{3/4})} + \|\tilde{g}\|_{L^\infty(B_{3/4})}\Bigr) \le C\biggl(\|u\|_{L^\infty(B_1)} + \int_{\mathbb{R}^n\setminus B_1} \frac{|u(y)|}{|y|^{n+2s+\alpha}}\,\mathrm{d}y + \operatorname*{osc}_{B_{3/4}} f\biggr).$$

Hence,

$$\|v_2\|_{L^\infty(B_{3/4})} \le \|u\|_{L^\infty(B_{3/4})} + \|v_1\|_{L^\infty(B_{3/4})} \le C\biggl(\|u\|_{L^\infty(B_1)} + \int_{\mathbb{R}^n\setminus B_1} \frac{|u(y)|}{|y|^{n+2s+\alpha}}\,\mathrm{d}y + \operatorname*{osc}_{B_{3/4}} f\biggr).$$

Then, by [Abatangelo and Ros-Oton 2020, Lemma 3.7], we deduce

$$\|p\|_{L^\infty(B_{3/4})} \le C\|v_2\|_{L^\infty(B_{3/4})} \le C\biggl(\|u\|_{L^\infty(B_1)} + \int_{\mathbb{R}^n\setminus B_1} \frac{|u(y)|}{|y|^{n+2s+\alpha}}\,\mathrm{d}y + \operatorname*{osc}_{B_{3/4}} f\biggr).$$

Altogether, we have shown

$$\|\tilde{f}\|_{L^\infty(B_{3/4})} \le \|\tilde{g}\|_{L^\infty(B_{3/4})} + \|p\|_{L^\infty(B_{3/4})} \le C\biggl(\|u\|_{L^\infty(B_1)} + \int_{\mathbb{R}^n\setminus B_1} \frac{|u(y)|}{|y|^{n+2s+\alpha}}\,\mathrm{d}y + \operatorname*{osc}_{B_{3/4}} f\biggr).$$

Finally, as a direct consequence of (2-10), we deduce

$$[\tilde{f}]_{C^\alpha(B_{3/4})} \le C\biggl(\|u\|_{L^\infty(B_1)} + \int_{\mathbb{R}^n\setminus B_1} \frac{|u(y)|}{|y|^{n+2s+\alpha}}\,\mathrm{d}y + [f]_{C^\alpha(B_{3/4})}\biggr),$$

which yields the claim (2-9).

Thus, by application of the interior regularity estimate [Fernández-Real and Ros-Oton 2024a, Theorem 2.4.1] to v, we obtain

$$\begin{aligned}\|u\|_{C^{2s+\alpha}(B_{1/2})} = \|v\|_{C^{2s+\alpha}(B_{1/2})} &\le c\big(\|v\|_{L^\infty(\mathbb{R}^n)} + \|\tilde{f}\|_{C^\alpha(B_{3/4})}\big)\\ &\le c\left(\|u\|_{L^\infty(B_1)} + \int_{\mathbb{R}^n\setminus B_1} \frac{|u(y)|}{|y|^{n+2s+\alpha}}\,\mathrm{d}y + [f]_{C^\alpha(B_{3/4})}\right),\end{aligned}$$

as desired. This proves (ii) in case $\alpha < 1$. The case $\alpha \ge 1$ goes in the same way by considering higher order incremental quotients in the arguments above. Statement (i) was proved in [Fernández-Real and Ros-Oton 2024a, Theorem 2.4.3]. The L^∞ norm can be replaced by the $L^1_{2s}(\mathbb{R}^n)$ norm by the same truncation argument we employed above. □

Next, we provide a lemma stating that equations up to a polynomial can be differentiated in the same way as classical nonlocal equations. This lemma will be used in the proof of Lemma 5.3.

Lemma 2.12. *Let $L \in \mathcal{L}_s^{\mathrm{hom}}(\lambda, \Lambda)$. Let $k \in \mathbb{N}$, $f \in C^1(B_1)$, and $K \in C^{k+\delta}(\mathbb{S}^{n-1})$ for some $\delta > 0$. Let $u \in C(B_1) \cap L^1_{2s+k+\delta}(\mathbb{R}^n)$ with $\partial_i u \in L^1_{2s+k-1+\delta}(\mathbb{R}^n)$. Then, it holds that*

$$Lu \overset{k+1}{=} f \quad \text{in } B_1,$$

and $\partial_i f_R \to \partial_i f$, if and only if

$$L(\partial_i u) \overset{k}{=} \partial_i f \quad \text{in } B_1.$$

Proof. Let us assume first that $\partial_i u \in L^1_{2s+k-1+\delta}(\mathbb{R}^n)$, and assume that $Lu \overset{k+1}{=} f$ in B_1. Then, there exist polynomials $p_R \in \mathcal{P}_k$ and functions $f_R \in L^\infty(B_1)$ with $f_R \to f$ such that

$$L(u\mathbb{1}_{B_R}) = f_R + p_R \quad \text{in } B_1.$$

Let us now consider difference quotients $D_i^h u(x) = \frac{u(x+e_i h)-u(x)}{|h|}$ and compute

$$L(D_i^h u\mathbb{1}_{B_R}) = L(D_i^h(u\mathbb{1}_{B_R})) - L(uD_i^h\mathbb{1}_{B_R}) = D_i^h f_R + D_i^h p_R - L(uD_i^h\mathbb{1}_{B_R}),$$

where, by following the proof of [Dipierro et al. 2022, Theorem 2.1], we can decompose

$$-L(uD_i^h\mathbb{1}_{B_R})(x) = \int_{\mathbb{R}^n\setminus B_3} uD_i^h\mathbb{1}_{B_R}(y)K(x-y)\,\mathrm{d}y = d_{R,h}(x) + g_{R,h}(x)$$

for functions $g_{R,h}$ such that

$$g_{R,h}(x) = \int_{\mathbb{R}^n} D_i^h(\mathbb{1}_{B_R})(y)u(y)\psi(x,y)\,\mathrm{d}y = -\int_{B_R} \big(D_{-h}^i u(y)\psi(x,y) + u(y)D_{-h}^i\psi(x,y)\big)\,\mathrm{d}y$$

for some function $\psi : B_1 \times (\mathbb{R}^n \setminus B_3) \to \mathbb{R}$ such that

$$\sup_{x\in B_1}\psi(x,y) \le C\sup_{x\in B_1}(1+|x-y|)^{-(n+2s+k-1+\delta)}, \qquad \sup_{x\in B_1}|\nabla_y\psi(x,y)| \le C\sup_{x\in B_1}(1+|x-y|)^{-(n+2s+k+\delta)},$$

and polynomials $d_{R,h} \in \mathcal{P}_{k-1}$ with

$$d_{R,h}(x) = \sum_{|\alpha|\le k-1}\kappa_{\alpha,h}x^\alpha, \qquad \kappa_{\alpha,h} = c_\alpha\int_{B_R} D_{-h}^i[u(y)\partial_x^\alpha K(x-y)]\,\mathrm{d}y, \qquad c_\alpha \in \mathbb{R}.$$

Clearly, it holds that $g_{R,h} \to g_R$, and $d_{R,h} \to d_R$, as $R \to \infty$, where

$$g_R(x) = \int_{B_R} \partial_i [u(y)\psi(x, y)] \, dy, \quad d_R(x) = \sum_{|\alpha| \le k-1} \kappa_\alpha x^\alpha, \quad \kappa_\alpha = c_\alpha \int_{B_R} \partial_i [u(y) \partial_x^\alpha K(x - y)] \, dy.$$

For the convergence $g_{R,h} \to g_R$ we are using that for any $x \in B_1$,

$$\begin{aligned}&\left|\mathbb{1}_{B_R}(y)(D^i_{-h} u(y)\psi(x, y) + \mathbb{1}_{B_R}(y)u(y)D^i_{-h}\psi(x, y))\right| \\ &\qquad \le C|\partial_i u(y)| \sup_{x\in B_1} (1 + |x - y|)^{-(n+2s+k-1+\delta)} + C|u(y)| \sup_{x\in B_1} (1 + |x - y|)^{-(n+2s+k+\delta)} \in L^1(\mathbb{R}^n)\end{aligned}$$

and dominated convergence. Moreover, from integrating by parts, we see that it holds for any $x \in B_1$

$$\begin{aligned}\int_2^\infty R^{-1} |g_R^{(2)}(x)| \, dR &\le \int_2^\infty R^{-1} \int_{\partial B_R} |u(y)||x - y|^{-(n+2s+k-1+\delta)} \, dy \, dR \\ &\le c \int_{B_2^c} |u(y)||y|^{-(n+2s+k+\delta)} \, dy < \infty,\end{aligned}$$

which implies that $g_R(x) \to 0$, as $R \to \infty$, uniformly in x.

Altogether, we have shown

$$L(\partial_i u \mathbb{1}_{B_R}) = \lim_{h\to 0} D_i^h f_R + \lim_{h\to 0} D_i^h p_R + \lim_{h\to 0} d_{R,h} + \lim_{h\to 0} g_{R,h} = \partial_i f_R + \partial_i p_R + d_R + g_R,$$

which implies that

$$L(\partial_i u \mathbb{1}_{B_R}) \overset{k}{=} f \quad \text{in } B_1,$$

as desired.

Let us now show the other implication, i.e., assume that $L(\partial_i u) \overset{k}{=} \partial_i f$ in B_1. Then, by [Dipierro et al. 2022] we observe that there are $F_R : \mathbb{R}^n \to \mathbb{R}$, and $P_R \in \mathcal{P}_k$ such that

$$L(u\mathbb{1}_{B_R}) = F_R + P_R \quad \text{in } B_1.$$

Clearly, by the same arguments as above, we have

$$L((D_i^h u)\mathbb{1}_{B_R}) = D_i^h L(u\mathbb{1}_{B_R}) - L(u D_i^h \mathbb{1}_{B_R}) = D_i^h F_R + D_i^h P_R + d_{R,h} + g_{R,h}$$

with $D_i^h P_R + d_{R,h} \in \mathcal{P}_{k-1}$ and $g_{R,h} \to g_R$, as $h \to 0$ with $g_R \to 0$, as $R \to \infty$. Thus, by the stability for viscosity solutions up to a polynomial (see [Abatangelo and Ros-Oton 2020, Lemma 3.5]), we have that

$$f_R + p_R = L(\partial_i u \mathbb{1}_{B_R}) = \partial_i F_R + \partial_i P_R + d_R + g_R,$$

where $d_R, p_R, \partial_i P_R \in \mathcal{P}_{k-1}$. Hence, after integrating the previous identity in x_i and denoting $\widetilde{F}_R(x) = \int_{-\infty}^{x_i} (f_R - g_R)(x', y_i) \, dy$, we can deduce

$$F_R = \widetilde{F}_R + \widetilde{P}_R \quad \text{in } B_1,$$

where $\widetilde{P}_R \in \mathcal{P}_k$ is such that $\partial_i \widetilde{P}_R = p_R - d_R - \partial_i P_R$. Then, since $f_R \to f$ and $g_R \to 0$, as $R \to \infty$, we deduce that $\widetilde{F}_R \to F$, where $\partial_i F = f$, and the proof is complete. □

2.5. ***Two lemmas on viscosity solutions.*** In this section, we prove two auxiliary lemmas for viscosity solutions to nonlocal equations with local Neumann boundary data, namely a stability result, and that sums of viscosity subsolutions are again viscosity subsolutions. Both results are standard for nonlocal equations in the interior of the solution domain (see [Fernández-Real and Ros-Oton 2024a]). However, since we consider equations at the boundary, where solutions satisfy a Neumann condition in the viscosity sense, both results require a proof. Both proofs heavily rely on the interaction of nonlocal operators with the distance function and the results in Section 2.2.

First, we prove a stability result, which will be crucial in the blow-up argument of our proof of the higher boundary regularity.

Lemma 2.13. *Let $k \in \mathbb{N} \cup \{0\}$, $\gamma \in (0,1)$ with $\gamma \neq s$, and $\Omega_j \subset \mathbb{R}^n$ be open, bounded domains with $\partial\Omega_j \in C^{2,\gamma}$ such that $0 \in \partial\Omega_j$, $\nu_0 = e_n$ for any $j \in \mathbb{N}$, and such that the $C^{2,\gamma}$ radii of Ω_j and $\operatorname{diam}(\Omega_j)$ are uniformly bounded. Given a sequence $r_j \searrow 0$, we set $\widetilde{\Omega}_j = r_j^{-1}\Omega_j$ and $\tilde{d}_j := d_{\widetilde{\Omega}_j}$. Let $v_j \in L^1_{2s+k}(\mathbb{R}^n)$ with $v_j/\tilde{d}_j^{s-1} \in C(\overline{\widetilde{\Omega}_j})$ be viscosity solutions to*

$$\begin{cases} L_j v_j \overset{k}{=} f_j & \text{in } \widetilde{\Omega}_j \cap B_1,\\ v_j = 0 & \text{in } \mathbb{R}^n \setminus \widetilde{\Omega}_j,\\ \partial_\nu(v_j/\tilde{d}_j^{s-1}) = g_j & \text{on } \partial\widetilde{\Omega}_j \cap B_1, \end{cases}$$

where $f_j \in C(\widetilde{\Omega}_j \cap B_1)$, $g_j \in C(\partial\widetilde{\Omega}_j \cap B_1)$, and $(L_j)_j \subset \mathcal{L}_s^{\text{hom}}(\lambda, \Lambda, k-1+\alpha)$ for some $\alpha > 0$. Moreover, assume that there are $v \in L^1_{2s+k}(\mathbb{R}^n)$ with $v/(x_n)_+^{s-1} \in C(\{x_n \geq 0\})$, $f \in C(\{x_n > 0\} \cap B_1)$, $g \in C(\{x_n = 0\} \cap B_1)$, $L \in \mathcal{L}_s^{\text{hom}}(\lambda, \Lambda, k-1+\alpha)$, and $\varepsilon_j \searrow 0$, $q_j \in \mathcal{P}_k$ such that

$$\begin{aligned} v_j/\tilde{d}_j^{s-1} &\to v/(x_n)_+^{s-1} && \text{in } L^\infty_{\text{loc}}(B_1),\\ v_j &\to v && \text{in } L^1_{2s+k}(\mathbb{R}^n),\\ |f_j - p_j - f| &\to 0 && \text{in } L^\infty_{\text{loc}}(B_1 \cap \{x_n > 0\}),\\ |g_j - q_j - g|(x) \leq c\varepsilon_j &\to 0 && \text{for all } x \in \partial\widetilde{\Omega}_j \cap B_1,\\ K_j &\to K && \text{in } C^{k-1+\alpha}(\mathbb{S}^{n-1}). \end{aligned}$$

Then, there exists $q \in \mathcal{P}_k$ such that v is a viscosity solution to

$$\begin{cases} Lv \overset{k}{=} f & \text{in } B_1 \cap \{x_n > 0\},\\ v = 0 & \text{in } \mathbb{R}^n \setminus \{x_n > 0\},\\ \partial_n(v/(x_n)_+^{s-1}) = g + q & \text{on } B_1 \cap \{x_n = 0\}. \end{cases}$$

If $k = 0$, the same result holds with $\tilde{d}_j^{s-\gamma} f_j \in L^\infty(\widetilde{\Omega}_j \cap B_1)$ and $(x_n)_+^{s-\gamma} f \in L^\infty(\{x_n > 0\} \cap B_1)$.

Proof. Let us define $u_j := v_j/\tilde{d}_j^{s-1}$ and $u := v/(x_n)_+^{s-1}$. Since $u_j \to u$ in $L^\infty_{\text{loc}}(B_1)$ it follows that $v_j = \tilde{d}_j^{s-1}u_j \to (x_n)_+^{s-1}u = v$ in $L^\infty_{\text{loc}}(B_1 \cap \{x_n > 0\})$. This property is enough to use the stability of viscosity solutions from [Fernández-Real and Ros-Oton 2024a, Proposition 3.2.12] to v_j and v. The higher order version which we require here follows from [Abatangelo and Ros-Oton 2020, Lemma 3.5]. Since $v_j \to v$ in $L^1_{2s}(\mathbb{R}^n)$, we also have that $v = 0$ in $B_1 \setminus \{x_n > 0\}$. Consequently, it only remains to prove the convergence of the Neumann boundary condition.

To do so, let $x_0 \in B_1 \cap \{x_n = 0\}$. In case $k \geq 1$, we first truncate v and v_j in $B_2(x_0)$ and apply [Abatangelo and Ros-Oton 2020, Lemma 3.6] to obtain the equations satisfied by $v\mathbb{1}_{B_2}(x_0)$ and $v_j\mathbb{1}_{B_2}(x_0)$. In order not to over-complicate the notation, let us denote the truncations still by v and v_j and the corresponding source terms by f and f_j. Then, let $\phi \in C^2(B_r(x_0))$ for some $r \in (0,1)$ with $\phi \leq u$ in $B_r(x_0)$, $\phi(x_0) = u(x_0)$, and $\phi \equiv u$ in $\mathbb{R}^n \setminus \overline{B_r(x_0)}$ be a test function. Given $\delta \in (0,1)$, $\eta \in (0,\gamma)$, we define now

$$\psi^{(\delta)}(x) = -\delta\mathbb{1}_{B_r(x_0)}(x)[(x_n)_+ - (x_n)_+^{1+\eta}], \quad \psi_j^{(\delta)}(x) = -\delta\mathbb{1}_{B_r(x_0)}(x)[\tilde{d}_j(x) - \tilde{d}_j^{1+\eta}(x)].$$

There exist $C > 0$ and $\varepsilon \in (0, r/2)$, independent of δ, j, such that

$$L_j(\tilde{d}_j^{s-1}\psi_j^{(\delta)}) \leq -C\delta\tilde{d}_j^{\eta-s} \quad \text{in } \widetilde{\Omega}_j \cap B_\varepsilon(x_0). \tag{2-11}$$

This is due to [Fernández-Real and Ros-Oton 2024a, Proposition B.2.1, Lemma B.2.6, Corollary B.2.8], and since $\widetilde{\Omega}_j \cap B_R(x_0)$ and the respective $C^{2,\gamma}$-radii of $\widetilde{\Omega}_j$ are uniformly bounded. Indeed, the aforementioned results yield the existence of $\varepsilon_0 > 0$ such that

$$-\delta L_j(\tilde{d}_j^{s-1}[\tilde{d}_j - \tilde{d}_j^{1+\eta}]) \leq -c_1\delta\tilde{d}_j^{\eta-s} \quad \text{in } \widetilde{\Omega}_j \cap B_{\varepsilon_0}(x_0).$$

Moreover, one computes by scaling from $\widetilde{\Omega}_j$ to Ω_j, denoting $d_j = d_{\Omega_j}$, and applying Lemma 2.2,

$$\begin{aligned}
-\delta L_j(\tilde{d}_j^{s-1}[\tilde{d}_j - \tilde{d}_j^{1+\eta}]\mathbb{1}_{\mathbb{R}^n \setminus B_r(x_0)}) &\leq c\delta \int_{\widetilde{\Omega}_j \setminus B_r(x_0)} (\tilde{d}_j^s(y) + \tilde{d}_j^{s+\eta}(y))|y|^{-n-2s}\,dy \\
&\leq c\delta \int_{\Omega_j \setminus B_{rr_j}(x_0)} (r_j^s d_j^s(y) + r_j^{s-\eta} d_j^{s+\eta}(y))|y|^{-n-2s}\,dy \\
&\leq c_2\delta(1 + r^{-s} + r^{\eta-s}) \quad \text{in } \widetilde{\Omega}_j \cap B_{r/2}(x_0),
\end{aligned} \tag{2-12}$$

where $c_2 > 0$ might depend on $\operatorname{diam}(\Omega_j)$, which we assumed to be bounded, but not on j. Thus, by combination of the previous two computations, we deduce (2-11) upon choosing $\varepsilon < \varepsilon_0$ if necessary.

Moreover, it is immediate by construction that

$$\psi^{(\delta)} \leq 0 \quad \text{in } \mathbb{R}^n. \tag{2-13}$$

Next, we set $\phi^{(\delta)} := \phi + \psi^{(\delta)}$. For any $\delta > 0$, it still holds $\phi^{(\delta)} \leq u$ by (2-13), and $\phi^{(\delta)}(x_0) = u(x_0)$, however $u - \phi^{(\delta)}$ has a strict minimum at x_0 in $\overline{B_r(x_0)}$.

It suffices to prove for any $\delta > 0$ small enough,

$$\partial_n\phi^{(\delta)}(x_0) \leq g(x_0) + q(x_0), \tag{2-14}$$

since then it follows that $\partial_n\phi(x_0) = \partial_n\phi^{(\delta)}(x_0) + \delta \leq g(x_0) + q(x_0) + \delta$, and we obtain the desired result upon taking the limit $\delta \searrow 0$.

Let us now construct test functions $\phi_j^{(\delta)}$ for any $j \in \mathbb{N}$ as

$$\phi_j^{(\delta)} = \begin{cases} u_j = u_j + \psi_j^{(\delta)} & \text{in } \mathbb{R}^n \setminus \overline{B_r(x_0)}, \\ \phi + c_j + \psi_j^{(\delta)} & \text{in } \overline{B_r(x_0)}, \end{cases}$$

where

$$c_j = \min\big\{c \in \mathbb{R} : \phi + c + \psi_j^{(\delta)} \le u_j \quad \text{in } \overline{B_r(x_0)}\big\}.$$

Since $\psi_j^{(\delta)} \to \psi^{(\delta)}$ (lower half-relaxed limits) in $\overline{B_r(x_0)}$, we obtain that $c_j \to 0$ and there exist $x_j \in \overline{B_r(x_0)}$ with $x_j \to x_0$ such that $\phi_j^{(\delta)}(x_j) = u_j(x_j)$ and $\phi_j^{(\delta)} \le u_j$ by [Fernández-Real and Ros-Oton 2024a, Lemma 3.2.10 and proof of Proposition 3.2.12].

Next, we argue that $x_j \in \partial\widetilde{\Omega}_j \cap B_1$. Without loss of generality, we can assume that $x_j \in B_\varepsilon(x_0)$ upon taking $j \in \mathbb{N}$ large enough. In fact, if $x_j \in \widetilde{\Omega}_j \cap B_\varepsilon(x_0)$, then we can compute using Corollary 2.5(i), and (2-11),

$$\begin{aligned}
L_j(\tilde{d}_j^{s-1}\phi_j^{(\delta)})(x_j) &= L_j(\tilde{d}_j^{s-1}\phi \mathbb{1}_{B_r(x_0)})(x_j) + c_j L_j(\tilde{d}_j^{s-1}\mathbb{1}_{B_r(x_0)})(x_j) \\
&\qquad\qquad + L_j(v_j \mathbb{1}_{\mathbb{R}^n\setminus B_r(x_0)})(x_j) + L_j(\tilde{d}_j^{s-1}\psi_j^{(\delta)})(x_j) \\
&\le L_j(\tilde{d}_j^{s-1}\phi)(x_j) + c_j L_j(\tilde{d}_j^{s-1})(x_j) + L_j(\tilde{d}_j^{s-1}u_j\mathbb{1}_{\mathbb{R}^n\setminus B_r(x_0)})(x_j) \\
&\qquad\qquad - c_j L_j(\tilde{d}_j^{s-1}\mathbb{1}_{\mathbb{R}^n\setminus B_r(x_0)})(x_j) + c\|v_j\|_{L^1_{2s}(\mathbb{R}^n)} - C\delta\tilde{d}_j^{\eta-s}(x_j) \\
&\le C_r\tilde{d}_j^{\gamma-s}(x_j) - C\delta\tilde{d}_j^{\eta-s}(x_j)
\end{aligned} \tag{2-15}$$

for some constant $C_r > 0$, depending also on $\|v_j\|_{L^1_{2s}(\mathbb{R}^n)}$ and $\|v\|_{L^1_{2s}(\mathbb{R}^n)}$. To estimate the fourth term in the last estimate, we used an argument similar to (2-12), namely

$$\begin{aligned}
-L_j(\tilde{d}_j^{s-1}\mathbb{1}_{\mathbb{R}^n\setminus B_r(x_0)})(x_j) &\le c\int_{\widetilde{\Omega}_j\setminus B_r(x_0)} \tilde{d}_j^{s-1}(y)|y|^{-n-2s}\,\mathrm{d}y \\
&\le c\int_{\Omega_j\setminus B_{rr_j}(x_0)} r_j^{s+1} d_j^{s-1}(y)|y|^{-n-2s}\,\mathrm{d}y \le cr^{-s-1} =: c_r
\end{aligned}$$

for some $c_r > 0$, where we applied Lemma 2.2. Let us now recall that $\eta < \gamma$.

Hence, upon making $\varepsilon > 0$ even smaller, we can have in $\widetilde{\Omega}_j \cap B_\varepsilon(x_0)$,

$$C\delta\tilde{d}_j^{\eta-\gamma} > \big(C_r + \mathbb{1}_{\{k=0\}}\|\tilde{d}_j^{s-\gamma} f_j\|_{L^\infty(\widetilde{\Omega}_j\cap B_1)} + \mathbb{1}_{\{k\ge1\}}\|f_j\|_{L^\infty(\widetilde{\Omega}_j\cap B_1)}\big).$$

Then it holds that

$$L_j(\tilde{d}_j^{s-1}\phi_j^{(\delta)})(x_j) < -\mathbb{1}_{\{k=0\}}\tilde{d}_j^{\gamma-s}(x_j)\|\tilde{d}_j^{s-\gamma} f_j\|_{L^\infty(\widetilde{\Omega}_j\cap B_1)} - \mathbb{1}_{\{k\ge1\}}\|f_j\|_{L^\infty(\widetilde{\Omega}_j\cap B_1)} < f_j(x_j). \tag{2-16}$$

However, by construction, $\tilde{d}_j^{s-1}\phi_j^{(\delta)}$ is a valid test function for the equation that is satisfied for $\tilde{d}_j^{s-1}u_j = v_j$ at x_j. Since we assumed that $x_j \in \widetilde{\Omega}_j \cap B_1$, it must hold that $L_j(\tilde{d}_j^{s-1}\phi_j^{(\delta)})(x_j) \ge f_j(x_j)$, which contradicts (2-16).

Therefore, it must be $x_j \in \partial\widetilde{\Omega}_j \cap B_1$, as we claimed before. Thus, by the boundary condition

$$\partial_{\nu_{x_j}}\phi_j^{(\delta)}(x_j) \le g_j(x_j).$$

Passing this inequality to the limit, and using the uniform convergence $|g_j - q_j - g| \to 0$, $\nu_{x_j} \to \nu_0 = e_n$, and $\widetilde{\Omega}_j \to \{x_n > 0\}$, we obtain

$$\partial_n(\phi^{(\delta)}(x_0) - q(x_0)) \le g(x_0),$$

where $q \in \mathcal{P}_k$ is the limit of the sequence of polynomials $(q_j)_j$. Thus, we have $\partial_n \phi^{(\delta)}(x_0) \le g(x_0) + q(x_0)$, i.e., (2-14), as desired. This concludes the proof. □

Second, we prove that the difference of two viscosity solutions is again a viscosity subsolution.

Lemma 2.14. *Let $k \in \mathbb{N} \cup \{0\}$, $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $\partial\Omega \in C^{2,\gamma}$ for some $\gamma > 0$. Let $L \in \mathcal{L}_s^{\text{hom}}(\lambda, \Lambda, k-1+\alpha)$ for some $\alpha > 0$. Let $v, w \in L^1_{2s}(\mathbb{R}^n)$ with $v/d^{s-1}, w/d^{s-1} \in C(\overline{\Omega})$ be viscosity solutions to*

$$\begin{cases} Lv \overset{k}{=} f_1 & \text{in } \Omega, \\ v = 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ v/d^{s-1} = g_1 & \text{on } \partial\Omega, \end{cases} \qquad \begin{cases} Lw \overset{k}{=} f_2 & \text{in } \Omega, \\ w = 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ w/d^{s-1} = g_2 & \text{on } \partial\Omega, \end{cases}$$

for some $f_1, f_2 \in C(\Omega)$ and $g_1, g_2 \in C(\partial\Omega)$. Then, $v - w$ is a viscosity solution to

$$\begin{cases} L(v-w) \overset{k}{=} f_1 - f_2 & \text{in } \Omega, \\ v - w = 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ (v-w)/d^{s-1} = g_1 - g_2 & \text{on } \partial\Omega. \end{cases}$$

Proof. We will only demonstrate the proof in case $k = 0$. The general case follows immediately by combining the arguments with Definition 2.8. For the nonlocal equation, the result follows for instance from [Fernández-Real and Ros-Oton 2024a, Lemma 3.4.14]. For the boundary condition, one can proceed as follows. First, we define the sup- and inf-convolutions (see [Fernández-Real and Ros-Oton 2024a, Lemma 3.2.16]),

$$(v/d^{s-1})_\varepsilon(x) := \inf_{\overline{D}} \left(\frac{v}{d^{s-1}}(z) + \frac{|x-z|^2}{\varepsilon} \right) \quad \text{for all } x \in \overline{D}, \quad (v/d^{s-1})_\varepsilon(x) = \frac{v}{d^{s-1}}(x) \quad \text{for all } x \in \mathbb{R}^n \setminus D,$$
$$(w/d^{s-1})^\varepsilon = \sup_{\overline{D}} \left(\frac{w}{d^{s-1}}(z) - \frac{|x-z|^2}{\varepsilon} \right) \quad \text{for all } x \in \overline{D}, \quad (w/d^{s-1})^\varepsilon(x) = \frac{w}{d^{s-1}}(x) \quad \text{for all } x \in \mathbb{R}^n \setminus D,$$

with $D \subset \Omega$ open, bounded such that $\overline{D} \cap \partial\Omega \neq \varnothing$. In analogy to [Fernández-Real and Ros-Oton 2024a, Proposition 3.2.17], we claim that for any $x \in \partial\Omega \cap \overline{D}$ it holds in the viscosity sense that

$$\partial_\nu (v/d^{s-1})_\varepsilon(x) \le g_1(x) + \delta_\varepsilon, \quad \partial_\nu (w/d^{s-1})^\varepsilon \ge g_2(x) + \delta^\varepsilon, \tag{2-17}$$

where $\delta_\varepsilon, \delta^\varepsilon \to 0$, as $\varepsilon \to 0$. Once (2-17) is proven, since $(v/d^{s-1})_\varepsilon$ and $-(w/d^{s-1})^\varepsilon$ are both semiconcave, we have that at any point $x \in \partial\Omega \cap \overline{D}$, where $(v/d^{s-1})_\varepsilon - (w/d^{s-1})^\varepsilon$ can be touched by a paraboloid from below, the functions $(v/d^{s-1})_\varepsilon$ and $-(w/d^{s-1})^\varepsilon$ must be in $C^{1,1}$. Hence, by the linearity of ∂_ν, and due to (2-17) it must hold that

$$\partial_\nu ((v/d^{s-1})_\varepsilon - (w/d^{s-1})^\varepsilon)(x) \le g_1(x) - g_2(x) + \delta_\varepsilon - \delta^\varepsilon \to g_1(x) - g_2(x) \quad \text{as } \varepsilon \to 0.$$

Thus, by the stability for viscosity solutions (which was provided in a significantly more general framework in Lemma 2.13), we deduce that $\partial_\nu((v-w)/d^{s-1}) \le (g_1 - g_2)$ in the viscosity sense. In a similar way, one can prove $\partial_\nu((v-w)/d^{s-1}) \ge (g_1 - g_2)$, and thus, we obtain the desired result.

Thus, it remains to give a proof of (2-17). To see it, for any test function $\phi \in C^2(B_r(x_0))$ touching $(v/d^{s-1})_\varepsilon$ from below at $x_0 \in \partial\Omega \cap \overline{D}$, we define

$$\psi^{(\delta)}(x) = -\delta \mathbb{1}_{B_1(x_0)}(x)[d(x) - d^{1+\eta}(x)]$$

for some $\eta \in (0, \gamma)$ and observe that $\phi^{(\delta)} = \phi + \psi^{(\delta)}$ is still a valid test function, touching $(v/d^{s-1})_\varepsilon$ (strictly) from below, at x_0. Then, there exists $x_\varepsilon \in \overline{D}$ with $x_\varepsilon \in B_{c\varepsilon}(x_0)$ for some $c > 0$, depending only on the oscillation of v/d^{s-1}, such that $\phi^{(\delta)}(\,\cdot\, + x_0 - x_\varepsilon) - \varepsilon^{-1}|x_0 - x_\varepsilon|^2$ touches v/d^{s-1} from below at x_ε. Indeed, from the definition of $(v/d^{s-1})_\varepsilon$ we deduce that there exist $x_\varepsilon \in \overline{D}$ with $x_\varepsilon \to x_0$ such that

$$\frac{v}{d^{s-1}}(x_0) \geq (v/d^{s-1})_\varepsilon(x_0) = \frac{v}{d^{s-1}}(x_\varepsilon) + \frac{|x_0 - x_\varepsilon|^2}{\varepsilon}.$$

Hence, the rate of convergence $x_\varepsilon \to x_0$ only depends on the oscillation of v/d^{s-1}. Then, since $\phi^{(\delta)}$ is a valid test function, we deduce that for any $x \in D$,

$$\phi^{(\delta)}(x + x_0 - x_\varepsilon) \leq (v/d^{s-1})_\varepsilon(x + x_0 - x_\varepsilon) \leq \frac{v}{d^{s-1}}(x) + \frac{|x_0 - x_\varepsilon|^2}{\varepsilon}$$

if $\varepsilon > 0$ is so small that $x + x_0 - x_\varepsilon \in D$. Since the aforementioned inequality becomes an equality in case $x = x_\varepsilon$, we deduce that indeed, $\phi^{(\delta)}(\,\cdot\, + x_0 - x_\varepsilon) - \varepsilon^{-1}|x_0 - x_\varepsilon|^2$ touches v/d^{s-1} from below at x_ε, as claimed.

We observe that $x_\varepsilon \notin \Omega$ since otherwise one would get a contradiction with the nonlocal equation satisfied by v, in the exact same way as in the proof of (2-16), if $\varepsilon > 0$ is small enough. Thus, $x_\varepsilon \in \partial\Omega \cap \overline{D}$, and from the boundary condition satisfied by v, it follows $\partial_\nu \phi^{(\delta)}(x_0) \leq g_1(x_\varepsilon)$. Thus, by the definition of $\phi^{(\delta)}$, we have $\partial_\nu \phi(x_0) = \partial_\nu \phi^{(\delta)}(x_0) + \delta \leq g_1(x_\varepsilon) + \delta$ for any $\delta > 0$. Thus, sending $\delta \to 0$ and recalling that $x_\varepsilon \to x_0$, as $\varepsilon \to 0$, this proves the first statement in (2-17) with $\delta_\varepsilon = g_1(x_\varepsilon) - g_1(x_0)$. Analogously, one proves the second claim in (2-17). □

3. Nonlocal maximum principles with local Dirichlet and Neumann conditions

In this section, we establish weak maximum principles for nonlocal equations with local Dirichlet and Neumann data (see Propositions 1.3 and 1.5).

First, we establish a weak maximum principle for solutions to the inhomogeneous Dirichlet problem in (1-10) (see Proposition 1.3). Its proof goes by sliding the barrier subsolution ϕ from Lemma 2.6 underneath v from below.

Proof of Proposition 1.3. By assumption on v, we have that $v/d^{s-1} \in C(\overline{\Omega})$ with $v/d^{s-1} \geq 0$ on $\partial\Omega$. Let $z \in \partial\Omega$ be such that $\min_{\partial\Omega} v/d^{s-1} = v/d^{s-1}(z) =: l \geq 0$. Let $\varepsilon \in (0, s)$ and $M > 1$ to be chosen later, and recall the subsolution $\phi_l \in C(\Omega)$ from Lemma 2.6. We define

$$c_0 := \inf\{c \in \mathbb{R} : \phi_l/d^{s-1} - c \leq v/d^{s-1} \text{in } \overline{\Omega}\}.$$

Since also $\phi_l/d^{s-1} \in C(\overline{\Omega})$, the above set is nonempty and $c_0 < \infty$. In fact, recalling the definition of ϕ_l, it must be

$$c_0 \le \|v/d^{s-1}\|_{L^\infty(\overline{\Omega})} + \|(\phi_l)_+/d^{s-1}\|_{L^\infty(\overline{\Omega})} \le \|v/d^{s-1}\|_{L^\infty(\overline{\Omega})} + l + c|\mathrm{diam}(\Omega)|^\varepsilon, \tag{3-1}$$

which is independent of M. Moreover, since $\phi_l/d^{s-1}(z) = l = v/d^{s-1}(z)$, we have that $c_0 \ge 0$. Then, in particular, we have

$$\phi_l/d^{s-1} - c_0 \le v/d^{s-1} \quad \text{in } \mathbb{R}^n, \qquad \text{and} \qquad \phi_l/d^{s-1}(x_0) - c_0 = v/d^{s-1}(x_0) \quad \text{for some } x_0 \in \overline{\Omega}.$$

In case $x_0 \in \Omega$, we have

$$\phi_l - c_0 d^{s-1} - v \le 0 \quad \text{in } \mathbb{R}^n \qquad \text{and} \qquad (\phi_l - c_0 d^{s-1} - v)(x_0) = 0,$$

so it must be

$$0 \le L(\phi_l - c_0 d^{s-1} - v)(x_0) \le L\phi_l(x_0) - c_0 L(d^{s-1})(x_0) \le -d^{\varepsilon-s-1}(x_0) - M + (l + c_0) c d^{\delta\gamma-s-1}(x_0),$$

where we used Lemma 2.6 and that $|L(d^{s-1})| \le c d^{\delta\gamma-s-1}$ for any $\delta \in (0, s)$ by Lemma 2.3. Next, we fix any $\delta \in (0, s)$, and take $\varepsilon < \delta\gamma$ and M so large, depending only on c_0, l, $\mathrm{diam}(\Omega)$ (but not on x_0), such that

$$-d^{\varepsilon-s-1}(x_0) - M + (l + c_0) c d^{\delta\gamma-s-1}(x_0) < 0.$$

Since c_0 is independent of M (see (3-1)), we obtain a contradiction. Thus, it must be $x_0 \in \partial\Omega$, which by construction yields that $c_0 = 0$, and therefore $\phi_l \le v$ in Ω. Since $l \ge 0$, by Lemma 2.6, there exists $\delta > 0$ such that $\phi_l \ge 0$ in $\Omega \cap \{d \le \delta\}$. Therefore, v is a viscosity solution to

$$\begin{cases} Lv \ge 0 & \text{in } \Omega \cap \{d > \delta\}, \\ v \ge 0 & \text{in } \mathbb{R}^n \setminus (\Omega \cap \{d > \delta\}). \end{cases}$$

Since $v \in C(\overline{\Omega \cap \{d > \delta\}})$, we can apply the maximum principle for viscosity solutions to v (see [Fernández-Real and Ros-Oton 2024a, Lemma 3.2.19]) and deduce that $v \ge 0$ in $\mathbb{R}^n$, as desired. □

In particular, we have the following comparison principle:

Lemma 3.1. *Let $L \in \mathcal{L}_s^{\mathrm{hom}}(\lambda, \Lambda)$. Let $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $\partial\Omega \in C^{1,\gamma}$ for some $\gamma > 0$. Let $v, b \in L^1_{2s}(\mathbb{R}^n)$ with $v/d^{s-1}, b/d^{s-1} \in C(\overline{\Omega})$ be viscosity solutions to*

$$\begin{cases} Lv \ge f & \text{in } \Omega, \\ v/d^{s-1} \ge 0 & \text{on } \partial\Omega, \end{cases} \qquad \begin{cases} Lb \le f & \text{in } \Omega, \\ b \le v & \text{in } \mathbb{R}^n \setminus \Omega, \\ b/d^{s-1} \le 0 & \text{on } \partial\Omega, \end{cases}$$

for some $f \in C(\Omega)$. Then, $v \ge b$ in $\mathbb{R}^n$.

Proof. Since by [Fernández-Real and Ros-Oton 2024a, Lemma 3.4.13] $w = v - b$ is a viscosity solution to $Lw \ge 0$ in Ω such that $w/d^{s-1} \ge 0$ on $\partial\Omega$, and $w \ge 0$ in $\mathbb{R}^n \setminus \Omega$, it satisfies the assumptions of Proposition 1.3. An application of this result concludes the proof. □

As an application, we have the following version of a nonlocal Hopf lemma for viscosity solutions. The proof follows in the same way as [Fernández-Real and Ros-Oton 2024a, Proposition 2.6.6], where the Hopf lemma was proved for bounded solutions.

Lemma 3.2. *Let $L \in \mathcal{L}_s^{\mathrm{hom}}(\lambda, \Lambda)$. Let $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $\partial\Omega \in C^{1,\gamma}$ for some $\gamma > 0$. Let $v \in L^1_{2s}(\mathbb{R}^n)$ with $v/d^{s-1} \in C(\overline{\Omega})$ satisfy, in the viscosity sense,*

$$\begin{cases} Lv = f \geq 0 & \text{in } \Omega, \\ v \geq 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ v/d^{s-1} \geq 0 & \text{on } \partial\Omega, \end{cases}$$

for some $f \in C(\Omega)$. Then, either $v \equiv 0$ in Ω, or

$$v(x) \geq C\Big(\inf_{\{x\in\Omega:\mathrm{dist}(x,\partial\Omega)\geq\delta\}} v\Big) d^s(x) \quad \text{in } \Omega$$

for some $C, \delta > 0$, which depend only on $n, s, \lambda, \Lambda, \gamma$, $\mathrm{diam}(\Omega)$, and the $C^{1,\gamma}$ radius of Ω.

Proof. First, by the weak maximum principle for viscosity solutions with boundary blow-up (see Proposition 1.3), we have $v \geq 0$ in $\mathbb{R}^n$. In order to deduce $v > 0$ in case $v \not\equiv 0$, one uses the nonlocal weak Harnack inequality (see [Fernández-Real and Ros-Oton 2024a, Theorem 3.3.1]). Then, we use the subsolution ϕ from [Fernández-Real and Ros-Oton 2024a, Corollary B.2.8] which satisfies

$$\begin{cases} L\phi \leq -1 & \text{in } N_\delta, \\ \max\{d^s, \delta^{-1}\} \geq \phi \geq \delta d^s & \text{in } \mathbb{R}^n, \end{cases}$$

for some $\delta > 0$ and where $N_\delta = \{0 < d < \delta\}$. Let us define

$$c_* = \min\{v(x) : x \in \Omega \setminus N_\delta\} > 0.$$

Then, we have

$$c_*\delta L\phi \leq Lv \quad \text{in } N_\delta \qquad \text{and} \qquad c_*\delta\phi \leq v \quad \text{in } \mathbb{R}^n \setminus N_\delta.$$

Hence, by the comparison principle in Lemma 3.1, we deduce that $c_*\delta\phi \leq u$ in $\mathbb{R}^n$, which implies the desired result. □

Given a $C^{1,\gamma}$ domain $\Omega \subset \mathbb{R}^n$, let us now consider functions $b : \mathbb{R}^n \to \mathbb{R}$, which arise as the solution to the Dirichlet problem

$$\begin{cases} Lb = f_b & \text{in } \Omega, \\ b_\Omega = e_b & \text{in } \mathbb{R}^n \setminus \Omega, \\ b_\Omega/d^{s-1} = g_b & \text{on } \partial\Omega, \end{cases} \tag{3-2}$$

for some $f_b \geq 0$ with $f_b \not\equiv 0$, $e_b \geq 0$, and $g_b \geq 0$. With the maximum principle (see Proposition 1.3) at hand, the existence of b can be established using standard techniques. For well-posedness results in case $L = (-\Delta)^s$, we refer to [Abatangelo 2015]. Moreover, by Proposition 1.3, we have $b \geq 0$ in Ω, and by the same argument as in the proof of (7-1), we have $b/d^{s-1} \in L^\infty(\Omega)$. Moreover, if $\partial\Omega \in C^{2,\gamma}$ and f_b, e_b, g_b are smooth, then by Theorem 1.4, we have $b_\Omega/d^{s-1} \in C^{1,\gamma}(\overline{\Omega})$, and $\partial_\nu(b/d^{s-1})$ exists in the classical sense.

In the following, we will denote by b_Ω the solution to (3-2) with $f_b = g_b = 1$ and $e_b = 0$.

As a corollary of the previous results, we obtain the following pointwise formulation of a nonlocal Hopf lemma for solutions with boundary blow-up.

Lemma 3.3. *Let $L \in \mathcal{L}_s^{\text{hom}}(\lambda, \Lambda)$. Let $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $\partial\Omega \in C^{1,\gamma}$ for some $\gamma > 0$. Let $v \in L^1_{2s}(\mathbb{R}^n)$ with $v/d^{s-1} \in C(\overline{\Omega})$ satisfy, in the viscosity sense,*

$$\begin{cases} Lv \geq 0 & \text{in } \Omega, \\ v \geq 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ v/d^{s-1} = g & \text{on } \partial\Omega, \end{cases}$$

for some $g \in C(\partial\Omega)$. Let $x_0 \in \partial\Omega$ be such that $\min_{\overline{\partial\Omega}} g = g(x_0) \leq 0$. Then, either $v \equiv 0$, or we have that in the viscosity sense

$$\partial_\nu (v/b)(x_0) > 0$$

for any b as in (3-2) *with $b/d^{s-1} = 1$ on $\partial\Omega \cap (\{g < 0\} \cup \{x_0\})$.*

In particular, Lemma 3.3 implies that for the regularized distance d,

$$\partial_\nu (v/d^{s-1})(x_0) = \partial_\nu (v/b)(x_0) + g(x_0)\partial_\nu (b/d^{s-1})(x_0) > g(x_0)\partial_\nu (b/d^{s-1})(x_0).$$

We stress that the sign of the right-hand side depends on the choice of the regularized distance d.

Proof. Since $g(x_0) \leq 0$ we have by the construction of b in (3-2)

$$\begin{aligned} L(v - g(x_0)b) \geq -g(x_0) \geq 0 \quad & \text{in } \Omega, \\ v - g(x_0)b \geq 0 \quad & \text{in } \mathbb{R}^n \setminus \Omega, \\ (v - g(x_0)b)/d^{s-1} = g - g(x_0) \geq 0 \quad & \text{on } \partial\Omega \cap \{g < 0\}, \\ (v - g(x_0)b)/d^{s-1} \geq g \geq 0 \quad & \text{on } \partial\Omega \cap \{g \geq 0\}. \end{aligned}$$

Thus, an application of Lemma 3.2 to $v - g(x_0)b$ yields that either $v - g(x_0)b \equiv 0$ in Ω, or

$$v - g(x_0)b \geq cd^s \quad \text{near } x_0. \tag{3-3}$$

We cannot have $v - g(x_0)b \equiv 0$, unless $g(x_0) = 0$ (in which case $v \equiv v - g(x_0)b \equiv 0$), since then

$$Lv = g(x_0)Lb \leq g(x_0) < 0 \quad \text{in } \Omega,$$

a contradiction. Thus, unless $v \equiv 0$, we have (3-3), and we compute, using that $b \geq 0$ and $(b/d^{s-1})(x_0) = 1$,

$$\partial_\nu (v/b)(x_0) = \lim_{x \to x_0} \frac{\frac{v(x)}{b(x)} - g(x_0)}{d(x)} = \lim_{x \to x_0} \frac{v(x) - g(x_0)b(x)}{b(x)d(x)} \geq c \lim_{x \to x_0} \frac{d^{s-1}(x)}{b(x)} = c > 0.$$

If the limit in the previous estimate does not exist, we need to interpret the boundary condition in the viscosity sense, i.e., take any smooth ψ with $\psi(x_0) = (v/d^{s-1})(x_0) = g(x_0)$ and $\psi \geq v/d^{s-1}$. Then, the limit $\partial_\nu \psi(x_0)$ exists, and an analogous computation as above yields $\partial_\nu \psi(x_0) \geq c > 0$, i.e., $\partial_\nu (v/b)(x_0) > 0$ in the viscosity sense. □

Finally, we are in a position to prove the main result of this section, a maximum principle for nonlocal equations with local Neumann conditions.

Lemma 3.4. *Let $L \in \mathcal{L}_s^{\text{hom}}(\lambda, \Lambda)$. Let $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $\partial\Omega \in C^{2,\gamma}$ for some $\gamma > 0$ and $K \in C^{5+2\gamma}(\mathbb{S}^{n-1})$. Let $\Gamma \subset \partial\Omega$, $v \in L^1_{2s}(\mathbb{R}^n)$ with $v/d^{s-1} \in C(\overline{\Omega})$ satisfy, in the viscosity sense,*

$$\begin{cases} Lv \ge f & \text{in } \Omega, \\ v \ge 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ \partial_\nu (v/b) \le g & \text{on } \partial\Omega \setminus \Gamma, \\ v/b \ge 0 & \text{on } \partial\Omega \cap \Gamma \end{cases}$$

for some $f \in C(\Omega)$ with $d^{s+1-\varepsilon} f \in L^\infty(\Omega)$ for some $\varepsilon \in (0, s]$, and $g \in C(\partial\Omega)$. Here, b is as in (3-2) *with $b/d^{s-1} = 1$ on $\partial\Omega \setminus \Gamma'$ for some $\Gamma' \Subset \Gamma$. Then, there exists $c > 0$, depending only on n, s, λ, Λ, γ, ε, and the $C^{2,\gamma}$ radius of Ω and* diam(Ω), *such that*

$$v/d^{s-1} \ge -c\|d^{s-\varepsilon} f\|_{L^\infty(\Omega)} - c\|g\|_{L^\infty(\partial\Omega\setminus\Gamma)} \quad \text{in } \Omega.$$

Proof. The case $f \ge 0$ and $g \le 0$ follows from the Hopf lemma (see Lemma 3.3). In fact, since $v/b \in C(\partial\Omega)$, there exists $x_0 \in \partial\Omega$ with $\min_{\partial\Omega}(v/b) = (v/b)(x_0)$. If $(v/b)(x_0) \ge 0$, then we have that $v/d^{s-1} \ge 0$ on $\partial\Omega$. Otherwise, $(v/b)(x_0) < 0$, and then by assumption it must be $x_0 \in \partial\Omega \setminus \Gamma$. However, in this case Lemma 3.3 implies that either $v \equiv 0$, (in which case we are done), or $\partial_\nu(v/b)(x_0) > 0$, which contradicts $g(x_0) \le 0$. Thus, we must have $v/d^{s-1} \ge 0$ on $\partial\Omega$. However, by the weak maximum principle (see Proposition 1.3), this implies $v \ge 0$, as desired.

Now, we explain how to get the result with general f, g. To do so, let $\widetilde{\psi}_1$ be the solution to

$$\begin{cases} L\widetilde{\psi}_1 = 0 & \text{in } \Omega, \\ \widetilde{\psi}_1 = 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ \widetilde{\psi}_1/d^{s-1} = h & \text{on } \partial\Omega, \end{cases}$$

for some smooth function h which satisfies $0 \le h \le 1$, and is such that $h = 1$ on $\partial\Omega \setminus \Gamma$, and $h = 0$ in $\partial\Omega \cap \Gamma'$.

From Lemma 3.3, we deduce that $\partial_\nu(\widetilde{\psi}_1/b) < 0$ on $\partial\Omega \setminus \Gamma$. Since $\partial\Omega \in C^{2,\gamma}$, by Theorem 1.4 we have that $\partial_\nu(\widetilde{\psi}_1/b) \in C^\gamma(\partial\Omega)$, and therefore, there is $c_0 > 0$ such that

$$\partial_\nu(\widetilde{\psi}_1/b) \le -c_0 < 0 \quad \text{on } \partial\Omega \setminus \Gamma.$$

Moreover, let us denote by $\widetilde{\psi}_2$ the function $\widetilde{\psi}$ from the second claim of Lemma 2.7, which satisfies for some $c_2 > 0$,

$$\begin{cases} L\widetilde{\psi}_2 \ge d^{\varepsilon-s} & \text{in } \Omega, \\ \widetilde{\psi}_2 = 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ \widetilde{\psi}_2/d^{s-1} = 0 & \text{on } \partial\Omega, \\ \partial_\nu(\widetilde{\psi}_2/b) \le c_2 & \text{on } \partial\Omega. \end{cases}$$

Hence, if we take $M = c_0^{-1}(c_2+1) > 0$ and define $\widetilde{\psi} := M\widetilde{\psi}_1 + \tilde{\psi}_2$, we obtain

$$\begin{cases} L\widetilde{\psi} \geq d^{\varepsilon-s} & \text{in } \Omega, \\ \widetilde{\psi} = 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ \widetilde{\psi}/d^{s-1} = Mh & \text{on } \partial\Omega, \\ \partial_\nu(\widetilde{\psi}/b) \leq -1 & \text{on } \partial\Omega \setminus \Gamma. \end{cases}$$

We apply the previous argument with v replaced by

$$w = v + \big(\|d^{s-\varepsilon} f\|_{L^\infty(\Omega)} + \|g\|_{L^\infty(\partial\Omega\setminus\Gamma)}\big)\widetilde{\psi}.$$

Then, we have that in the viscosity sense,

$$\begin{cases} Lw \geq f + d^{\varepsilon-s}\big(\|d^{s-\varepsilon} f\|_{L^\infty(\Omega)} + \|g\|_{L^\infty(\partial\Omega\setminus\Gamma)}\big) \geq 0 & \text{in } \Omega, \\ w \geq v \geq 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ \partial_\nu(w/b) \leq g - \big(\|d^{s-\varepsilon} f\|_{L^\infty(\Omega)} + \|g\|_{L^\infty(\partial\Omega\setminus\Gamma)}\big) \leq 0 & \text{on } \partial\Omega \setminus \Gamma, \\ w/b \geq Mh \geq 0 & \text{on } \partial\Omega \cap \Gamma. \end{cases}$$

Altogether, by the same argument as at the beginning of the proof, we have $w \geq 0$ in Ω. Let us now observe that by construction and the same argument as in the proof of (7-1) we have

$$\widetilde{\psi} \leq C d^{s-1} \quad \text{in } \Omega$$

for some $C > 0$. Therefore, we obtain

$$v \geq -\widetilde{\psi}\big(\|d^{s-\varepsilon} f\|_{L^\infty(\Omega)} + \|g\|_{L^\infty(\partial\Omega\setminus\Gamma)}\big) \geq -Cd^{s-1}\big(\|d^{s-\varepsilon} f\|_{L^\infty(\Omega)} + \|g\|_{L^\infty(\partial\Omega\setminus\Gamma)}\big) \quad \text{in } \Omega,$$

as desired. ☐

Proof of Proposition 1.5. This is a special case of Lemma 3.4. ☐

4. Hölder estimates up to the boundary

The previous maximum principle for nonlocal equations with local Neumann conditions (see Lemma 3.4) puts us in a position to establish a Harnack inequality for solutions to (1-7) at the boundary, which will eventually lead to the Hölder regularity estimate in Theorem 1.6.

To prove it, we adapt some of the ideas in [Lian and Zhang 2023] to the framework of solutions to nonlocal problems which blow up at the boundary.

For $\delta > 0$, let us define $\Omega_\delta = \{x \in \Omega : \operatorname{dist}(x, \partial\Omega) \geq \delta\}$.

Lemma 4.1. *Let $L \in \mathcal{L}_s^{\mathrm{hom}}(\lambda, \Lambda)$. Let $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $0 \in \partial\Omega$ and $\partial\Omega \in C^{2,\gamma}$ for some $\gamma > 0$ and $K \in C^{5+2\gamma}(\mathbb{S}^{n-1})$. Let $v \in L^1_{2s}(\mathbb{R}^n)$ with $v/d^{s-1} \in C(\overline{\Omega})$ be a viscosity solution to*

$$\begin{cases} Lv \geq f & \text{in } \Omega \cap B_1, \\ v \geq 0 & \text{in } \mathbb{R}^n, \\ \partial_\nu(v/b_\Omega) \leq g & \text{on } \partial\Omega \cap B_1 \end{cases}$$

for some $f \in C(\Omega \cap B_1)$ *with* $d^{s-\alpha} f \in L^\infty(\Omega \cap B_1)$ *for some* $\alpha \in (0, s]$, *and* $g \in C(\overline{\partial\Omega \cap B_1})$. *Assume that* $0 \in \partial\Omega$. *Then,*

$$\fint_{\Omega_{1/2}\cap B_1} (v/b_\Omega)\,\mathrm{d}x \le c \inf_{\Omega\cap B_{\eta^{-1}}} (v/b_\Omega) + c\big(\|d^{s-\alpha} f_-\|_{L^\infty(\Omega\cap B_1)} + \|g_+\|_{L^\infty(\partial\Omega\cap B_1)}\big),$$

where $\eta > 1$ *and* $c > 0$ *depend only on* $n, s, \lambda, \Lambda, \gamma, \alpha$, *and the* $C^{2,\gamma}$ *radius of* Ω. *Here,* b_Ω *is defined as in* (3-2).

Proof. The interior weak Harnack inequality for viscosity supersolutions (see [Fernández-Real and Ros-Oton 2024a, Theorem 3.3.1]) applied with v implies

$$\fint_{\Omega_{1/2}\cap B_1} v(x)\,\mathrm{d}x \le c \inf_{x\in\Omega_{1/2}\cap B_1} v(x) + c\|f\|_{L^\infty(\Omega_{1/2}\cap B_1)},$$

where $c > 0$ depends on $n, s, \lambda, \Lambda, \eta, \alpha$. Moreover, since $b \asymp c > 0$ in $\Omega_{1/2} \cap B_1$, it follows for $u := v/b$ by Lemma 3.2 that

$$\fint_{\Omega_{1/2}\cap B_1} u(x)\,\mathrm{d}x \le c \inf_{x\in\Omega_{1/2}\cap B_1} u(x) + c\|d^{s-\alpha} f\|_{L^\infty(\Omega_{1/2}\cap B_1)}.$$

Thus, it remains to show

$$\inf_{x\in\Omega_{1/2}\cap B_1} u(x) \le c \inf_{x\in\Omega\cap B_{\eta^{-1}}} u(x) + c\big(\|d^{s-\alpha} f\|_{L^\infty(\Omega\cap B_1)} + \|g\|_{L^\infty(\partial\Omega\cap B_1)}\big). \tag{4-1}$$

Since $v \ge 0$, by the weak Harnack inequality, either $v \equiv 0$ in $\Omega_{1/2} \cap B_1$, or $\inf_{\Omega_{1/2}\cap B_1} v > 0$. Therefore, without loss of generality, we can assume that $\inf_{\Omega_{1/2}\cap B_1} v = 1$.

To prove (4-1), let us take a set $D \subset \mathbb{R}^n$ with $\partial D \in C^{2,\gamma}$ such that

$$\Omega \cap B_{1/2} \subset D \subset \Omega \cap B_1,$$

Let w be a function such that

$$\begin{cases} Lw = 0 & \text{in } D,\\ w \le 1 & \text{in } (\Omega_{1/2}\cap B_1)\setminus D,\\ w = 0 & \text{in } \mathbb{R}^n \setminus (D \cup (\Omega_{1/2}\cap B_1)),\\ \partial_\nu(w/b_\Omega) \ge 0 & \text{on } \partial D \cap B_{2\eta^{-1}},\\ w/b_\Omega \le 0 & \text{on } \partial D \setminus B_{2\eta^{-1}},\\ w/b_\Omega \ge c_1 & \text{in } \Omega \cap B_{\eta^{-1}}. \end{cases}$$

We construct w as follows. Let $h : \partial D \to \mathbb{R}$ and $e : \mathbb{R}^n \setminus D \to \mathbb{R}$ be smooth functions such that for some $\eta < \frac{1}{8}$

$$h = \begin{cases} 0 & \text{on } \partial D \setminus B_{2\eta^{-1}},\\ c_1 & \text{on } \partial D \cap B_{\eta^{-1}}, \end{cases} \qquad e = \begin{cases} 1 & \text{in } T,\\ 0 & \text{in } \mathbb{R}^n \setminus (D \cup (\Omega_{1/2}\cap B_1)), \end{cases}$$

where $T \Subset (\Omega_{1/2} \cap B_1) \setminus D$, $0 \le h \le c_1$, and $0 \le e \le 1$. We let w be the solution to

$$\begin{cases} Lw = 0 & \text{in } D,\\ w = e & \text{in } \mathbb{R}^n \setminus D,\\ w/b_D = h & \text{on } \partial D. \end{cases}$$

Then, we can show that $\partial_\nu(w/b_\Omega) \ge C > 0$ in $\partial D \cap B_{2\eta^{-1}}$ (for any given $C > 0$) by making $c_1 > 0$ small enough. Indeed, if w_1 solves the Dirichlet problem with boundary data zero and exterior data e, then by the Hopf lemma (see Lemma 3.2), we have since $w_1/d_D^s \in C^{1,\gamma}(\overline{D})$ by the boundary regularity results in [Abatangelo and Ros-Oton 2020], and since $\partial D \cap B_{2\eta^{-1}} \Subset \partial\Omega$,

$$\begin{aligned}\partial_\nu(w_1/b_\Omega) &= \partial_\nu(w_1/d_D^{s-1})(d_D^{s-1}/b_\Omega) + (w_1/d_D^{s-1})\partial_\nu(d_D^{s-1}/b_\Omega)\\ &= \partial_\nu(w_1/d_D^s)d_D + (w_1/d_D^s)\partial_\nu(d_D) = w_1/d_D^s \ge c_0 > 0 \quad \text{on } \partial D \cap B_{2\eta^{-1}}.\end{aligned}$$

Moreover, if w_2 solves the Dirichlet problem with boundary data h and exterior data zero, we get from Theorem 1.4 that $|\partial_\nu(w_2/b_\Omega)| \le c_3 c_1$ in $B_{2\eta^{-1}}$ for some $c_3 > 0$. Hence, choosing $c_1 > 0$ small enough, we deduce the claim for $w = (C/c_0)w_1 + w_2$.

Thus, we have by construction, and using that $\inf_{\Omega_{1/2}\cap B_1} v = 1$, and $w \asymp d_D^s$ near $\partial D \setminus \partial\Omega$,

$$\begin{cases} L(v-w) \ge f & \text{in } D,\\ v - w \ge 0 & \text{in } \mathbb{R}^n \setminus D,\\ \partial_\nu((v-w)/b_\Omega) \le g & \text{on } \partial D \cap B_{2\eta^{-1}},\\ (v-w)/b_\Omega \ge 0 & \text{on } \partial D \setminus B_{2\eta^{-1}}.\end{cases}$$

Note that b_Ω satisfies

$$\begin{cases} Lb_\Omega \ge 0 & \text{in } D,\\ Lb_\Omega \not\equiv 0 & \text{in } D,\\ b_\Omega \ge 0 & \text{in } \mathbb{R}^n \setminus D,\\ b_\Omega/d_D^{s-1} = 1 & \text{on } \partial D \cap B_{4\eta^{-1}},\\ b_\Omega/d_D^{s-1} \ge 0 & \text{on } \partial D.\end{cases}$$

Since $(\partial D \cap B_{4\eta^{-1}}) \Supset (\partial D \cap B_{2\eta^{-1}})$, we can apply the maximum principle for the Neumann problem Lemma 3.4 with $\Gamma = \partial D \setminus B_{2\eta^{-1}}$ and $b = b_\Omega$, and deduce

$$(v-w)/b_\Omega \ge -c\|d^{s-\alpha} f_-\|_{L^\infty(D\cap B_1)} - c\|g_+\|_{L^\infty(\partial D\cap B_1)} \quad \text{in } D \cap B_1.$$

Since, by construction, we also have

$$w/b_\Omega \ge c_1 = c_1 \inf_{\Omega_{1/2}\cap B_1} v \ge c_2 \inf_{\Omega_{1/2}\cap B_1} u \quad \text{in } \Omega \cap B_{\eta^{-1}},$$

for some $c_2 > 0$, since $b_\Omega \asymp c > 0$ in $\Omega_{1/2} \cap B_1$, we deduce

$$\begin{aligned} v/b_\Omega &= (w + v - w)/b_\Omega\\ &\ge c_2 \inf_{\Omega_{1/2}\cap B_1} u - c\|d^{s-\alpha} f_-\|_{L^\infty(D\cap B_1)} - c\|g_+\|_{L^\infty(\partial D\cap B_1)}\\ &\ge c_2 \inf_{\Omega_{1/2}\cap B_1} u - c\|d^{s-\alpha} f_-\|_{L^\infty(\Omega\cap B_1)} - c\|g_+\|_{L^\infty(\partial\Omega\cap B_1)} \quad \text{in } \Omega \cap B_{\eta^{-1}},\end{aligned}$$

where we used $D \cap B_1 \subset \Omega \cap B_1$. Hence, we obtain (4-1), as desired. □

As a corollary of the previous weak Harnack inequality at the boundary, we obtain a growth lemma.

Lemma 4.2. *Let $L \in \mathcal{L}_s^{\mathrm{hom}}(\lambda, \Lambda)$. Let $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $\partial\Omega \in C^{2,\gamma}$ for some $\gamma > 0$ and $K \in C^{5+2\gamma}(\mathbb{S}^{n-1})$. Let $\eta > 1$ be as in Lemma 4.1. Assume that $x_0 \in \partial\Omega$ and let $0 < R \le 1$. Let $v \in L^1_{2s}(\mathbb{R}^n)$ with $v/d^{s-1} \in C(\overline{\Omega})$ be a viscosity solution to*

$$\begin{cases} Lv \ge f & \text{in } \Omega \cap B_R(x_0), \\ \partial_\nu(v/b_\Omega) \le g & \text{on } \partial\Omega \cap B_R(x_0), \\ v \ge 0 & \text{in } B_R(x_0), \\ v \ge b_\Omega(1-\eta^{j\beta}) & \text{in } B_{\eta^j R}(x_0) \cap \Omega \text{ for all } j \ge 1, \\ v \ge (1-\eta^{j\beta}) & \text{in } B_{\eta^j R}(x_0) \setminus \Omega \text{ for all } j \ge 1, \\ |\Omega_{R/4} \cap B_{R/2}(x_0) \cap \{v/b_\Omega \ge \frac{1}{4}\}| \ge \frac{1}{2}|\Omega_{R/4} \cap B_{R/2}(x_0)| \end{cases}$$

for some $f \in C(\Omega \cap B_R(x_0))$ with $d^{s-\alpha} f \in L^\infty(\Omega \cap B_R(x_0))$ for some $\alpha \in (0, s]$, and $g \in C(\overline{\partial\Omega \cap B_R(x_0)})$. Then, there exist $\delta > 0$, and $\beta \in (0,1)$, depending only on $n, s, \lambda, \Lambda, \gamma, \alpha$, and the $C^{2,\gamma}$ radius of Ω, such that

$$\inf_{\Omega \cap B_{\eta^{-1}R}(x_0)} (v/b_\Omega) + R^{1+\alpha} \|d^{s-\alpha} f_-\|_{L^\infty(\Omega \cap B_R(x_0))} + R\|g_+\|_{L^\infty(\partial\Omega \cap B_R(x_0))} \ge \delta.$$

Proof. Let us assume without loss of generality that $x_0 = 0$. The proof follows from an application of the weak Harnack inequality (see Lemma 4.1) to v_+. It is slightly involved due to the appearance of the tail term.

Indeed, we have

$$Lv_+(x) \ge f(x) - \int_{\mathbb{R}^n \setminus B_R} v_-(y) K(x-y)\,\mathrm{d}y =: \tilde{f}(x),$$

where we used that by assumption, $v \ge 0$ in B_R. Then, we obtain from Lemma 4.1 (after scaling), using the last assumption and setting $u := v/b_\Omega$,

$$\inf_{\Omega \cap B_{\eta^{-1}R}} u + R^{1+\alpha}\|d^{s-\alpha}\tilde{f}_-\|_{L^\infty(\Omega \cap B_{R/2})} + R\|g_+\|_{L^\infty(\partial\Omega \cap B_{R/2})} \ge c_0 \fint_{\Omega_{R/4} \cap B_{R/2}} u\,\mathrm{d}x \ge \frac{c_0}{8}, \tag{4-2}$$

where $c_0 > 0$ is the constant from the weak Harnack inequality.

Next, we estimate $\|d^{s-\alpha}\tilde{f}\|_{L^\infty(\Omega \cap B_R)}$. To do so, we apply a similar reasoning as in the proof of Lemma 2.2. First, we recall that for any $x \in B_{R/2}$, there exists $\kappa > 0$ such that for any $t \in (0, \kappa)$,

$$\mathcal{H}^{n-1}(\{d = t\} \cap B_{\eta^j R} \setminus B_{\eta^{j-1}R}) \le C(\eta^j R)^{n-1},$$

where $C > 0$ depends only on n and the $C^{2,\gamma}$ radius of Ω (we refer to [Fernández-Real and Ros-Oton 2024a, Lemma B.2.4] for a reference of this fact). Next, we observe that by the coarea formula, and since $0 \le b_\Omega \le C d^{s-1}$,

$$\begin{aligned} &R^{1+s} \int_{\Omega \setminus B_R} v_-(y) K(x-y)\,\mathrm{d}y \\ &\le c \sum_{j \ge 1} (1-\eta^{j\beta}) R^{1+s} \int_{\Omega \cap (B_{\eta^j R} \setminus B_{\eta^{j-1}R})} d^{s-1}(y)|y|^{-n-2s}\,\mathrm{d}y \\ &\le c \sum_{j \ge 1} (1-\eta^{j\beta}) R^{1+s} \left((\eta^j R)^{-n-2s} \int_{(B_{\eta^j R} \setminus B_{\eta^{j-1}R}) \cap \{d \le \kappa\}} d^{s-1}(y)|\nabla d(y)|\,\mathrm{d}y + \kappa^{s-1}(\eta^j R)^{-2s} \right) \end{aligned}$$

$$\leq c \sum_{j\geq 1} (1-\eta^{j\beta}) R^{1+s} \Big((\eta^j R)^{-n-2s} \int_0^{\min\{\eta^j R,\kappa\}} t^{s-1} \Big(\int_{(B_{\eta^j R} \setminus B_{\eta^{j-1} R}) \cap \{d=t\}} \mathrm{d}\mathcal{H}^{n-1}(y) \Big) \mathrm{d}t + (\eta^j R)^{-2s} \Big)$$
$$\leq c \sum_{j\geq 1} (1-\eta^{j\beta}) R^{1+s} \big((\eta^j R)^{-1-s} + (\eta^j R)^{-2s} \big) \leq c \sum_{j\geq 1} (1-\eta^{j\beta}) \eta^{-2sj}$$

for some $c > 0$, depending only on $n, s, \lambda, \Lambda, \kappa, C, \eta$, where we also used that $R \leq 1$. Similarly,

$$R^{1+s} \int_{(\mathbb{R}^n \setminus \Omega) \setminus B_R} v_-(y) K(x-y) \,\mathrm{d}y \leq c \sum_{j\geq 1} (1-\eta^{j\beta}) R^{1+s} \int_{\mathbb{R}^n \cap (B_{\eta^j R} \setminus B_{\eta^{j-1} R})} |y|^{-n-2s} \,\mathrm{d}y$$
$$\leq c \sum_{j\geq 1} (1-\eta^{j\beta}) R^{1+s} (\eta^j R)^{-2s} \leq c \sum_{j\geq 1} (1-\eta^{j\beta}) \eta^{-2js},$$

where we used that $R^{1-s} \leq 1$, and $c > 0$ depends only on n, s, Λ. Therefore, we obtain

$$R^{1+s} \int_{\mathbb{R}^n \setminus B_R} d^{s-1}(y) v_-(y) K(x-y) \,\mathrm{d}y \leq c \sum_{j\geq 1} (1-\eta^{j\beta}) \eta^{-2js}.$$

Since this quantity vanishes as $\beta > 0$ goes to zero, we can make the whole expression smaller than $c_0/16$, which implies, by recalling the definition of $\tilde{f}$,

$$R^{1+\alpha} \| d^{s-\alpha} \tilde{f}_- \|_{L^\infty(\Omega \cap B_{R/2})} \leq R^{1+\alpha} \| d^{s-\alpha} f_- \|_{L^\infty(\Omega \cap B_{R/2})} + R^{1+s} \Big\| \int_{\Omega \setminus B_R} v_-(y) K(\cdot - y) \,\mathrm{d}y \Big\|_{L^\infty(B_{R/2})}$$
$$\leq R^{1+\alpha} \| d^{s-\alpha} f_- \|_{L^\infty(\Omega \cap B_R)} + \frac{c_0}{16},$$

and therefore by the estimate (4-2)

$$\inf_{\Omega \cap B_{\eta^{-1} R}} u + R^{1+\alpha} \| d^{s-\alpha} f_- \|_{L^\infty(\Omega \cap B_R)} + R \| g_+ \|_{L^\infty(\partial\Omega \cap B_R)} \geq \frac{c_0}{8} - \frac{c_0}{16} = \frac{c_0}{16},$$

as desired. □

We are now in a position to prove the boundary Hölder regularity.

Lemma 4.3. *Let $L \in \mathcal{L}_s^{\mathrm{hom}}(\lambda, \Lambda)$. Let $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $\partial\Omega \in C^{2,\gamma}$ for some $\gamma > 0$ and $K \in C^{5+2\gamma}(\mathbb{S}^{n-1})$. Assume that $x_0 \in \partial\Omega$ and let $0 < R \leq 1$. Let $v \in L^1_{2s}(\mathbb{R}^n)$ with $v/d^{s-1} \in C(\overline{\Omega})$ be a viscosity solution to*

$$\begin{cases} Lv = f & \text{in } \Omega \cap B_R(x_0), \\ v = 0 & \text{in } B_R(x_0) \setminus \Omega, \\ \partial_\nu (v/b_\Omega) = g & \text{on } \partial\Omega \cap B_R(x_0) \end{cases}$$

for some $f \in C(\Omega \cap B_R(x_0))$ and $g \in C(\overline{\partial\Omega \cap B_R(x_0)})$. Then, there exist $c > 0$, and $\alpha_0 \in (0,1)$, depending only on $n, s, \lambda, \Lambda, \gamma$, and the $C^{2,\gamma}$ radius of Ω, such that if $d^{s-\alpha} f \in L^\infty(\Omega \cap B_R(x_0))$ for some $\alpha \in (0, \alpha_0]$, then it holds that

$$[v/d^{s-1}]_{C^\alpha(\Omega \cap B_{R/2}(x_0))}$$
$$\leq c R^{-\alpha} \big(\| v/d^{s-1} \|_{L^\infty(\Omega)} + \| v \|_{L^\infty(\mathbb{R}^n \setminus \Omega)} + R^{1+\alpha} \| d^{s-\alpha} f \|_{L^\infty(\Omega \cap B_R(x_0))} + R \| g \|_{L^\infty(\partial\Omega \cap B_R(x_0))} \big).$$

Proof. Let us assume without loss of generality that $x_0 = 0$. We will prove the desired result in two steps. Let us denote by $\eta > 1$ the constant from Lemma 4.2.

Step 1. We claim that for any $k \in \mathbb{N}$,

$$\operatorname*{osc}_{B_{\eta^{-k}R}} (v/b_\Omega) \le c\eta^{-\alpha k}\big(\|v/d^{s-1}\|_{L^\infty(\Omega)} + \|v\|_{L^\infty(\mathbb{R}^n\setminus\Omega)} + R^{1+\alpha}\|d^{s-\alpha} f\|_{L^\infty(\Omega\cap B_R)} + R^\alpha + R\|g\|_{L^\infty(\partial\Omega\cap B_R)}\big),$$

for some constant $c > 0$, depending only on $n, s, \lambda, \Lambda, \gamma$, and the $C^{2,\gamma}$ radius of Ω. To prove it, we set $\alpha_0 := \min\{\beta, \gamma s, 1 - s[-\log_\eta(1-\delta'/2)]\}$, and $\delta := 1 - \eta^{-\alpha_0}$, where δ', β, η are the constants from Lemma 4.2. This yields

$$(1-\delta) = \eta^{-\alpha_0}, \quad \alpha_0 \le \min\{\beta, \gamma s, 1-s\}, \quad \delta \le \delta'/2. \tag{4-3}$$

Let us set $u = v/b_\Omega$, take $\alpha \in (0, \alpha_0]$, and

$$M := 4\delta^{-1}c_1\big(\|v/d^{s-1}\|_{L^\infty(\Omega)} + \|v\|_{L^\infty(\mathbb{R}^n\setminus\Omega)} + R^{1+\alpha}\|d^{s-\alpha} f\|_{L^\infty(\Omega\cap B_R(x_0))} + R^\alpha + R\|g\|_{L^\infty(\partial\Omega\cap B_R(x_0))}\big),$$

where $c_1 > 0$ denotes the constant c_1 from Lemma 2.3.

The claim of Step 1 will follow immediately, once we construct an increasing sequence $(m_k)_k$ and a decreasing sequence $(M_k)_k$ such that for any $k \in \mathbb{N}$,

$$m_k \le u \le M_k \quad \text{in } B_{\eta^{-k}R}, \tag{4-4}$$

$$M_k - m_k = M\eta^{-\alpha k}. \tag{4-5}$$

We prove (4-4) and (4-5) by induction. Setting $m_0 = -(\delta/2c_1)M,\ M_0 = (\delta/2c_1)M$, we obtain the desired results for $k = 0$. Let us now assume that (4-4) and (4-5) hold true for any $j \le k-1$.

We will now prove it for k. Clearly, one of the following two options always holds true:

$$\big|\Omega_{\eta^{-(k-1)}R/4} \cap B_{\eta^{-(k-1)}R/2} \cap \big\{u \ge \tfrac12(M_{k-1}+m_{k-1})\big\}\big| \ge \tfrac12\big|\Omega_{\eta^{-(k-1)}R/4} \cap B_{\eta^{-(k-1)}R/2}\big|,$$
$$\big|\Omega_{\eta^{-(k-1)}R/4} \cap B_{\eta^{-(k-1)}R/2} \cap \big\{u \ge \tfrac12(M_{k-1}+m_{k-1})\big\}\big| \le \tfrac12\big|\Omega_{\eta^{-(k-1)}R/4} \cap B_{\eta^{-(k-1)}R/2}\big|.$$

In the first case, and in the second case, we define

$$w = \frac{v - (b_\Omega + \mathbb{1}_{\mathbb{R}^n\setminus\Omega}\mathbb{1}_{\{m_{k-1}<0\}})m_{k-1}}{M_{k-1}-m_{k-1}}, \quad w = \frac{(b_\Omega + \mathbb{1}_{\mathbb{R}^n\setminus\Omega}\mathbb{1}_{\{M_{k-1}>0\}})M_{k-1} - v}{M_{k-1}-m_{k-1}}, \quad \text{respectively.}$$

Let us assume that we are in the first case. The proof of the second case goes via the same arguments, and we will skip it. Let us verify that w satisfies the assumptions of Lemma 4.2. First, if $u(x) \ge \frac12(M_{k-1}+m_{k-1})$ for some $x \in \Omega$, it follows that

$$\frac{w}{b_\Omega}(x) = \frac{u(x)-m_{k-1}}{M_{k-1}-m_{k-1}} \ge \frac{u(x)-m_{k-1}}{M_{k-1}-m_{k-1}} \ge \frac{\frac{M_{k-1}+m_{k-1}}{2} - m_{k-1}}{M_{k-1}-m_{k-1}} = \frac12,$$

Thus, as an immediate consequence of being in the first case, we get

$$\Big|\Omega_{\eta^{-(k-1)}R/4} \cap B_{\eta^{-(k-1)}R/2} \cap \Big\{\frac{w}{b_\Omega} \ge \frac12\Big\}\Big| \ge \tfrac12\big|\Omega_{\eta^{-(k-1)}R/4} \cap B_{\eta^{-(k-1)}R/2}\big|.$$

Moreover, by (4-4) (for $k-1$), we have

$$w = \frac{v - b_\Omega m_{k-1}}{M_{k-1} - m_{k-1}} \geq 0 \quad \text{in } B_{\eta^{-(k-1)}R} \cap \Omega.$$

Nonnegativity of w in $B_{\eta^{-(k-1)}R} \setminus \Omega$ follows by assumption and construction. We obtain

$$|L(b_\Omega + \mathbb{1}_{\mathbb{R}^n \setminus \Omega})| \leq c_1 \quad \text{in } \Omega,$$

and therefore $d^{s-\alpha} L(b_\Omega + \mathbb{1}_{\mathbb{R}^n\setminus\Omega}) \in L^\infty(\Omega \cap B_R)$. Then, by (4-5) (for $k-1$) we have

$$Lw = \frac{f - L(b_\Omega + \mathbb{1}_{\mathbb{R}^n\setminus\Omega}\mathbb{1}_{\{m_{k-1}<0\}})m_{k-1}}{M_{k-1} - m_{k-1}} \geq \frac{f - c_1 m_{k-1}}{M_{k-1} - m_{k-1}} \quad \text{in } \Omega \cap B_R. \tag{4-6}$$

Moreover, clearly

$$\partial_\nu(w/b_\Omega) = \frac{g - \partial_\nu(b_\Omega/b_\Omega)m_{k-1}}{M_{k-1} - m_{k-1}} = \frac{g}{M_{k-1} - m_{k-1}} \quad \text{on } \partial\Omega \cap B_R.$$

It remains to verify the fourth and fifth assumption of Lemma 4.2. Let us first consider $j \leq k-1$. In that case, for any $x \in B_{\eta^{-(k-1)+j}R} \cap \Omega$ it holds by (4-4) and (4-5) that

$$\begin{aligned} \frac{w}{b_\Omega}(x) &= \frac{u(x) - m_{k-1}}{M_{k-1} - m_{k-1}} \geq \frac{m_{k-j-1} - m_{k-1}}{M_{k-1} - m_{k-1}} \\ &\geq \frac{M_{k-1} - M_{k-j-1} + m_{k-j-1} - m_{k-1}}{M_{k-1} - m_{k-1}} = 1 - \frac{M_{k-j-1} - m_{k-j-1}}{M_{k-1} - m_{k-1}} = 1 - \eta^{\alpha j}. \end{aligned}$$

Clearly, for any $x \in B_{\eta^{-(k-1)+j}R} \setminus \Omega$ and in case $m_{k-1} < 0$, by the same arguments as above, using (4-4), we have

$$w(x) = \frac{v(x) - m_{k-1}}{M_{k-1} - m_{k-1}} \geq \frac{m_{k-j-1} - m_{k-1}}{M_{k-1} - m_{k-1}} \geq 1 - \eta^{\alpha j}.$$

If however $m_{k-1} \geq 0$, then we can use that $v = 0$ in $B_R \setminus \Omega$. Moreover, if $j > k-1$ we compute for $x \in B_{\eta^{-(k-1)+j}R} \cap \Omega$,

$$\begin{aligned} \frac{w}{b_\Omega}(x) &= \frac{u(x) - m_{k-1}}{M_{k-1} - m_{k-1}} \geq \frac{m_0 - m_{k-1}}{M_{k-1} - m_{k-1}} \\ &\geq \frac{(M_{k-1} - m_{k-1}) - (M_0 - m_0)}{M_{k-1} - m_{k-1}} = 1 - \eta^{\alpha(k-1)} \geq 1 - \eta^{\alpha j}. \end{aligned}$$

Finally, for $x \in B_{\eta^{-(k-1)+j}R} \setminus \Omega$, again by the same arguments as above, and using that $v \geq m_0$ by construction, we have

$$w(x) = \frac{v(x) - m_{k-1}\mathbb{1}_{\{m_{k-1}<0\}}}{M_{k-1} - m_{k-1}} \geq \frac{m_0 - m_{k-1}}{M_{k-1} - m_{k-1}} \geq 1 - \eta^{\alpha j}.$$

Consequently, all assumptions of Lemma 4.2 are satisfied for w with radius $\eta^{-(k-1)}R$. Thus, we deduce from Lemma 4.2 and the choice of δ,

$$\begin{aligned} u - m_{k-1} &= (M_{k-1} - m_{k-1})\frac{w}{b_\Omega} \\ &\geq 2\delta(M_{k-1} - m_{k-1}) - (\eta^{-(k-1)}R)^{1+\alpha}\big(\|d^{s-\alpha} f\|_{L^\infty(\Omega\cap B_{\eta^{-(k-1)}R})} + c_1|m_{k-1}|\big) \\ &\qquad - (\eta^{-(k-1)}R)\|g\|_{L^\infty(\partial\Omega\cap B_{\eta^{-(k-1)}R})} \quad \text{in } \Omega\cap B_{\eta^{-k}R}. \end{aligned}$$

Moreover, by (4-3), the choice of M, (4-5), and the estimate $|m_{k-1}| \leq M_0 = (\delta/2c_1)M$, we estimate

$$\begin{aligned} (\eta^{-(k-1)}R)^{1+\alpha}\big(\|d^{s-\alpha} f\|_{L^\infty(\Omega\cap B_{\eta^{-(k-1)}R})} + c_1|m_{k-1}|\big) + (\eta^{-(k-1)}R)\|g\|_{L^\infty(\partial\Omega\cap B_{\eta^{-(k-1)}R})} \\ \leq \eta^{-\alpha(k-1)}\delta M = \delta(M_{k-1} - m_{k-1}). \end{aligned}$$

Therefore, we deduce

$$m_k := \delta(M_{k-1} - m_{k-1}) + m_{k-1} \leq u \leq M_{k-1} =: M_k \quad \text{in } \Omega\cap B_{\eta^{-k}R},$$

which proves (4-4) for k. Equation (4-5) for k follows from (4-3). The proof of Step 1 is complete.

Step 2. Now that we have established the claim of Step 1, let us show how to conclude the proof. Let us take $x, y \in B_{R/2}$. We define $k \in \mathbb{N}$ as

$$\inf\{k \in \mathbb{N} : |x-y| \geq \eta^{-k}(R/2)\}.$$

Then, $|x-y| \leq \eta^{-k+1}(R/2)$ and by Step 1, it holds that

$$\begin{aligned} \frac{|u(x)-u(y)|}{|x-y|^\alpha} &\leq \eta^{k\alpha}(R/2)^{-\alpha} \operatorname*{osc}_{B_{\eta^{-k+1}(R/2)}} u \\ &\leq cR^{-\alpha}\big(\|u\|_{L^\infty(\Omega)} + \|v\|_{L^\infty(\mathbb{R}^n\setminus\Omega)} + R^{1+\alpha}\|d^{s-\alpha} f\|_{L^\infty(\Omega\cap B_R)} + R^{1+\alpha} + R\|g\|_{L^\infty(\partial\Omega\cap B_R)}\big). \end{aligned}$$

We can omit the additional summand $+R^{1+\alpha}$ by an additional scaling and normalization argument, i.e., by assuming that $R=1$ and $\|u\|_{L^\infty(\Omega)} + \|v\|_{L^\infty(\mathbb{R}^n\setminus\Omega)} + \|d^{s-\alpha} f\|_{L^\infty(\Omega\cap B_1)} + \|g\|_{L^\infty(\partial\Omega\cap B_1)} = 1$, applying the previous estimate, and rescaling to general R. This concludes the proof after using that by Theorem 1.4 it holds that $b_\Omega/d^{s-1} \in C^\alpha(\Omega\cap B_{R/2}(x_0))$. □

We are now in a position to deduce the boundary Hölder regularity estimate in $C^{1,\gamma}$ domains.

Proof of Theorem 1.6. Note that

$$\partial_\nu(v/b_\Omega) = \partial_\nu(v/d^{s-1}) - \partial_\nu(b_\Omega/d^{s-1})(v/d^{s-1}),$$

and recall that $|\partial_\nu(b_\Omega/d^{s-1})| \leq C$. Hence, we can apply Lemma 4.3 (with $R = \frac{1}{2}$ and varying $x_0 \in \partial\Omega$). Combining it with the interior regularity results from [Fernández-Real and Ros-Oton 2024a, Theorem 2.4.3], and a covering argument, we deduce the desired result. In order to produce the tail-term in the estimate, we employ a truncation argument in the same way as in the proof of Corollary 4.4. □

We end this section with a boundary Hölder regularity estimate for solutions that are defined up to a polynomial and might grow fast at infinity.

Corollary 4.4. *Let $L \in \mathcal{L}_s^{\hom}(\lambda, \Lambda)$. Let $k \in \mathbb{N} \cup \{0\}$. Let $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $\partial\Omega \in C^{2,\gamma}$ for some $\gamma > 0$ and $K \in C^{5+2\gamma}(\mathbb{S}^{n-1})$. Let $f \in C(\Omega \cap B_4)$, $g \in C(\overline{\partial\Omega \cap B_4})$, and v with $v/d^{s-1} \in C(\overline{\Omega})$ be a viscosity solution to*

$$\begin{cases} Lv \overset{k}{=} f & \text{in } \Omega \cap B_4, \\ v = 0 & \text{in } B_4 \setminus \Omega, \\ \partial_\nu(v/d^{s-1}) = g & \text{on } \partial\Omega \cap B_4. \end{cases}$$

Then, there exists $\alpha_0 > 0$ such that if for some $\alpha \in (0, \alpha_0]$ we have $d^{s+1-\alpha} f \in L^\infty(\Omega \cap B_4)$, then the following holds true: If $k = 0$, and $v \in L^1_{2s}(\mathbb{R}^n)$, then $v/d^{s-1} \in C^\alpha_{\mathrm{loc}}(\overline{\Omega} \cap B_4)$, and

$$\left\| \frac{v}{d^{s-1}} \right\|_{C^\alpha(\overline{\Omega} \cap B_1)} \le c\left(\left\| \frac{v}{d^{s-1}} \right\|_{L^\infty(\Omega \cap B_4)} + \|v\|_{L^1_{2s}(\mathbb{R}^n \setminus B_4)} + \|d^{s+1-\alpha} f\|_{L^\infty(\Omega \cap B_4)} + \|g\|_{L^\infty(\partial\Omega \cap B_4)} \right).$$

If $k \in \mathbb{N}$, $K \in C^{k-1+\delta}(\mathbb{S}^{n-1})$, and $v \in L^1_{2s+k-1+\delta}(\mathbb{R}^n)$ for some $\delta > 0$, then $v/d^{s-1} \in C^\alpha_{\mathrm{loc}}(\overline{\Omega} \cap B_4)$, and

$$\left\| \frac{v}{d^{s-1}} \right\|_{C^\alpha(\overline{\Omega} \cap B_1)} \le c\left(\left\| \frac{v}{d^{s-1}} \right\|_{L^\infty(\Omega \cap B_4)} + \|v\|_{L^1_{2s+k-1+\delta}(\mathbb{R}^n \setminus B_4)} + \|d^{s+1-\alpha} f\|_{L^\infty(\Omega \cap B_4)} + \|g\|_{L^\infty(\partial\Omega \cap B_4)} \right),$$

where $c > 0$ and α_0, depend only on $n, s, \lambda, \Lambda, \gamma, k, \delta$, and the $C^{2,\gamma}$ radius of Ω.

Proof. In case $k = 0$, the proof follows by a truncation argument. Indeed, let us define $w = v\mathbb{1}_{B_4}$ and observe that

$$Lw = f - L(v\mathbb{1}_{\mathbb{R}^n \setminus B_4}) =: \tilde{f} \quad \text{in } \Omega \cap B_2.$$

Moreover, we can estimate

$$\|d^{s+1-\alpha} \tilde{f}\|_{L^\infty(\Omega \cap B_2)} \le c\|d^{s-1+\alpha} f\|_{L^\infty(\Omega \cap B_2)} + c\|v\|_{L^1_{2s}(\mathbb{R}^n \setminus B_4)}.$$

Thus, the desired result follows immediately by application of Theorem 1.6 to w, using that $v = 0$ in $B_4 \setminus \Omega$, by assumption.

Let now $k \in \mathbb{N}$. Again, we define $w = v\mathbb{1}_{B_4}$, but this time, since the equation only holds up to a polynomial, we obtain for any $R > 4$,

$$Lw = f_R - L(v\mathbb{1}_{B_R \setminus B_4}) + p_R =: \tilde{f} \quad \text{in } \Omega \cap B_3,$$

where $f_R \to f$ in $d^{s+1-\alpha} L^\infty(\Omega \cap B_3)$, as $R \to \infty$, and $p_R \in \mathcal{P}_{k-1}$. As in the proof of Lemma 2.10 (see also [Abatangelo and Ros-Oton 2020, Lemma 3.6; Kukuljan 2021, Lemma 4.8]), taking difference quotients of order $k - 1 + \delta$ of the equation for w, and using crucially that $K \in C^{k-1+\delta}(\mathbb{S}^{n-1})$, we can find a polynomial $p \in \mathcal{P}_{\lfloor k-1+\delta \rfloor}$ and h with $d^{s+1-\alpha} h \in L^\infty(\Omega \cap B_3)$ such that

$$\begin{cases} Lw = h + p & \text{in } \Omega \cap B_3, \\ w = 0 & \text{in } \mathbb{R}^n \setminus (\Omega \cap B_4), \end{cases}$$

and moreover, h satisfies the estimate

$$\|d_\Omega^{s+1-\alpha} h\|_{L^\infty(\Omega \cap B_3)} \le C\left(\|d_\Omega^{s+1-\alpha} f\|_{L^\infty(\Omega \cap B_3)} + \|v| \cdot |^{-n-2s-(k-1+\delta)}\|_{L^1(\mathbb{R}^n \setminus B_4)} \right). \tag{4-7}$$

Next, let us take a bounded domain $D \subset \mathbb{R}^n$ with $\partial D \in C^{1,\gamma}$ such that $\Omega \cap B_2 \subset D \subset \Omega \cap B_3$. Moreover, we find w_1, w_2 such that $w_1/d_D^{s-1}, w_1/d_D^{s-1} \in C(\overline{D})$ and $w = w_1 + w_2$ satisfying

$$\begin{cases} Lw_1 = h & \text{in } D, \\ w_1 = w & \text{in } \mathbb{R}^n \setminus D, \\ w_1/d_D^{s-1} = v/d_D^{s-1} & \text{on } \partial D, \end{cases} \quad \text{and} \quad \begin{cases} Lw_2 = p & \text{in } D, \\ w_2 = 0 & \text{in } \mathbb{R}^n \setminus D, \\ w_2/d_D^{s-1} = 0 & \text{on } \partial D. \end{cases}$$

The existence of $w_2 \in L^\infty(\mathbb{R}^n)$ follows from [Fernández-Real and Ros-Oton 2024a, Theorem 3.2.27], and we obtain $w_2/d_D^s \in C^\gamma(\overline{D})$ from [Fernández-Real and Ros-Oton 2024a, Theorem 2.7.1], which yields $w_2/d_D^{s-1} = d_D(w_2/d_D^s) \in C^\gamma(\overline{D})$ since $\partial D \in C^{1,\gamma}$. Then, we can define $w_1 := w - w_2$. We claim that

$$\|w_1/d_D^{s-1}\|_{L^\infty(D)} \le c\big(\|v/d_\Omega^{s-1}\|_{L^\infty(\Omega\cap B_4)} + \|d_\Omega^{s+1-\alpha} h\|_{L^\infty(\Omega\cap B_3)}\big). \tag{4-8}$$

To see this, let us recall the function ψ_1 (with respect to D) from Lemma 2.7, and observe that by Lemma 2.3, we can take it in such a way that

$$L(\psi_1 + d_\Omega^{s-1}) \ge c_0 d_D^{\alpha-s-1} \quad \text{in } D \tag{4-9}$$

for some $c_0 > 0$. Moreover, recall $\psi_1/d_D^{s-1} = 1$ on ∂D. Then, let us define

$$\Psi(x) = c_1\psi_1(x)\big(\|v/d_D^{s-1}\|_{L^\infty(\partial D)} + \|d_D^{s+1-\alpha} h\|_{L^\infty(D)} + \|w/d_\Omega^{s-1}\|_{L^\infty(\Omega\cap B_4)}\big) \\ + c_1 d_\Omega^{s-1}(x)\|w/d_\Omega^{s-1}\|_{L^\infty(\Omega\cap B_4)},$$

where $c_1 := \max\{c_0^{-1}, 1\}$, and observe that by (4-9) we have

$$\begin{cases} Lw_1 \le L\Psi & \text{in } D, \\ w_1 \le \Psi & \text{in } \mathbb{R}^n \setminus D, \\ w_1/d_D^{s-1} \le \Psi/d_D^{s-1} & \text{on } \partial D, \end{cases}$$

which, recalling that $\psi_1 \le c_1 d_D^{s-1}$ in D, and $d_D \le d_\Omega$, as well as the definition of D, imply that

$$\begin{aligned} \frac{w_1}{d_D^{s-1}} &\le c_2c_1\big(\|v/d_D^{s-1}\|_{L^\infty(\partial D)} + \|d_D^{s+1-\alpha} h\|_{L^\infty(D)} + \|w/d_\Omega^{s-1}\|_{L^\infty(\Omega\cap B_4)}\big) + c_2c_1\frac{d_\Omega^{s-1}}{d_D^{s-1}}\|w/d_\Omega^{s-1}\|_{L^\infty(\Omega\cap B_4)} \\ &\le c\big(\|v/d_\Omega^{s-1}\|_{L^\infty(\partial\Omega\cap B_3)} + \|d_\Omega^{s+1-\alpha} h\|_{L^\infty(\Omega\cap B_3)} + \|v/d_\Omega^{s-1}\|_{L^\infty(\Omega\cap B_4)}\big), \end{aligned}$$

which yields our claim in (4-8). As a direct consequence of (4-8), we deduce

$$\begin{aligned} \|w_2/d_D^{s-1}\|_{L^\infty(D)} &\le \|w/d_D^{s-1}\|_{L^\infty(D)} + \|w_1/d_D^{s-1}\|_{L^\infty(D)} \\ &\le c\big(\|v/d_\Omega^{s-1}\|_{L^\infty(\Omega\cap B_4)} + \|d_\Omega^{s+1-\alpha} h\|_{L^\infty(\Omega\cap B_3)}\big). \end{aligned} \tag{4-10}$$

Finally, we claim that

$$\|p\|_{L^\infty(D)} \le c\|w_2/d_D^{s-1}\|_{L^\infty(D)}. \tag{4-11}$$

Once we show (4-11), then the proof is complete after combination of (4-11), (4-10), (4-7), and application of the boundary Hölder regularity estimate (see Theorem 1.6) to w in Ω, as in the case $k = 0$. We prove

(4-11) by contradiction. Suppose there are sequences $(L_j)_j$, $(w_j)_j$, $(p_j)_j$ with

$$\|p_j\|_{L^\infty(D)} = 1, \quad \text{and} \quad \begin{cases} L_j w_j = p_j & \text{in } D, \\ w_j = 0 & \text{in } \mathbb{R}^n \setminus D, \\ w_j / d_\Omega^{s-1} = 0 & \text{on } \partial D, \\ \lim_{j\to\infty} \|w_j / d_D^{s-1}\|_{L^\infty(D)} = 0. \end{cases}$$

Then, up to subsequences, it holds that $L_{j_m} \rightharpoonup L$, $w_{j_m}/d_D^{s-1} \to u_0$ in $L^\infty(D)$ for some $u_0 \in L^\infty(D)$, $p_{j_m} \to p_0$ in $L^\infty(D)$. While the first convergence statement follows from [Abatangelo and Ros-Oton 2020, Lemma 3.7], the second convergence statement follows from Theorem 1.6 and the Arzelà–Ascoli theorem, and the third one is immediate from the boundedness of (p_{j_m}) in a finite dimensional space.

We can now make use of the stability result in [Fernández-Real and Ros-Oton 2024a, Proposition 2.2.36], and deduce that for $w_0 = d_D^{s-1} u_0$, it holds that

$$\|p_0\|_{L^\infty(D)} = 1, \quad \text{and} \quad \begin{cases} L w_0 = p_0 & \text{in } D, \\ w_0 = 0 & \text{in } \mathbb{R}^n \setminus D, \\ w_0 / d_D^{s-1} = 0 & \text{on } \partial D, \\ \|w_0 / d_D^{s-1}\|_{L^\infty(D)} = 0. \end{cases}$$

Clearly, $w_0 = 0$ is not a solution to $Lw_0 = p_0$ in D, so we have obtained a contradiction, and conclude the proof of (4-11). □

5. Liouville theorem in the half-space

The proof of our main result (see Theorem 1.2) is based on a blow-up argument. A crucial ingredient in such proof is a suitable Liouville theorem in the half-space. In this section, we will establish such a result for nonlocal problems with local Neumann boundary conditions:

Theorem 5.1. *Let $L \in \mathcal{L}_s^{\text{hom}}(\lambda, \Lambda)$. Let $k \in \mathbb{N}$, $\gamma \in (0,1)$ with $\gamma \neq s$, and $K \in C^{k-1+\gamma-s+\delta}(\mathbb{S}^{n-1})$ for some $\delta > 0$. Let $u \in C(\mathbb{R}^n)$ be a viscosity solution to*

$$\begin{cases} L((x_n)_+^{s-1} u) \overset{k-1+\lceil \gamma - s \rceil}{=} 0 & \text{in } \{x_n > 0\}, \\ \partial_n u = p & \text{in } \{x_n = 0\}, \\ |u(x)| \le C(1+|x|)^{k+\gamma} & \text{for all } x \in \{x_n > 0\}, \end{cases}$$

for some $C > 0$, $p \in \mathcal{P}_{k-1}$. Then, there exist $a_\beta \in \mathbb{R}$ for any $\beta \in (\mathbb{N} \cup \{0\})^n$ with $|\beta| \le k$ such that

$$u(x) = \sum_{|\beta| \le k} a_\beta x_1^{\beta_1} \cdots x_n^{\beta_n} \quad \text{for all } x \in \{x_n > 0\}.$$

In order to prove Theorem 5.1, we first establish the following one-dimensional version, which can be proved by combination of the arguments in [Ros-Oton and Serra 2016a, Lemma 6.2; Abatangelo and Ros-Oton 2020, Lemma 3.3].

Lemma 5.2. *Let $k \in \mathbb{N}$, $\gamma \in (0,1)$ with $\gamma \neq s$, and $u \in C(\mathbb{R})$ satisfying*

$$\begin{cases} (-\Delta)^s((x_+)^{s-1}u) \overset{k-1+\lceil \gamma - s\rceil}{=} 0 & \text{in } (0,\infty), \\ |u(x)| \le C(1+|x|)^{k+\gamma} & \text{for all } x > 0, \end{cases}$$

for some $C > 0$. Then, there exist $a_0, a_1, \dots, a_k \in \mathbb{R}$ such that

$$u(x) = \sum_{j=0}^{k} a_j x^j \quad \text{for all } x > 0.$$

Proof. In case $k = 1$ and $\gamma < s$, the proof is an application of [Ros-Oton and Serra 2016a, Lemma 6.2] with $u(x) := (x_+)^{s-1}u(x)$, and $\delta = s > 0$, $\beta = s + \gamma \in (0, 2s)$.

In case $k > 1$ or $\gamma > s$, we have $k - 1 + \lceil \gamma - s \rceil \ge 1$. Let us define $v(x) = (x_+)^{s-1}u(x)$, let $V : \mathbb{R} \times [0,\infty) \to \mathbb{R}$ be the harmonic extension of v in the sense of [Abatangelo and Ros-Oton 2020, Lemma 3.3], and finally define $\widetilde{V}(x,y) = \int_{-\infty}^{x} V(z,y)\,\mathrm{d}z$. Note that $\widetilde{V}$ satisfies (see [Abatangelo and Ros-Oton 2020, Lemma 3.3])

$$\begin{cases} \operatorname{div}(y^{1-2s}\nabla \widetilde{V}(x,y)) = 0 & \text{in } \mathbb{R}\times(0,\infty), \\ \widetilde{V}(x,y) = v(x) & \text{on } \mathbb{R}\times\{0\}, \\ |\widetilde{V}(x,y)| \le C\big(1 + |x|^{2(k-1+\lceil\gamma-s\rceil)+1+\gamma+s} + |y|^{(k-1+\lceil\gamma-s\rceil)+1+\gamma+s}\big) & \text{in } \mathbb{R}\times(0,\infty). \end{cases}$$

Next, by [Ros-Oton and Serra 2016a, Lemma 6.2] (see also [Fernández-Real and Ros-Oton 2024a, Theorem 1.10.16]), we have the representation formula

$$\widetilde{V}(x,y) = \widetilde{V}(r\cos\theta, r\sin\theta) = \sum_{j=0}^{\infty} a_j \Theta_j(\theta) r^{j+s}, \quad \text{for all } x \in \mathbb{R},\ y \in [0,\infty),$$

where $a_j \in \mathbb{R}$, and $(\Theta_j)_j$ is a complete orthogonal system in the subspace of even functions in $L^2\big((0,\pi), (\sin\theta)^{1-2s}\,\mathrm{d}\theta\big)$. By the Parseval identity, the bounds on $|\widetilde{V}|$ imply

$$\sum_{j=0}^{\infty} a_j^2 R^{2+2j} = \int_{\partial B_R \cap \{y>0\}} \widetilde{V}(x,y)^2 y^{1-2s}\,\mathrm{d}\sigma \le C R^{4(k-1+\lceil\gamma-s\rceil)+2+2\gamma+2} = C R^{4(k+\lceil\gamma-s\rceil)+2\gamma}.$$

Therefore, it must be $a_j = 0$ for any $j > j_0$, where $j_0 = \min\big\{j \in \mathbb{N} : 2 + 2j > 4(k + \lceil\gamma - s\rceil) + 2\gamma\big\}$, which implies

$$\widetilde{V}(x,y) = \sum_{j=0}^{j_0} a_j \Theta_j(\theta) r^{j+s} \quad \text{for all } x \in \mathbb{R},\ y \in [0,\infty).$$

Upon recalling the definition of V and $\widetilde{V}$, this implies

$$v(x) = (x_+)^s \sum_{j=0}^{j_0-1} b_j x^j$$

for some $b_j \in \mathbb{R}$, and since $|v(x)| \le C(1+|x|)^{k+\gamma-1+s}$ and $\gamma \in (0,1)$ by assumption, it must be $b_j = 0$ for any $j \ge k$. Recalling that by definition $u(x) = v(x)(x_+)^{1-s}$, we deduce that u must be a polynomial of degree at most k in $\{x > 0\}$, as desired. □

Moreover, we will need the following lemma (see also [Kukuljan 2021, Proposition 4.3]):

Lemma 5.3. *Let $L \in \mathcal{L}_s^{\mathrm{hom}}(\lambda, \Lambda)$. Let $k \in \mathbb{N}$, $K \in C^{k-2+\delta}(\mathbb{S}^{n-1})$ for some $\delta > 0$. Let $f \in \mathcal{P}_k$. Then,*

$$L((x_n)_+^{s-1} f) \overset{k-1}{=} 0 \quad \text{in } \{x_n > 0\}.$$

Proof. Let us first give a simple proof in case $k = 1$. Then, it suffices to prove that for any $i \in \{1, \dots, n\}$

$$L((x_n)_+^{s-1} x_i) = 0 \quad \text{in } \{x_n > 0\}.$$

First, by integrating $x \mapsto (x_n)_+^{s-1}$ in x_i, and using that $L((x_n)_+^{s-1}) = 0$, we deduce

$$L((x_n)_+^{s-1} x_i) \equiv c \quad \text{in } \{x_n > 0\}$$

for some constant $c \in \mathbb{R}$. Then, since $x \mapsto (x_n)_+^{s-1} x_i$ is homogeneous of degree s, we deduce that for any $\lambda > 0$ and $x \in \{x_n > 0\}$,

$$c = L((x_n)_+^{s-1} x_i)(\lambda x) = \lambda^{-2s} L((\lambda x_n)_+^{s-1} \lambda x_i)(x) = \lambda^{-s} L((x_n)_+^{s-1} x_i)(x) = \lambda^{-s} c.$$

This implies that $c = 0$, as desired.

For $k \geq 2$, we prove the result by induction. Assume that we know already

$$L((x_n)_+^{s-1} p) \overset{k-2}{=} 0 \quad \text{in } \{x_n > 0\} \tag{5-1}$$

for every $p \in \mathcal{P}_{k-1}$. Now, let $q \in \mathcal{P}_k$. Then, by integrating (5-1) with $p := \partial_i q$ for $i \in \{1, \dots, n\}$, by Lemma 2.12 we find that there exists a constant $c \in \mathbb{R}$ such that

$$L((x_n)_+^{s-1} q) \overset{k-1}{=} c \quad \text{in } \{x_n > 0\}.$$

Since $c \overset{k-1}{=} 0$ for any $k \geq 2$, we conclude the proof. □

Finally, we state a Hölder regularity estimate in the half-space, which follows from Corollary 4.4.

Corollary 5.4. *Let $L \in \mathcal{L}_s^{\mathrm{hom}}(\lambda, \Lambda)$. Let $k \in \mathbb{N} \cup \{0\}$, $\gamma > 0$, and $K \in C^{k-1+\delta}(\mathbb{S}^{n-1})$ for some $\delta > 0$. Let $f \in C(\{x_n > 0\} \cap B_2)$, $g \in C(\overline{\{x_n = 0\} \cap B_2})$, and $u \in C(\{x_n \geq 0\})$ be a viscosity solution to*

$$\begin{cases} L((x_n)_+^{s-1} u) \overset{k}{=} f & \text{in } \{x_n > 0\} \cap B_2, \\ \partial_n u = g & \text{on } \{x_n = 0\} \cap B_2. \end{cases}$$

Then, there exists $\alpha_0 > 0$ such that if $(x_n)_+^{s+1-\alpha} f \in L^\infty(\{x_n > 0\} \cap B_2)$ for some $\alpha \in (0, \alpha_0]$, then the following holds true: if $k = 0$ and $(x_n)_+^{s-1} u \in L^1_{2s}(\mathbb{R}^n)$ it holds that $u \in C^\alpha_{\mathrm{loc}}(\{x_n \geq 0\} \cap B_2)$, and

$$\|u\|_{C^\alpha(\{x_n \geq 0\} \cap B_1)} \leq c\big(\|u\|_{L^\infty(\{x_n > 0\} \cap B_4)} + \|(x_n)_+^{s-1} u\|_{L^1_{2s}(\mathbb{R}^n \setminus B_4)} + \|(x_n)_+^{s+1-\alpha} f\|_{L^\infty(\{x_n > 0\} \cap B_2)} + \|g\|_{L^\infty(\{x_n = 0\} \cap B_2)}\big),$$

and if $k \in \mathbb{N}$ and $(x_n)_+^{s-1} u \in L^1_{2s+(k-1+\delta)}(\mathbb{R}^n)$ it holds that $u \in C^\alpha_{\mathrm{loc}}(\{x_n \geq 0\} \cap B_2)$, and

$$\|u\|_{C^\alpha(\{x_n \geq 0\} \cap B_1)} \leq c\big(\|u\|_{L^\infty(\{x_n > 0\} \cap B_4)} + \big\|[(x_n)_+^{s-1} u]|\cdot|^{-n-2s-(k-1+\delta)}\big\|_{L^1(\{x_n > 0\} \setminus B_4)} + \|(x_n)_+^{s+1-\alpha} f\|_{L^\infty(\{x_n > 0\} \cap B_2)} + \|g\|_{L^\infty(\{x_n = 0\} \cap B_2)}\big),$$

where $c > 0$ and α_0 depend only on $n, s, \lambda, \Lambda, \gamma, k, \delta$.

Proof. The result follows directly from Corollary 4.4 applied to some domain $\Omega \subset \mathbb{R}^n$ with $\partial\Omega \in C^{1,\gamma}$, which satisfies $\{x_n > 0\} \cap B_2 \subset \Omega \subset \{x_n > 0\} \cap B_4$. □

With the help of the one-dimensional Liouville theorem in the half-space and the Hölder regularity estimate up to the boundary (see Corollary 5.4), the proof of Theorem 5.1 follows by a standard procedure, which is explained in detail for instance in [Abatangelo and Ros-Oton 2020, proof of Theorem 3.10].

Proof of Theorem 5.1. First, we observe that by scaling Corollary 5.4, we obtain that for any $R \geq 1$,

$$\begin{aligned}[u]_{C^\alpha(B_R)} \leq cR^{-\alpha}\big[\|u\|_{L^\infty(B_{4R})} + R^{1+s}\|(x_n)_+^{s-1}u|\cdot|^{-n-2s}\|_{L^1(\mathbb{R}^n\setminus B_{4R})}\mathbb{1}_{\{k=1\text{and }\gamma<s\}} \\ + R^{s+k-1+\lceil\gamma-s\rceil+\eta}\big\|[(x_n)_+^{s-1}u]|\cdot|^{-n-2s-(k-2+\lceil\gamma-s\rceil+\eta)}\big\|_{L^1(\{x_n>0\}\setminus B_{4R})}\mathbb{1}_{\{k\geq 2\text{or }\gamma>s\}} \\ + R\|p\|_{L^\infty(\{x_n=0\}\cap B_{4R})}\big] \\ \leq cR^{k+\gamma-\alpha},\end{aligned} \tag{5-2}$$

where we take $\eta = 1+\gamma-s-\lceil\gamma-s\rceil+\delta$ and used in the last estimate the growth condition on u, the fact that $\|p\|_{L^\infty(\{x_n=0\}\cap B_R)} \leq cR^{k-1}$, and the following computation using polar coordinates with $y_n = r\cos\theta$ for some $\theta \in [0, 2\pi)$ (similar to the proof of Lemma 4.2), which is slightly different in case ($k = 1$ and $\gamma < s$) and ($k \geq 2$ or $\gamma > s$). In case $k = 1$ and $\gamma < s$, we obtain

$$\begin{aligned}R^{1+s}\|(x_n)_+^{s-1}u|\cdot|^{-n-2s}\|_{L^1(\mathbb{R}^n\setminus B_{4R})} &\leq CR^{1+s}\int_{\mathbb{R}^n\setminus B_{4R}}(y_n)_+^{s-1}|y|^{-n-2s+1+\gamma}\,\mathrm{d}y \\ &\leq cR^{1+s}\int_0^{2\pi}\cos(\theta)_+^{s-1}\left(\int_{4R}^\infty r^{s-1}r^{-1-2s+1+\gamma}\,\mathrm{d}r\right)\mathrm{d}\theta \\ &\leq cR^{1+s}R^{\gamma-s}\left(\int_0^{2\pi}\cos(\theta)_+^{s-1}\,\mathrm{d}\theta\right) \leq cR^{1+\gamma}.\end{aligned} \tag{5-3}$$

In case ($k \geq 2$ or $\gamma > s$), we obtain, using that $\eta > 1+\gamma-s-\lceil\gamma-s\rceil$,

$$\begin{aligned}&R^{s+k-1+\lceil\gamma-s\rceil+\eta}\big\|[(x_n)_+^{s-1}u]|\cdot|^{-n-2s-(k-2+\lceil\gamma-s\rceil+\eta)}\big\|_{L^1(\{x_n>0\}\setminus B_4)} \\ &\qquad\leq CR^{s+k-1+\lceil\gamma-s\rceil+\eta}\int_{\mathbb{R}^n\setminus B_{4R}}(y_n)_+^{s-1}|y|^{-n-2s-(k-2+\lceil\gamma-s\rceil+\eta)+k+\gamma}\,\mathrm{d}y \\ &\qquad\leq cR^{s+k-1+\lceil\gamma-s\rceil+\eta}\int_0^{2\pi}\cos(\theta)_+^{s-1}\left(\int_{4R}^\infty r^{s-1}r^{-1-2s+2-\lceil\gamma-s\rceil+\gamma-\eta}\,\mathrm{d}r\right)\mathrm{d}\theta \\ &\qquad\leq cR^{k+s}R^{\gamma-s}\left(\int_0^{2\pi}\cos(\theta)_+^{s-1}\,\mathrm{d}\theta\right) \leq cR^{k+\gamma}.\end{aligned}$$

Next, let us take any $\tau \in \mathbb{S}^{n-1}$ such that $\tau_n = 0$ and $0 < h < R/2$. We consider the difference quotients

$$w_{1,\tau}(x) = \frac{u(x+h\tau)-u(x)}{h^\alpha}, \quad p_{1,\tau}(x) = \frac{p(x+h\tau)-p(x)}{h^\alpha}$$

and deduce from (5-2) (after applying the estimate to smaller balls of radius comparable to R inside B_R) that

$$\|w_{1,\tau}\|_{L^\infty(B_R)} \leq cR^{k+\gamma-\alpha} \quad \text{for all } R \geq 1.$$

Clearly, since $\tau_n = 0$, $w_{1,\tau}$ satisfies in the viscosity sense

$$\begin{cases} L((x_n)_+^{s-1} w_{1,\tau}) \overset{k-1+\lceil\gamma-s\rceil}{=} 0 & \text{in } \{x_n > 0\}, \\ \partial_n w_{1,\tau} = p_{1,\tau} & \text{on } \{x_n = 0\}. \end{cases} \tag{5-4}$$

Here, we are using that sums of viscosity solutions are again viscosity solutions by Lemma 2.14. Using (5-4) and also that $|p_{1,\tau}(x)| \le c|x|^{k-1-\alpha}$ since $p \in \mathcal{P}_{k-1}$, we can apply the previous arguments to $w_{1,\tau}$. Eventually, this implies that $w_{2,\tau}(x) = (w_{1,\tau}(x+h\tau) - w_{1,\tau}(x))/h^{\alpha}$ satisfies $\|w_{2,\tau}\|_{L^\infty(B_R)} \le cR^{k+\gamma-2\alpha}$. This way, we obtain higher order difference quotients $w_{j,\tau}$, $j \in \mathbb{N}$, and they satisfy

$$\begin{cases} L((x_n)_+^{s-1} w_{j,\tau}) \overset{k-1+\lceil\gamma-s\rceil}{=} 0 & \text{in } \{x_n > 0\}, \\ \partial_n w_{j,\tau} = p_{j,\tau} & \text{on } \{x_n = 0\}, \\ \|w_{j,\tau}\|_{L^\infty(B_R)} \le cR^{k+\gamma-j\alpha} & \text{for all } R \ge 1, \\ \|p_{j,\tau}\|_{L^\infty(B_R)} \le cR^{k-1-j\alpha} & \text{for all } R \ge 1. \end{cases}$$

Then, taking $j_0 \in \mathbb{N}$ as the smallest number such that $j_0\alpha > k+\gamma$, and upon taking the limit $R \to \infty$, we deduce that

$$\lim_{R\to\infty} \|w_{j_0,\tau}\|_{L^\infty(B_R)} \le c \lim_{R\to\infty} R^{k+\gamma-j_0\alpha} = 0,$$

i.e., $w_{j_0,\tau} \equiv 0$ in $\mathbb{R}^n$. Thus, $w_{j_0-1,\tau}$ is a function that is constant in the τ-direction. Clearly, we can also take difference quotients of $w_{j_0-1,\tau}$ in other directions $\tau' \in \mathbb{S}^{n-1}$ with $\tau'_n = 0$, and the same arguments as before apply. Therefore, $w_{j_0-1,\tau}(x) = w_{j_0-1,\tau}(x_n)$ is one-dimensional for any $\tau \in \mathbb{S}^{n-1}$ with $\tau_n = 0$.

Unraveling the higher order difference quotients, we get that $w_{j_0-2,\tau}(x) = (V_1(x_n), x') + V_2(x_n)$ for some one-dimensional functions $V_1 : \mathbb{R} \to \mathbb{R}^{n-1}$ and $V_2 : \mathbb{R} \to \mathbb{R}$, and continuing this argument $j_0 - 1$ times, we deduce that u must be a polynomial in x' with coefficients that are one-dimensional functions from $\mathbb{R} \to \mathbb{R}$ in x_n.

Then, by the growth condition on u, for any multi-index $\beta \in (\mathbb{N} \cup \{0\})^{n-1}$ with $|\beta| \le k$, we obtain functions A_β in x_n such that

$$u(x) = \sum_{|\beta|\le k} (x')^{\beta} A_\beta(x_n).$$

In particular, this implies that $D^{\beta}_{x'} u(x) = c(\beta) A_\beta(x_n)$ for any $|\beta| = k$ and some constant $c(\beta) > 0$, where $D^{\beta}_{x'}$ denotes an incremental quotient approximating the partial derivative $\partial^{\beta}_{x'}$ in the x'-variables. Therefore, discretely differentiating the equation for u, we deduce

$$c(\beta) L((x_n)_+^{s-1} A_\beta)(x) = L((x_n)_+^{s-1} D^{\beta}_{x'} u)(x) = L(D^{\beta}_{x'}[(x_n)_+^{s-1} u])(x) \overset{k-1+\lceil\gamma-s\rceil}{=} 0 \quad \text{in } \{x_n > 0\}.$$

By the growth condition on u, it must be $|A_\beta(x_n)| \le c(1+|x_n|)^{k-|\beta|+\gamma} = c(1+|x|)^{\gamma}$, and since A_β was also one-dimensional, i.e., $LA_\beta = (-\Delta)^s_{\mathbb{R}} A_\beta$, we can apply Lemma 5.2 to A_β, which yields $A_\beta(x_n) = p_\beta(x_n)$ for some polynomial $p_\beta \in \mathcal{P}_{k-|\beta|} = \mathcal{P}_0$. Next, we recall from Lemma 5.3,

$$L((x_n)_+^{s-1} (x')^{\beta} p_\beta(x_n)) \overset{k-1+\lceil\gamma-s\rceil}{=} 0 \quad \text{in } \{x_n > 0\}.$$

Thus, repeating the arguments from above, we deduce that, for every β with $|\beta| \le k$ it holds that

$$\begin{cases} L((x_n)_+^{s-1} A_\beta) \overset{k-1+\lceil \gamma - s \rceil}{=} 0 & \text{in } \{x_n > 0\}, \\ |A_\beta(x)| \le C(1+|x|)^{k-|\beta|+\gamma} & \text{for all } x \in \{x_n > 0\}, \end{cases}$$

and hence $A_\beta(x_n) = p_\beta(x_n)$ for some polynomial $p_\beta \in \mathcal{P}_{k-|\beta|}$. This implies $u(x) = p(x)$ for some polynomial p, and by the growth condition on u, it must be $p \in \mathcal{P}_k$, as desired. □

6. Higher order boundary regularity

The goal of this section is to prove the desired higher order boundary regularity for nonlocal equations with local Neumann conditions (see Theorem 1.2). The proof goes by a blow-up argument and heavily uses the Liouville theorem in the half-space (see Theorem 5.1), as well as the boundary Hölder estimate (see Theorem 1.6).

Lemma 6.1. *Let $L \in \mathcal{L}_s^{\hom}(\lambda, \Lambda)$. Let $k \in \mathbb{N}$ and $\Omega \subset \mathbb{R}^n$ be an open, bounded domain with $\partial\Omega \in C^{k+1,\gamma}$ for some $\gamma \in (0,1)$ with $\gamma \neq s$, and $K \in C^{2k+2\gamma+3}(\mathbb{S}^{n-1})$. Let $v \in L^1_{2s}(\mathbb{R}^n)$ with $v/d^{s-1} \in C(\overline{\Omega})$ be a viscosity solution to*

$$\begin{cases} Lv = f & \text{in } \Omega \cap B_1, \\ v = 0 & \text{in } B_1 \setminus \Omega, \\ \partial_\nu(v/d^{s-1}) = g & \text{on } \partial\Omega \cap B_1. \end{cases}$$

(i) *If $k = 1$ and $\gamma < s$, $f \in C(\Omega \cap B_1)$ with $d^{s-\gamma} f \in L^\infty(\Omega \cap B_1)$, $g \in C^\gamma(\partial\Omega \cap B_1)$, then for any $x_0 \in \partial\Omega \cap B_{1/2}$ and $x \in \Omega \cap B_{1/2}$ it holds that*

$$\begin{aligned} &\Big|\frac{v}{d^{s-1}}(x) - \Big(\frac{v}{d^{s-1}}(x_0) - A(x_0)\cdot(x-x_0)\Big)\Big| \\ &\qquad \le c\Big(\Big\|\frac{v}{d^{s-1}}\Big\|_{L^\infty(\Omega)} + \|v\|_{L^\infty(\mathbb{R}^n\setminus\Omega)} + \|d^{s-\gamma} f\|_{L^\infty(\Omega\cap B_1)} + \|g\|_{C^\gamma(\partial\Omega\cap B_1)}\Big)|x-x_0|^{1+\gamma} \end{aligned}$$

for some $c > 0$, which only depends on $n, s, \lambda, \Lambda, \gamma$, and the $C^{2,\gamma}$ radius of Ω. If in addition, $g \equiv 0$, then $A(x_0)\cdot \nu_{x_0} = 0$.

(ii) *If $k \ge 2$ or $\gamma > s$, $f \in C^{(k-1)-s+\gamma}(\Omega \cap B_1)$, $g \in C^{k-1+\gamma}(\partial\Omega \cap B_1)$, then for any $x_0 \in \partial\Omega \cap B_{1/2}$, there is $Q(\,\cdot\,; x_0) \in \mathcal{P}_k$ such that for any $x \in \Omega \cap B_{1/2}$ it holds that*

$$\begin{aligned} &\Big|\frac{v}{d^{s-1}}(x) - Q(x; x_0)\Big| \\ &\qquad \le c\Big(\Big\|\frac{v}{d^{s-1}}\Big\|_{L^\infty(\Omega)} + \|v\|_{L^\infty(\mathbb{R}^n\setminus\Omega)} + \|f\|_{C^{(k-1)-s+\gamma}(\Omega\cap B_1)} + \|g\|_{C^{k-1+\gamma}(\partial\Omega\cap B_1)}\Big)|x-x_0|^{k+\gamma} \end{aligned}$$

for some $c > 0$, which only depends on $n, s, \lambda, \Lambda, \gamma, k$, and the $C^{k+1,\gamma}$ radius of Ω.

Proof. Let us assume without loss of generality that $x_0 = 0 \in \partial\Omega$ with $\partial_{\nu_0} = e_n$. We set $u := v/d^{s-1}$.

We will prove the desired result by a blow-up argument. To do so, we assume by contradiction that for any $j \in \mathbb{N}$ there exist $C^{k+1,\gamma}$ domains $\Omega_j \subset \mathbb{R}^n$, $f_j \in C^{k-1}(\Omega_j \cap B_1)$, $g_j \in C^{k-1+\gamma}(\partial\Omega_j \cap B_1)$, $r_j > 0$, operators L_j with ellipticity constants λ, Λ, and $v_j \in C(\Omega_j) \cap L^1_{2s}(\mathbb{R}^n)$ viscosity solutions to

$$\begin{cases} L_j v_j = f_j & \text{in } \Omega_j \cap B_1, \\ v_j = 0 & \text{in } B_1 \setminus \Omega_j, \\ \partial_\nu (v_j / d_j^{s-1}) = g_j & \text{on } \partial\Omega_j \cap B_1, \end{cases}$$

such that

$$|\operatorname{diam} \Omega_j| + \|u_j\|_{L^\infty(\Omega_j)} + \|v_j\|_{L^\infty(\mathbb{R}^n \setminus \Omega_j)} + \mathbb{1}_{\{k=1 \text{and } \gamma<s\}} \|d_j^{s-\gamma} f_j\|_{L^\infty(\Omega_j \cap B_1)} \\ + \mathbb{1}_{\{k\geq 2 \text{or } \gamma>s\}} \|f_j\|_{C^{(k-1)-s+\gamma}(\Omega_j \cap B_1)} + \|g_j\|_{C^{k-1+\gamma}(\Omega_j \cap B_1)} + \|d_j\|_{C^{k+1,\gamma}(\Omega_j \cap B_1)} \leq C$$

for some $C > 0$, denoted $d_{\Omega_j} = d_j$, and used that $d_j \in C^{k+1,\gamma}$ by [Fernández-Real and Ros-Oton 2024a, Definition 2.7.5]. Finally, we assume by contradiction

$$\sup_{j\in\mathbb{N}} \sup_{r>0} r^{-k-\gamma} \|u_j - Q\|_{L^\infty(\Omega_j \cap B_r)} = \infty \quad \text{for all } Q \in \mathcal{P}_k.$$

Observe that up to a rotation, $r_m^{-1}\Omega_{j_m} \cap B_{r_m^{-1}} \to \{x_n > 0\}$. Moreover, we will write

$$\tilde{d}_{j_m} \mathbb{1}_{r_m^{-1}\Omega_{j_m}} := \tilde{d}_{j_m} =: r_m^{-1} d_{j_m}(r_m\,\cdot\,)$$

for the (regularized) distance with respect to $r_m^{-1}\Omega_{j_m}$.

We consider the $L^2(\Omega_j \cap B_r)$-projections of u_j over $\mathcal{P}_k$, and denote them by $Q_{j,r} \in \mathcal{P}_k$. They satisfy the following properties:

$$\|u_j - Q_{j,r}\|_{L^2(\Omega_j\cap B_r)} \leq \|u_j - Q\|_{L^2(\Omega_j \cap B_r)} \quad \text{for all } Q \in \mathcal{P}_k,$$
$$\int_{\Omega_j \cap B_r} (u_j(x) - Q_{j,r}(x)) Q(x)\,\mathrm{d}x = 0 \quad \text{for all } Q \in \mathcal{P}_k.$$

Next, we introduce

$$\theta(r) := \sup_{j\in\mathbb{N}} \sup_{\rho \geq r} \rho^{-k-\gamma} \|u_j - Q_{j,\rho}\|_{L^\infty(\Omega_j \cap B_r)}. \tag{6-1}$$

Observe that $\theta(r) \nearrow \infty$, as $r \searrow 0$. This follows from [Abatangelo and Ros-Oton 2020, Lemma 4.3] applied with $s = 0$ (the proof remains exactly the same in this case).

As a consequence, there exist sequences $(r_m)_m$ and $(j_m)_m$ such that

$$\frac{\|u_{j_m} - Q_{j_m,r_m}\|_{L^\infty(\Omega_{j_m} \cap B_{r_m})}}{r_m^{k+\gamma}\theta(r_m)} \geq \tfrac{1}{2} \quad \text{for all } m \in \mathbb{N}. \tag{6-2}$$

Let us define for any $m \in \mathbb{N}$,

$$w_m(x) = \frac{u_{j_m}(r_m x) - Q_{j_m,r_m}(r_m x)}{r_m^{k+\gamma}\theta(r_m)}, \tag{6-3}$$

and observe that by construction, we have

$$\|w_m\|_{L^\infty(r_m^{-1}\Omega_{j_m} \cap B_1)} \geq \tfrac{1}{2}, \quad \int_{r_m^{-1}\Omega_{j_m}\cap B_1} w_m(x) Q(r_m x)\,\mathrm{d}x = 0 \quad \text{for all } m \in \mathbb{N},\ Q \in \mathcal{P}_k. \tag{6-4}$$

Next, we claim that

$$\|w_m\|_{L^\infty(r_m^{-1}\Omega_{j_m} \cap B_R)} \leq c R^{k+\gamma} \quad \text{for all } R \geq 1,\ m \in \mathbb{N}. \tag{6-5}$$

To see this, we estimate for any $R \geq 1$, using the definitions of $\theta(Rr_m)$ and w_m (see (6-1) and (6-3)),

$$\begin{aligned}\|w_m\|_{L^\infty(r_m^{-1}\Omega_{j_m}\cap B_R)} &\leq \frac{\|u_{j_m} - Q_{j_m,Rr_m}\|_{L^\infty(\Omega_{j_m}\cap B_{Rr_m})}}{r_m^{k+\gamma}\theta(r_m)} + \frac{\|Q_{j_m,Rr_m} - Q_{j_m,r_m}\|_{L^\infty(\Omega_{j_m}\cap B_{Rr_m})}}{r_m^{k+\gamma}\theta(r_m)} \\ &\leq \frac{(Rr_m)^{k+\gamma}\theta(Rr_m)}{r_m^{k+\gamma}\theta(r_m)} + \frac{\|Q_{j_m,Rr_m} - Q_{j_m,r_m}\|_{L^\infty(\Omega_{j_m}\cap B_{Rr_m})}}{r_m^{k+\gamma}\theta(r_m)}. \end{aligned} \tag{6-6}$$

Moreover, it follows that for any $j \in \mathbb{N}$, $r > 0$, and $R \geq 1$,

$$\|Q_{j,Rr} - Q_{j,r}\|_{L^\infty(\Omega_j\cap B_{Rr})} \leq c\theta(r)(Rr)^{k+\gamma}. \tag{6-7}$$

Indeed, if we write

$$Q_{j,r}(x) = \sum_{|\beta|\leq k} a_{j,r}^{(\beta)} x_1^{\beta_1}\cdots x_n^{\beta_n}, \quad \beta \in \mathbb{N}^n,\ a_{j,r}^{(\beta)} \in \mathbb{R},$$

then by [Abatangelo and Ros-Oton 2020, Lemma A.10] we have for any $|\alpha| \leq k$

$$\begin{aligned} r^{|\beta|}|a_{j,r}^{(\beta)} - a_{j,2r}^{(\beta)}| &\leq c\|Q_{j,r} - Q_{j,2r}\|_{L^\infty(\Omega_j\cap B_r)} \\ &\leq c\|u_j - Q_{j,r}\|_{L^\infty(\Omega_j\cap B_r)} + c\|u_j - Q_{j,2r}\|_{L^\infty(\Omega_j\cap B_{2r})} \\ &\leq c\theta(r)r^{k+\gamma} + c\theta(2r)(2r)^{k+\gamma} \leq c\theta(r)(2r)^{k+\gamma}. \end{aligned}$$

By iteration of this inequality, we obtain for any $l \in \mathbb{N}$

$$\begin{aligned} |a_{j,r}^{(\beta)} - a_{j,2^l r}^{(\beta)}| &\leq \sum_{i=0}^{l-1} |a_{j,2^i r}^{(\beta)} - a_{j,2^{i+1}r}^{(\beta)}| \leq c\sum_{i=0}^{l-1}\theta(2^i r)(2^i r)^{k+\gamma-|\beta|} \\ &\leq c\theta(r)r^{k+\gamma-|\beta|}\sum_{i=0}^{l-1}\frac{\theta(2^i r)}{\theta(r)}2^{i(k+\gamma-|\beta|)} \leq c\theta(r)(2^l r)^{k+\gamma-|\beta|}. \end{aligned}$$

This yields for any $R > 1$

$$|a_{j,r}^{(\beta)} - a_{j,Rr}^{(\beta)}| \leq c\theta(r)(Rr)^{k+\gamma-|\beta|},$$

which implies (6-7).

Thus, combining (6-6) and (6-7),

$$\|w_m\|_{L^\infty(\Omega_{j_m}\cap B_R)} \leq \frac{(Rr_m)^{k+\gamma}\theta(Rr_m)}{r_m^{k+\gamma}\theta(r_m)} + c\frac{(Rr_m)^{k+\gamma}\theta(r_m)}{r_m^{k+\gamma}\theta(r_m)} \leq cR^{k+\gamma},$$

where we used in the last step that $t \mapsto \theta(r)$ is monotone decreasing, proving (6-5).

Next, using (6-5), we will estimate the $L^1_{2s+(k+\lceil\gamma-s\rceil-1)}$ norm of w_m. We have the estimate

$$\begin{aligned} &\int_{(\Omega_{j_m}\setminus B_{Rr_m})\cap\{d_{j_m}\geq\kappa\}} d_{j_m}^{s-1}(y)|y|^{-n-2s-\lceil\gamma-s\rceil+1+\gamma}\,\mathrm{d}y \\ &\qquad\leq \kappa^{s-1}\int_{(\Omega_{j_m}\setminus B_{Rr_m})}|y|^{-n-s+\gamma-\lceil\gamma-s\rceil}|y|^{1-s}\,\mathrm{d}y \\ &\qquad\leq c\kappa^{s-1}\operatorname{diam}(\Omega_{j_m})^{1-s}\int_{\mathbb{R}^n\setminus B_{Rr_m}}|y|^{-n-s+\gamma-\lceil\gamma-s\rceil} \leq c(Rr_m)^{\gamma-s-\lceil\gamma-s\rceil}, \end{aligned}$$

where we used that always $\gamma < s + \lceil\gamma - s\rceil < 0$. Moreover, by a similar computation as in Lemma 2.2

(with $\gamma := s-1 < 2s + \lceil \gamma - s \rceil - 1 - \gamma =: \beta$), we have

$$\int_{(\Omega_{j_m} \setminus B_{Rr_m}) \cap \{d_{j_m} < \kappa\}} d_{j_m}^{s-1}(y)|y|^{-n-2s-\lceil \gamma - s\rceil + 1 + \gamma} \, \mathrm{d}y \le c(Rr_m)^{\gamma - s - \lceil \gamma - s \rceil}.$$

Thus, altogether, using (6-5) and $\gamma \in (0,1)$ we obtain

$$\begin{aligned}
&\big\| \tilde{d}_{j_m}^{s-1} w_m |\cdot|^{-n-2s-(k+\lceil \gamma - s\rceil - 1)} \big\|_{L^1(\mathbb{R}^n \setminus B_R)} \\
&\quad \le c \int_{r_m^{-1}\Omega_{j_m} \setminus B_R} \tilde{d}_{j_m}^{s-1}(y)|y|^{-n-2s-\lceil \gamma - s\rceil + 1 + \gamma} \, \mathrm{d}y \\
&\quad \le c r_m^{1-s} \int_{r_m^{-1}\Omega_{j_m} \setminus B_R} d_{j_m}^{s-1}(r_m y)|y|^{-n-2s-\lceil \gamma - s\rceil + 1 + \gamma} \, \mathrm{d}y \\
&\quad = c r_m^{s-\gamma+\lceil \gamma - s \rceil} \int_{\Omega_{j_m} \setminus B_{Rr_m}} d_{j_m}^{s-1}(y)|y|^{-n-2s-\lceil \gamma - s\rceil + 1 + \gamma} \, \mathrm{d}y \\
&\quad \le c r_m^{s-\gamma+\lceil \gamma - s \rceil} \int_{(\Omega_{j_m} \setminus B_R) \cap \{d_{j_m} \ge \kappa\}} d_{j_m}^{s-1}(y)|y|^{-n-2s-\lceil \gamma - s\rceil + 1 + \gamma} \, \mathrm{d}y \\
&\qquad + c r_m^{s-\gamma+\lceil \gamma - s \rceil} \int_{(\Omega_{j_m} \setminus B_R) \cap \{d_{j_m} < \kappa\}} d_{j_m}^{s-1}(y)|y|^{-n-2s-\lceil \gamma - s\rceil + 1 + \gamma} \, \mathrm{d}y \\
&\quad \le c r_m^{s-\gamma+\lceil \gamma - s \rceil} (Rr_m)^{\gamma - s - \lceil \gamma - s\rceil} \le R^{\gamma - s - \lceil \gamma - s \rceil} \to 0 \quad \text{as } R \to \infty.
\end{aligned} \tag{6-8}$$

Now, we investigate the equation that is satisfied by w_m. We claim that

$$\frac{|a_{j_m,r_m}^{(\beta)}|}{\theta(r_m)} \to 0, \quad \text{as } m \to \infty \quad \text{for all } |\beta| \le k. \tag{6-9}$$

Indeed, from the considerations above, we deduce that for any $m, l \in \mathbb{N}$,

$$\frac{|a_{j_m,r_m}^{(\beta)} - a_{j_m,2^l r_m}^{(\beta)}|}{\theta(r_m)} \le c \sum_{i=1}^{l} \frac{\theta(2^{l-i} r_m)}{\theta(r_m)} (2^{l-i} r_m)^{k+\gamma-|\beta|}.$$

Hence, choosing $l \in \mathbb{N}$ such that $2^l r_m \in [1,2)$, we deduce

$$\begin{aligned}
\frac{|a_{j_m,r_m}^{(\beta)}|}{\theta(r_m)} &\le \frac{|a_{j_m,2^l r_m}^{(\beta)}|}{\theta(r_m)} + \frac{|a_{j_m,r_m}^{(\beta)} - a_{j_m,2^l r_m}^{(\beta)}|}{\theta(r_m)} \\
&\le c\theta(r_m)^{-1} \bigg(|a_{j_m,2^l r_m}^{(\beta)}| + \sum_{i=1}^{l} \theta(2^{-i})(2^{-i})^{k+\gamma-|\beta|} \bigg) \to 0 \quad \text{as } m \to \infty,
\end{aligned}$$

which implies (6-9).

Let us now distinguish between the cases ($k = 1$ and $\gamma < s$) and ($k \ge 2$ or $\gamma > s$). In case $k = 1$ and $\gamma < s$, we find that it holds in the viscosity sense

$$\begin{aligned}
\tilde{d}_{j_m}^{s-\gamma} L_{j_m}(\tilde{d}_{j_m}^{s-1} w_m) &= r^{\gamma - s} d_{j_m}^{s-\gamma}(r_m \cdot) r_m^{1-s} L_{j_m}(d_{j_m}^{s-1}(r_m \cdot) w_m) \\
&= d_{j_m}^{s-\gamma}(r_m \cdot) \frac{L_{j_m}(d_{j_m}^{s-1} u_{j_m}(r_m \cdot)) - L_{j_m}(d_{j_m}^{s-1} Q_{j_m,r_m}(r_m \cdot))}{r_m^{2s}\theta(r_m)} \\
&= d_{j_m}^{s-\gamma}(r_m \cdot) \frac{f_{j_m}(r_m \cdot) - L_{j_m}(d_{j_m}^{s-1} Q_{j_m,r_m})(r_m \cdot)}{\theta(r_m)} \quad \text{in } r_m^{-1}\Omega_{j_m} \cap B_{r_m^{-1}}.
\end{aligned} \tag{6-10}$$

Moreover, by Corollary 2.5(i),

$$\|d_{j_m}^{s-\gamma} L_{j_m}(d_{j_m}^{s-1} Q_{j_m,r_m})(r_m\,\cdot\,)\|_{L^\infty(r_m^{-1}\Omega_{j_m}\cap B_{r_m^{-1}})} = \|d_{j_m}^{s-\gamma} L_{j_m}(d_{j_m}^{s-1} Q_{j_m,r_m})\|_{L^\infty(\Omega_{j_m}\cap B_1)} \le c \sum_{|\beta|\le 1} |a_{j_m,r_m}^{(\beta)}|. \tag{6-11}$$

Therefore, recalling $\|d_{j_m}^{s-\gamma} f_{j_m}\|_{L^\infty(\Omega_{j_m}\cap B_1)} \le C$, and combining (6-10), (6-11), and (6-9), we obtain

$$\|\tilde{d}_{j_m}^{s-\gamma} L_{j_m}(\tilde{d}_{j_m}^{s-1} w_m)\|_{L^\infty(r_m^{-1}\Omega_{j_m}\cap B_{r_m^{-1}})} \le c\frac{\|d_{j_m}^{s-\gamma} f_{j_m}\|_{L^\infty(\Omega_{j_m}\cap B_1)} + \sum_{|\beta|\le 1}|a_{j_m,r_m}^{(\beta)}|}{\theta(r_m)} \to 0 \quad \text{as } m\to\infty. \tag{6-12}$$

In case $k \ge 2$ or $\gamma > s$, we first deduce by an argument analogous to (6-10),

$$L_{j_m}(\tilde{d}_{j_m}^{s-1} w_m) = \frac{f_{j_m}(r_m\,\cdot\,) - L_{j_m}(d_{j_m}^{s-1} Q_{j_m,r_m})(r_m\,\cdot\,)}{r_m^{(k-1)-s+\gamma}\theta(r_m)} \quad \text{in } r_m^{-1}\Omega_{j_m} \cap B_{r_m^{-1}}. \tag{6-13}$$

Next, using again Corollary 2.5(ii), we obtain

$$r^{-(k-1)+s-\gamma}[L_{j_m}(d_{j_m}^{s-1} Q_{j_m,r_m})(r_m\,\cdot\,)]_{C^{k-1-s+\gamma}(r_m^{-1}\Omega_{j_m}\cap B_{r_m^{-1}})} = [L_{j_m}(d_{j_m}^{s-1} Q_{j_m,r_m})]_{C^{k-1-s+\gamma}(\Omega_{j_m}\cap B_1)} \le c \sum_{|\beta|\le k} |a_{j_m,r_m}^{(\beta)}|, \tag{6-14}$$

in analogy to (6-11). Finally, recalling

$$r^{-(k-1)+s-\gamma}[f_j(r_m\,\cdot\,)]_{C^{(k-1)-s+\gamma}(r_m^{-1}\Omega_{j_m}\cap B_{r_m^{-1}})} = [f_j]_{C^{(k-1)-s+\gamma}(\Omega_{j_m}\cap B_1)} \le C,$$

and combining (6-13), (6-14), and (6-9), we obtain

$$[L_{j_m}(\tilde{d}_{j_m}^{s-1} w_m)]_{C^{k-1-s+\gamma}(r_m^{-1}\Omega_{j_m}\cap B_{r_m^{-1}})} \le c\frac{[f_j]_{C^{(k-1)-s+\gamma}(\Omega_{j_m}\cap B_1)} + \sum_{|\beta|\le 1}|a_{j_m,r_m}^{(\beta)}|}{\theta(r_m)} \to 0 \quad \text{as } m\to\infty.$$

Thus, there exists a polynomial $p_m \in \mathcal{P}_{k-2+\lceil\gamma-s\rceil}$ such that

$$|L_{j_m}(\tilde{d}_{j_m}^{s-1} w_m) - p_m| \to 0, \quad \text{as } m\to\infty \quad \text{in } L^\infty_{\mathrm{loc}}(\{x_n>0\}). \tag{6-15}$$

Next, considering again all values for γ, k at the same time, we treat the Neumann boundary condition:

$$\partial_\nu w_m = \frac{\partial_\nu u_{j_m}(r_m\,\cdot\,) - \partial_\nu(Q_{j_m,r_m})(r_m\,\cdot\,)}{r_m^{(k-1)+\gamma}\theta(r_m)} = \frac{g_{j_m}(r_m\,\cdot\,) - \partial_\nu(Q_{j_m,r_m})(r_m\,\cdot\,)}{r_m^{(k-1)+\gamma}\theta(r_m)} \quad \text{on } \partial r_m^{-1}\Omega_{j_m}\cap B_{r_m^{-1}}.$$

We obtain

$$r_m^{-(k-1)-\gamma}[\partial_\nu Q_{j_m,r_m}(r_m\,\cdot\,)]_{C^{(k-1)+\gamma}(\partial r_m^{-1}\Omega_{j_m}\cap B_{r_m^{-1}})} = [\partial_\nu Q_{j_m,r_m}]_{C^{(k-1)+\gamma}(\partial\Omega_{j_m}\cap B_1)} \le c\sum_{|\beta|\le k}|a_{j_m,r_m}^{(\beta)}|,$$

and using also that $g_{j_m} \in C^{k-1+\gamma}(\Omega_{j_m}\cap B_1)$ by the boundary condition, we deduce

$$[\partial_\nu w_m]_{C^{(k-1)+\gamma}(\partial r_m^{-1}\Omega_{j_m}\cap B_{r_m^{-1}})} \le c\frac{[g_{j_m}]_{C^{(k-1)+\gamma}(\partial\Omega_{j_m}\cap B_1)} + \sum_{|\beta|\le k}|a_{j_m,r_m}^{(\beta)}|}{\theta(r_m)} \le c\theta(r_m)^{-1} \to 0,$$

as $m \to \infty$. Consequently, for any $m \in \mathbb{N}$ there exists a polynomial $q_m \in \mathcal{P}_{k-1}$ such that

$$|\partial_\nu w_m(x) - q_m| \le c\frac{|x|^\gamma}{\theta(r_m)} \to 0 \quad \text{for all } x \in \partial r_m^{-1}\Omega_{j_m} \cap B_{r_m^{-1}}. \tag{6-16}$$

Finally, we are in a position to apply the stability theorem (see Lemma 2.13) to w_m. The convergence results in (6-12), (6-15) and (6-16) establish the required convergence of the source terms and the Neumann boundary data.

Moreover, the operators L_{j_m} converge to an operator L with the same ellipticity constants. By the boundary Hölder regularity estimate for solutions to the nonlocal Neumann problem (see Corollary 4.4 applied with $k := k + \lceil \gamma - s\rceil$, $\delta := 0$, $\Omega := r_m^{-1}\Omega_{j_m}$, $v := \tilde{d}_{j_m}^{s-1} w_m$, $f := L_{j_m}(\tilde{d}_{j_m}^{s-1} w_m)$, and $g := \partial_\nu w_m$), together with the Arzelà–Ascoli theorem, the sequence $(w_m)_m$ converges in $L^\infty_{\text{loc}}(\{x_n \ge 0\})$ to some $w \in C(\{x_n \ge 0\})$. All the quantities on the right-hand side of the estimate in Corollary 4.4 will be bounded uniformly in k, due to (6-8), (6-12), (6-15), and (6-16). Thus, in particular $\tilde{d}_{j_m}^{s-1}(r_m\,\cdot) w_m \to (x_n)_+^{s-1} w$ locally uniformly in $\{x_n > 0\}$. Finally, in order to apply the stability result in Lemma 2.13, it remains to establish $\tilde{d}_{j_m}^{s-1}(r_m\,\cdot) w_m \to (x_n)_+^{s-1} w$ in $L^1_{2s+(k+\lceil\gamma-s\rceil-1)}(\mathbb{R}^n)$. To see this, we also observe that by (6-5),

$$|w(x)| \le C(1+|x|)^{k+\gamma} \quad \text{for all } x \in \{x_n > 0\}. \tag{6-17}$$

Therefore, using also (6-8) and a computation based on polar coordinates (along the lines of (5-3)) we obtain, since $\gamma < 1$,

$$\begin{aligned}\int_{\mathbb{R}^n\setminus B_R} &\big|\tilde{d}_{j_m}^{s-1}(y) w_m(y) - (y_n)_+^{s-1} w(y)\big| |y|^{-n-2s-(k+\lceil\gamma-s\rceil-1)}\,\mathrm{d}y \\ &\le C\int_{\mathbb{R}^n\setminus B_R} (y_n)_+^{s-1} |y|^{-n-2s-\lceil\gamma-s\rceil+1+\gamma}\,\mathrm{d}y + C\int_{(r_m^{-1}\Omega_{j_m})\setminus B_R} \tilde{d}_{j_m}^{s-1}(y)|y|^{-n-2s-\lceil\gamma-s\rceil+1+\gamma}\,\mathrm{d}y \\ &\le CR^{\gamma-s-\lceil\gamma-s\rceil} \to 0 \quad \text{as } R \to \infty.\end{aligned}$$

This implies $\tilde{d}_{j_m}^{s-1} w_m \to (x_n)_+^{s-1} w$ in $L^1_{2s+(k+\lceil\gamma-s\rceil-1)}(\mathbb{R}^n)$, by combining it with the locally uniform convergence in $L^\infty_{\text{loc}}(\{x_n \ge 0\})$.

Thus, by stability of viscosity solutions (see Lemma 2.13), we deduce that in the viscosity sense

$$\begin{cases} L((x_n)_+^{s-1} w) \overset{k-1+\lceil\gamma-s\rceil}{=} 0 & \text{in } \{x_n > 0\}, \\ \partial_n w = p & \text{on } \{x_n = 0\}, \end{cases}$$

where $p \in \mathcal{P}_{k-1}$ is a polynomial, and moreover, by (6-4), it must be that

$$\|w\|_{L^\infty(B_1 \cap \{x_n > 0\})} \ge \tfrac{1}{2}. \tag{6-18}$$

An application of the Liouville theorem (see Theorem 5.1, using (6-17)) yields now that $w \in \mathcal{P}_k$. Thus, we can choose $Q(x) = w(r_m^{-1}x)$ in (6-4). This implies that

$$0 = \lim_{m\to\infty}\int_{B_1\cap r_m^{-1}\Omega_{j_m}} w_m(x) Q(r_m x)\,\mathrm{d}x = \lim_{m\to\infty}\int_{B_1\cap r_m^{-1}\Omega_{j_m}} w_m(x) w(x)\,\mathrm{d}x = \int_{B_1\cap\{x_n>0\}} w^2(x)\,\mathrm{d}x,$$

where we used in the last step $w_m \to w$ and $r_m^{-1}\Omega_{j_m} \to \{x_n > 0\}$. This yields $w = 0$, which however contradicts (6-18), and thus, we conclude the proof of (ii).

Finally, if $k=1$ and $\gamma < s$, then by the Liouville theorem (see Theorem 5.1), there exist $a \in \mathbb{R}^n$ and $b \in \mathbb{R}$ such that

$$w(x) = (a, x) + b.$$

Moreover, if $g_j \equiv 0$, then also $g \equiv 0$. Thus, it must be that $\partial_n w = 0$ in $\{x_n = 0\}$, which implies $a_n = 0$. ☐

We are now in a position to prove our main result.

Proof of Theorem 1.2. We define $u := v/d^{s-1}$. Let us assume that

$$\|u\|_{L^\infty(\mathbb{R}^n)} + \|d^{s-\gamma} f\|_{L^\infty(\Omega\cap B_2)} \mathbb{1}_{\{1+\gamma<2s\}} + \|f\|_{C^{k-2s+\gamma}(\Omega\cap B_2)} \mathbb{1}_{\{1+\gamma>2s\}} + \|g\|_{C^{k-1+\gamma}(\partial\Omega\cap B_2)} \le 1.$$

First, we claim that for any $x_0 \in \Omega \cap B_{1/2}$ with $z \in \partial\Omega \cap B_{1/2}$ such that $|x_0 - z| = d(x_0) =: r \le 1$, there exists a polynomial $Q \in \mathcal{P}_k$ of degree k such that

$$[u - Q]_{C^{k+\gamma}(B_{r/2}(x_0))} \le c \tag{6-19}$$

for some constant $c > 0$, depending only on $n, s, \lambda, \Lambda, \gamma, \Omega, k$, where we assume without loss of generality that $\nu_z = e_n$. This estimate already yields the desired result since it implies

$$[u]_{C^{k+\gamma}(B_{r/2}(x_0))} \le [u - Q]_{C^{k+\gamma}(B_{r/2}(x_0))} + [Q]_{C^{k+\gamma}(B_{r/2}(x_0))} \le c.$$

From here, a covering argument (see [Fernández-Real and Ros-Oton 2024a, Lemma A.1.4]) together with Hölder interpolation (recall that $\|u\|_{L^\infty(\mathbb{R}^n)} \le 1$) yields the desired regularity estimate in $\overline{\Omega} \cap B_1$. Improving the global L^∞ norm to the $L^1_{2s}(\mathbb{R}^n)$ norm, or the $L^1_{k+\gamma}(\mathbb{R}^n \setminus B_2)$ norm, respectively, in the estimate goes by the exact same arguments as in the proofs of Lemma 2.10 and Corollary 4.4.

To see (6-19), let us take $z \in \partial\Omega \cap B_{1/2}$ such that $|x_0 - z| = d(x_0) = r$, and apply Lemma 6.1 to see that there exists a polynomial $Q \in \mathcal{P}_k$ such that the function

$$u_r(x) := \frac{u(x_0 + rx) - Q(x_0 + rx)}{r^{k+\gamma}} \quad \text{satisfies} \quad \|u_r\|_{L^\infty(B_R)} \le C R^{k+\gamma} \quad \text{for all } R \in [1, r^{-1}].$$

Moreover, since $\|u\|_{L^\infty(\mathbb{R}^n)} \le 1$, and $Q \in \mathcal{P}_k$, we deduce

$$\|u_r\|_{L^\infty(B_R)} \le C r^{-k-\gamma}(1 + (rR)^k) \le C R^{k+\gamma} \quad \text{for all } R \ge r^{-1}.$$

Together, this implies

$$\begin{aligned}\int_{\mathbb{R}^n \setminus B_{3/4}} \frac{d^{s-1}(x_0+rx)|u_r(x)|}{|x|^{n+k+\gamma}} \, dx \le c \int_{\mathbb{R}^n \setminus B_{3/4}} \frac{d^{s-1}(x_0+rx)}{|x|^n} \, dx &= c \int_{\mathbb{R}^n \setminus B_{3r/4}} \frac{d^{s-1}(x_0+x)}{|x|^n} \, dx \\ &\le c(1 + r^{s-1}),\end{aligned}$$

where we used Lemma 2.2 with $\gamma := s - 1 < 0 =: \beta$. Moreover, we have by the definition of r,

$$\|d^{s-1}(x_0 + r\,\cdot\,) u_r\|_{L^\infty(B_{3/4})} \le c r^{s-1}.$$

Now, we apply the interior regularity theory for nonlocal problems (see Lemma 2.10). To do so, we distinguish between the cases (i) $k = 1$ and $k + \gamma = 1 + \gamma \le 2s$ and (ii) $k + \gamma > 2s$. In case (i), we apply

Lemma 2.10(i) with $\beta = 1+\gamma$, observe that automatically $\gamma < s$, and obtain

$$\begin{aligned}
[d^{s-1}(u-Q)]_{C^{1+\gamma}(B_{r/2}(x_0))} &= [d^{s-1}(x_0+r\,\cdot\,)u_r]_{C^{1+\gamma}(B_{1/2})} \\
&\le c\|d^{s-1}(x_0+r\,\cdot\,)u_r\|_{L^\infty(B_{3/4})} + c\left\| \frac{d^{s-1}(x_0+r\,\cdot\,)u_r}{|x|^{n+1+\gamma}} \right\|_{L^1(\mathbb{R}^n\setminus B_{3/4})} \\
&\qquad + c\|L(d^{s-1}(x_0+r\,\cdot\,)u_r)\|_{L^\infty(B_{3/4})} \\
&\le cr^{s-1} + cr^{2s-(1+\gamma)}\|Lv\|_{L^\infty(B_{3r/4}(x_0))} + cr^{2s-(1+\gamma)}\|L(d^{s-1}Q)\|_{L^\infty(B_{3r/4}(x_0))} \\
&\le cr^{s-1} + cr^{s-1}\|d^{s-\gamma}f\|_{L^\infty(B_r(x_0))} + cr^{s-1} \le cr^{s-1},
\end{aligned}$$

where we used Corollary 2.5(i) and that $d \ge r/4$ in $B_{3r/4}(x_0)$ by construction, and $r \le 1$.

In case (ii), we apply Lemma 2.10(ii) with $\alpha := k+\gamma-2s > 0$ and obtain

$$\begin{aligned}
[d^{s-1}(u-Q)]_{C^{k+\gamma}(B_{r/2}(x_0))} &= [d^{s-1}(x_0+r\,\cdot\,)u_r]_{C^{k+\gamma}(B_{1/2})} \\
&\le c\|d^{s-1}(x_0+r\,\cdot\,)u_r\|_{L^\infty(B_{3/4})} + c\left\| \frac{d^{s-1}(x_0+r\,\cdot\,)u_r}{|x|^{n+k+\gamma}} \right\|_{L^1(\mathbb{R}^n\setminus B_{3/4})} \\
&\qquad + c[L(d^{s-1}(x_0+r\,\cdot\,)u_r)]_{C^{k+\gamma-2s}(B_{3/4})} \\
&\le cr^{s-1} + c[Lv]_{C^{k+\gamma-2s}(B_{3r/4}(x_0))} + c[L(d^{s-1}Q)]_{C^{k+\gamma-2s}(B_{3r/4}(x_0))} \\
&\le cr^{s-1} + cr^{s-1}\|f\|_{C^{k+\gamma-2s}(B_r(x_0))} + cr^{s-1} \le cr^{s-1},
\end{aligned}$$

where we used Corollary 2.5(iii) in the second to last step.

Moreover, using again the L^∞ estimate for u_r with $R=1$, we have

$$\|d^{s-1}(u-Q)\|_{L^\infty(B_{r/2}(x_0))} \le cr^{s-1}\|u-Q\|_{L^\infty(B_{r/2}(x_0))} \le cr^{s+(k-1)+\gamma}\|u_r\|_{L^\infty(B_1)} \le cr^{s+(k-1)+\gamma},$$

and hence by Hölder interpolation, we obtain that for any $\delta \in (0, k+\gamma)$ it holds that

$$[d^{s-1}(u-Q)]_{C^\delta(B_{r/2}(x_0))} \le cr^{s-1+k+\gamma-\delta}.$$

Therefore, altogether by the product rule,

$$\begin{aligned}
[(u-Q)]_{C^{k+\gamma}(B_{r/2}(x_0))} &= [D^k(d^{1-s}d^{s-1}(u-Q))]_{C^\gamma(B_{r/2}(x_0))} \\
&\le \sum_{|\beta|=k}\sum_{\alpha\le\beta}[(\partial^\alpha d^{1-s})(\partial^{\beta-\alpha}d^{s-1}(u-Q))]_{C^\gamma(B_{r/2}(x_0))} \\
&\le \sum_{|\beta|=k}\sum_{\alpha\le\beta}\big(\|\partial^\alpha d^{1-s}\|_{L^\infty(B_{r/2}(x_0))}[\partial^{\beta-\alpha}d^{s-1}(u-Q)]_{C^\gamma(B_{r/2}(x_0))} \\
&\qquad + \|\partial^{\beta-\alpha}d^{s-1}(u-Q)\|_{L^\infty(B_{r/2}(x_0))}[\partial^\alpha d^{1-s}]_{C^\gamma(B_{r/2}(x_0))}\big) \\
&\le c\sum_{|\beta|=k}\sum_{\alpha\le\beta}\big(r^{1-s-|\alpha|}r^{s-1+k+\gamma-(k-|\alpha|+\gamma)} + r^{s-1+k+\gamma-(k-|\alpha|)}r^{1-s-|\alpha|-\gamma}\big) \\
&\le c\sum_{|\beta|=k}\sum_{\alpha\le\beta} \le c,
\end{aligned} \tag{6-20}$$

where we used that $r \le 1$, and the following observation based on the fact that $d \in C^{k+1,\gamma}(\overline{\Omega})$ together with corresponding estimates $|D^j d| \le c_j d^{1-j}$ (resp. $|D^j d^{1-s}| \le c_j d^{1-s-j}$) in Ω for every $j \le k$ (see [Fernández-Real and Ros-Oton 2024a, Lemma B.0.1]):

$$\begin{aligned}[][\partial^\alpha d^{1-s}]_{C^\gamma(B_{r/2}(x_0))} &\le \|D^{|\alpha|+1} d^{1-s}\|_{L^\infty(B_{r/2}(x_0))} \sup_{x,y \in B_{r/2}(x_0)} |x-y|^{1-\gamma} \\ &\le c r^{1-s-|\alpha|-\gamma} \qquad \text{for all } |\alpha| \le k. \end{aligned} \tag{6-21}$$

This proves our claim (6-19). We can replace the L^∞ norm of u in $\mathbb{R}^n \setminus B_2$ by the $L^1_{2s}(\mathbb{R}^n)$ norm via a truncation argument, as in the proof of Corollary 4.4. We conclude the proof. □

Finally, we explain how to prove Theorem 1.7.

Proof of Theorem 1.7. The result follows immediately from Theorem 1.2, however it remains to prove that the result only requires $K \in C^{k-2s+\gamma}(\mathbb{S}^{n-1})$ if $\Omega = \{x_n = 0\}$. First of all, we recall the Hölder estimate (see Corollary 5.4), which holds true without any regularity assumption on K if $k = 0$. For the Liouville theorem (see Theorem 5.1), we only require $K \in C^{k-1-s+\gamma+\delta}(\mathbb{S}^{n-1})$ for an arbitrarily small $\delta > 0$ and $k-1-s+\gamma < k-2s+\gamma$. In Lemma 6.1, additional regularity for K is assumed in order to apply Corollary 2.5. However, if $\Omega = \{x_n > 0\}$, we have

$$L(d^{s-1}Q) = L((x_n)_+^{s-1}Q) \overset{k-1}{=} 0 \quad \text{in } \{x_n > 0\}$$

for any $Q \in \mathcal{P}_k$. Hence, in case $k = 1$ and $\gamma < s$, the proof goes through exactly as before, without any restrictions on K. If $k \ge 2$ or $\gamma > s$, (6-13) needs to be interpreted as an equation up to a polynomial, but the rest of the proof remains the same. Moreover, we apply the Hölder estimate (see Corollary 5.4), which would force us to impose $K \in C^{k-1}(\mathbb{S}^{n-1})$ in case $k \ge 2$ or $\gamma > s$. Therefore, in this case, we need to proceed a little differently. Indeed, we replace the computation in (6-8) by the following estimate, based on polar coordinates (see also (5-3)) for $\eta = 1 + \gamma - s - \lceil \gamma - s \rceil + \delta$ for some very small $\delta > 0$:

$$\begin{aligned} \big\| (x_n)_+^{s-1} w_m |\cdot|^{-n-2s-(k-2+\lceil\gamma-s\rceil+\eta)} \big\|_{L^1(\mathbb{R}^n \setminus B_R)} &\le c \int_{\mathbb{R}^n \setminus B_R} (x_n)_+^{s-1} |x|^{-n-2s-\lceil\gamma-s\rceil+2+\gamma+\eta} \,\mathrm{d}x \\ &\le c \int_0^{2\pi} \cos(\theta)_+^{s-1} \left(\int_R^\infty r^{s-1} r^{-1-2s-\lceil\gamma-s\rceil+2+\gamma+\eta} dr \right) \mathrm{d}\theta \\ &= c \int_0^{2\pi} \cos(\theta)_+^{s-1} \left(\int_R^\infty r^{-1-\delta} dr \right) \mathrm{d}\theta \le c R^{-\delta} \to 0, \end{aligned}$$

as $R \to \infty$. Then, we can apply Corollary 5.4 with $k := k-1$ and $\delta := \eta$ and only need to assume that $K \in C^{k-2+\eta}(\mathbb{S}^{n-1})$, which is fine by the same reasoning as for the Liouville theorem above. Moreover, the stability theorem (see Lemma 2.13) can still be applied since $k - 2 + \eta \le k - 1$ if we choose $\delta < s - \eta$.

Finally, the proof of Theorem 1.2 relies on an application of the interior regularity result (see Lemma 2.10). In case $k = 1$ and $1 + \gamma \le 2s$, we apply Lemma 2.10(i), so in this case, no regularity assumption on K is required, at all. In case $1 + \gamma > 2s$, we apply Lemma 2.10(ii) with $\alpha := k + \gamma - 2s$ (and interpret the equation up to a polynomial of degree $k - 1$, which is possible due to Remark 2.11), so in this case, we need to assume only that $K \in C^{k-2s+\gamma}(\mathbb{S}^{n-1})$, as desired. □

7. Nonlocal equations with local Dirichlet boundary conditions

Finally, we give the proof of the boundary regularity for nonlocal equations with Dirichlet boundary conditions (see Theorem 1.4).

Proof of Theorem 1.4. Let us first extend h in such a way that $h \in C^{k+\gamma}(\mathbb{R}^n)$. Then, we define $w := v - d^{s-1}h$ and observe that w solves

$$\begin{cases} Lw = \tilde{f} & \text{in } \Omega, \\ w = 0 & \text{in } \mathbb{R}^n \setminus \Omega, \\ w/d^{s-1} = 0 & \text{on } \partial\Omega, \end{cases}$$

where $\tilde{f} := f - L(d^{s-1}h)$. Moreover, for $x_0 \in \Omega$ an application of Corollary 2.5 yields $|\tilde{f}(x_0)| \le c_1 d^{\gamma-s}(x_0)$ in case $k+\gamma < 1+s$, as well as $[\tilde{f}]_{C^{k-1-s+\gamma}(\overline{\Omega})} \le c_2$ in case $k+\gamma > 1+s$, and also $[\tilde{f}]_{C^{k-2s+\gamma}(B_{d(x_0)/2}(x_0))} \le c_3 d^{s-1}(x_0)$ in case $k+\gamma > 2s$. Since $w/d^{s-1} = 0$ on $\partial\Omega$, by the maximum principle (see Proposition 1.3) and a barrier argument (see for instance the proof of [Fernández-Real and Ros-Oton 2024a, Lemma 2.3.9], using the barrier from [Fernández-Real and Ros-Oton 2024a, Lemma 2.3.10] in case $k+\gamma > 1+s$ and the barrier $\widetilde{\psi}$ from the second claim in Lemma 2.7 in case $k+\gamma < 1+s$) it holds that $w \in L^\infty(\Omega)$ and

$$\|w\|_{L^\infty(\Omega)} \le C\|d^{s-\gamma}\tilde{f}\|_{L^\infty(\Omega)}. \tag{7-1}$$

Thus w is a solution in the setting of [Ros-Oton and Serra 2017; Abatangelo and Ros-Oton 2020]. We assume without loss of generality

$$\|w\|_{L^\infty(\Omega)} + \|d^{s-\gamma}\tilde{f}\|_{L^\infty(\overline{\Omega})}\mathbb{1}_{\{k+\gamma<1+s\}} + \|\tilde{f}\|_{C^{k-1-s+\gamma}(\Omega)}\mathbb{1}_{\{k+\gamma>1+s\}} \le 1.$$

Then, [Ros-Oton and Serra 2017; Abatangelo and Ros-Oton 2020] imply that for any $z \in \partial\Omega$ there exists a polynomial $Q_z \in \mathcal{P}_{k-1}$ such that

$$|w(x) - Q_z(x)d^s| \le c|x-z|^{k-1+\gamma+s} \le c|x-z|^{k+\gamma}d^{s-1}(x) \quad \text{for all } x \in B_1(z).$$

By adjusting the proof of [Ros-Oton and Serra 2017, Proposition 3.2] in case $k+\gamma < 1+s$, or the second part of the proof of [Abatangelo and Ros-Oton 2020, Proposition 4.1] in case $k+\gamma > 1+s$, respectively, according to the slight modification of the upper bound in the previous estimate, we get that for any $x_0 \in \Omega \cap B_1(z)$, letting $r := d(x_0)$,

$$\|w - Q_z d^s\|_{L^\infty(B_{r/2}(x_0))} \le cr^{k+\gamma+s-1}, \quad [w - Q_z d^s]_{C^{k+\gamma}(B_{r/2}(x_0))} \le cr^{s-1}. \tag{7-2}$$

Indeed, while the first estimate is immediate from the expansion, the second result follows by letting

$$v_r(x) = r^{-k-\gamma}\big(u(x_0+rx) - Q_z(x_0+rx)d^s(x_0+rx)\big),$$

and observing that by the previous estimate and the properties of $\tilde{f}$ it holds that

$$\|v_r\|_{L^\infty(B_R)} \le c(1+r^{s-1}) \quad \text{for all } R > 0, \qquad [\tilde{f}]_{C^{k+\gamma-2s}(B_{r/2}(x_0))}\mathbb{1}_{\{k+\gamma>2s\}} \le cr^{s-1}.$$

Plugging these findings into the remainder of [Ros-Oton and Serra 2017, proof of Theorem 1.2; Abatangelo and Ros-Oton 2020, proof of Theorem 1.4], we obtain (7-2). From there we can show, using Hölder interpolation, and also $d \in C^{k+1+\gamma}(\overline{\Omega})$, that for any $\delta \in (0, k+\gamma]$ it holds that

$$[w - Q_z d^s]_{C^\delta(B_{r/2}(x_0))} \le c r^{k+\gamma+s-1-\delta}, \quad \|d^{1-s}\|_{L^\infty(B_{r/2}(x_0))} \le c r^{1-s}, \quad [d^{1-s}]_{C^\delta(B_{r/2}(x_0))} \le c r^{1-s-\delta}.$$

Thus, proceeding in a similar way as in the proof of Theorem 1.2, and using (7-2) as well as the previous estimate, we obtain

$$\begin{aligned}\left[\frac{w}{d^{s-1}} - Q_z d\right]_{C^{k+\gamma}(B_{r/2}(x_0))} &= [D^k(d^{1-s}(w - Q_z d^s))]_{C^\gamma(B_{r/2}(x_0))} \\ &\le \sum_{|\beta|=k}\sum_{\alpha\le\beta}[(\partial^\alpha d^{1-s})(\partial^{\beta-\alpha}(w - Q_z d^s))]_{C^\gamma(B_{r/2}(x_0))} \\ &\le \sum_{|\beta|=k}\sum_{\alpha\le\beta}\big(\|\partial^\alpha d^{1-s}\|_{L^\infty(B_{r/2}(x_0))}[\partial^{\beta-\alpha}(w - Q_z d^s)]_{C^\gamma(B_{r/2}(x_0))} \\ &\qquad\qquad + [\partial^\alpha d^{1-s}]_{C^\gamma(B_{r/2}(x_0))}\|\partial^{\beta-\alpha}(w - Q_z d^s)\|_{L^\infty(B_{r/2}(x_0))}\big) \\ &\le c\sum_{|\beta|=k}\sum_{\alpha\le\beta}\big(r^{1-s-|\alpha|}r^{s-1+|\alpha|} + r^{1-s-|\alpha|-\gamma}r^{\gamma+s-1+|\alpha|}\big) \le c.\end{aligned}$$

From here, by a covering argument, and using the continuity of the extension operator,

$$\begin{aligned}\left\|\frac{v}{d^{s-1}}\right\|_{C^{k,\gamma}(\overline{\Omega})} &\le c\big(\|v - d^{s-1}h\|_{L^\infty(\mathbb{R}^n)} + \|f\|_{C^{k-1-s+\gamma}(\Omega)} + \|h\|_{C^{k+\gamma}(\partial\Omega)}\big) \\ &\le c(\|f\|_{C^{k-1-s+\gamma}(\Omega)} + \|h\|_{C^{k+\gamma}(\partial\Omega)}).\end{aligned}$$ □

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