DIFFRACTION FOR THE DIRAC-COULOMB PROPAGATOR

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Abstract. The Dirac equation in $\mathbb{R}^{1,3}$ with potential Z/r is a relativistic field equation modeling the hydrogen atom. We analyze the singularity structure of the propagator for this equation, showing that the singularities of the Schwartz kernel of the propagator are along an expanding spherical wave away from rays that miss the potential singularity at the origin, but also may include an additional spherical wave of *diffracted* singularities emanating from the origin. This diffracted wavefront is $1-\epsilon$ derivatives smoother than the main singularities, for all $\epsilon > 0$, and is a conormal singularity.

1. Introduction

In this paper we study the structure of the propagator for the Dirac–Coulomb equation on $\mathbb{R}^{1,3}$. This equation, a description of the hydrogen atom with a relativistic electron, was explicitly solved by Darwin [11] in 1928 using separation of variables, giving a mode-by-mode description of the solutions with the radial functions defined by infinite series. Such an approach, while computationally useful for the spectral theory of the hydrogen atom, yields little concrete information about the structure of the Schwartz kernel of the propagator.

In this paper we derive the following results about the structure of the propagator. Notation involving the Dirac equation will be explained in detail below. Let η denote the (mostly plus) Minkowski metric on $\mathbb{R}^4$, whose coordinates are $t \equiv x^0, x^1, x^2, x^3$. Let $r = r(x) \equiv \left((x^1)^2 + (x^2)^2 + (x^3)^2\right)^{1/2}$ denote radius in the space coordinates.

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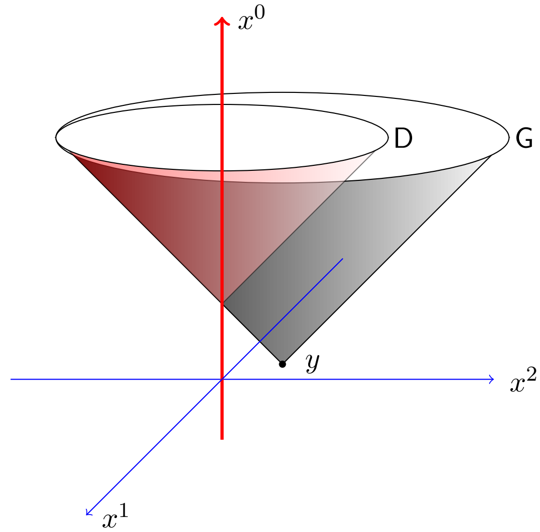

FIGURE 1. The "geometric" (G) and "diffracted" (D) wavefronts for the fundamental solution with initial pole at y. Note that the main and diffracted fronts intersect along a single ray, the continuation of the null geodesic from y straight through the potential singularity.

Theorem 1. *Consider a real-valued vector potential* $\mathbf{A} = (A_0 = \mathsf{Z}/r + V, A_1, A_2, A_3)$ *with* $V, A_1, A_2, A_3 \in C^\infty(\mathbb{R}^3)$*, and let* $m, \mathsf{Z} \in \mathbb{R}$*, with* $|\mathsf{Z}| < 1/2$.

Let ψ *be the admissible fundamental solution of the Dirac equation minimally coupled to the electric potential* V*:*

$$\big(i\big(\gamma_0(\partial_0 + iA_0) + \gamma_j(\partial_j + iA_j)\big) - m\big)\psi = 0,$$

with initial condition

$$\psi_{x^0=0} = \psi_0 \delta_y$$

for some four-spinor ψ_0 *and point* $y \in \mathbb{R}^3$.

For $x^0 > r(y)$,

$$\mathrm{WF}\,\psi \subset \mathsf{G} \cup \mathsf{D}$$

with $\mathsf{G} = N^*\{\eta_{\alpha\beta}(x^\alpha - y^\alpha)(x^\beta - y^\beta) = 0\}$ *given by the "geometric" (i.e., directly propagated) light cone emanating from* y *and* $\mathsf{D} = N^*\{r(x) = x^0 - r(y)\}$ *a secondary "diffracted" wavefront. The singularity on* $\mathsf{D}\backslash\mathsf{G}$ *is conormal and is* $1 - 0$ *derivatives smoother than the singularity at* G.

(Here, as throughout the paper, we use the notation $a - 0$ to mean "$a - \epsilon$ for all $\epsilon > 0$.") The notion of admissibility of solutions, which simply refers to lying in the scale of energy spaces defined by the self-adjoint Hamiltonian, is defined in §4.2 below.

The proof uses tools originally developed for the analysis of diffraction by cone and edge singularities [32], [30]. In particular, the analysis proceeds in two main steps:

(1) We show that the singularities of ψ can at most lie in $\mathsf{G} \cup \mathsf{D}$. This proceeds by a positive commutator argument using commutants in Melrose's b-calculus of pseudodifferential operators, inspired by the methods of Vasy [42].
(2) We show that the diffracted singularity is conormal and weaker than the main front. This uses methods of Melrose and the second author from [32], involving Mazzeo's edge calculus of pseudodifferential operators, and a propagation of module regularity (as employed by Melrose–Vasy–Wunsch [30])) to obtain both the conormality and the regularity of the diffracted front.

The Dirac–Coulomb equation describes spin-$\frac{1}{2}$ particles (such as electrons and positrons) in the presence of a point charge Z. Much of the literature about the Dirac–Coulomb system and related operators focuses on characterizing its eigenvalues and eigenstates. This description is unfortunately insufficient to describe diffractive phenomena. Darwin [11] used separation of variables to characterize the generalized eigenfunctions of the exact Dirac–Coulomb system in terms of confluent hypergeometric functions and spinor spherical harmonics. One could in principle derive our theorem in that setting by a careful analysis of the special functions but to our knowledge this has not been done.

Kato in his book [21] provided one of the first results showing that the Hamiltonian governing the evolution of the Dirac–Coulomb system is essentially self adjoint in the range $|\mathsf{Z}| < 1/2$ (corresponding to atomic charge less than 68.5). Weidmann [44] extended this result to $|\mathsf{Z}| < \sqrt{3}/2$; beyond this value of Z the Hamiltonian is no longer self-adjoint. We provide in Section 4.1 another proof of the essential self-adjointness in this optimal range.

Other interest in the Dirac–Coulomb system as an evolution equation has come from the dispersive equations community. Their work has largely focused on proving dispersive and Strichartz estimates for solutions by treating the components as solving systems of coupled wave equations. We mention here the work of D'Ancona and collaborators [5, 6, 10] as well as the work of Cacciafesta–Séré [7] and Erdoğan–Green–Toprak [13].

There is now a significant body of work describing the propagation of singularities on singular spaces, where diffraction occurs; the problem of the wave equation on conic manifolds (or the wave equation with an inverse square potential) is the singular setting most closely resembling the Dirac–Coulomb problem. The first diffraction problems were rigorously analyzed by Sommerfeld [37], with many other examples subsequently studied by Friedlander [14] and Keller [23]. The use made by these authors of separation of variables and Bessel function analysis was generalized to cones of arbitrary cross section by Cheeger–Taylor [8, 9], who established the analogous result to Theorem 1 in the setting of “product cones,” where the metric on the link does not vary with the radius. The non-product situation, where scaling invariance in r is lost, requires different methods, and in consequence the b-pseudodifferential analysis used in this paper can be viewed as a continuation of a line of work beginning with Melrose–Sjöstrand [28, 29], Melrose [27], and Taylor [40] describing the propagation of singularities on manifolds with smooth boundary. Melrose and the second author [32] used such commutator methods to generalize the results of Cheeger–Taylor to the non-product setting (see also Qian [35] in the case of inverse square potentials). This work was expanded to include corners and edge singularities by Vasy [42] and Melrose–Vasy–Wunsch [31], [30]. The functional framework for our estimates is especially inspired by Vasy’s work.

One of the original applications for the careful analysis of singularity propagation was to the problem of wave decay. Indeed, in certain settings Lax–Phillips [24] and Vainberg [41] (later generalized by Tang–Zworski [39]) provided a blueprint for obtaining decay estimates on “perturbations” of odd-dimensional Euclidean spaces from propagation estimates using as input the weak Huygens principle, which dictates that a solution with compactly supported Cauchy data eventually becomes smooth in a fixed compact set. More recent approaches to wave decay applying to spacetimes with ends that are not flat Minkowski space (again following the work of Vasy [43]) give new ways to extract decay rates for solutions of wave equations from propagation estimates. Work of the authors and Vasy [3, 4] and the first author and Marzuola [2] use related techniques to describe the radiation field on asymptotically Minkowski spaces and on product cones, respectively. Similar techniques played a key role in the work of Hintz–Vasy [18] establishing the global stability of the Kerr–de Sitter spacetime.

We thus hope to use the results obtained here to study the decay rates and asymptotics of the Dirac equation with one or more Coulomb-type singularities. Additionally, there are potential applications of our results to quantum field theory, viz., the construction of Hadamard states for the Dirac–Coulomb problem (see, e.g., [15]). These physically acceptable states are characterized by their wavefront sets, with the separation between $\tau \gtrless 0$ components (with τ dual to t) playing an essential role.

Even though the square of the Dirac–Coulomb system is principally scalar, the Dirac–Coulomb problem poses a number of difficulties not present with scalar wave equations on singular backgrounds. Many of these can be described in terms of the form of the second order equation obtained by (approximately) squaring the system (described in Section 4.3 below). In the case of the exact Dirac–Coulomb system, this second order operator has the form

$$-(\partial_t + i\frac{\mathsf{Z}}{r})^2 - \Delta - m^2 - i\frac{\mathsf{Z}}{r^2}\begin{pmatrix} 0 & \sigma_r \\ \sigma_r & 0 \end{pmatrix},$$

where Δ is the (positive) Laplacian on $\mathbb{R}^3$ and σ_r are 2×2 Pauli-type matrices that square to the identity. The equation differs from the Klein–Gordon equation in two significant ways. The first way is that the potential is coupled via the "minimal coupling" formalism, which introduces cross terms of the form $\frac{\mathsf{Z}}{r}D_t$; this does not present much additional difficulty, although it does need to be controlled in the b-calculus propagation arguments. More significant is the second difference, namely the order zero term

$$-i\frac{\mathsf{Z}}{r^2}\begin{pmatrix} 0 & \sigma_r \\ \sigma_r & 0 \end{pmatrix}.$$

As the Hardy inequality on $\mathbb{R}^3$ suggests that factors of $1/r$ should be treated as *derivatives*, this term is principal from the point of view of scaling. Moreover, it is anti-self-adjoint and cannot have a sign because σ_r has eigenvalues ± 1. Dealing with it directly can cause significant headaches. In trying to prove the diffractive theorem (Theorem 21 below) for the second order equation, this anti-self-adjoint term creates what should be viewed as the top order term and cannot be controlled by the positive terms in the commutator estimate. This term even makes global energy estimates difficult, as the derivative of the energy can no longer be controlled by the energy.

The complications of the Klein–Gordon system suggest that one ought to work with the first order system directly. On the other hand, the "energy estimates" obtained via the first order system are not as simple to work with as those arising from the second order equation. We therefore use both equations in this paper. For the elliptic part of the diffractive theorem (Section 5.2.2) and the geometric improvement (Section 6.1) we work with the second order equation, but for the "hyperbolic" part of the diffractive theorem (Section 5.2.3) we work directly with the first order equation.

In Section 2 we introduce the Dirac–Coulomb equation and fix some notation. Section 3 provides an introduction to the b- and edge-pseudodifferential calculi and describes the interaction of the b-calculus with differential operators on $\mathbb{R}^3$. In Section 4 we return to the equation and provide some preliminary results: we show that the Hamiltonian governing the evolution is essentially self-adjoint for $|\mathsf{Z}| < \sqrt{3}/2$, discuss the available energy estimates, introduce the second order operator, and describe how singularities propagate away from the origin. Sections 5 and 6 are the heart of the paper; Section 5 proves the diffractive theorem in which we show that singularities propagating through the origin must lie on the union of the diffracted and propagated fronts and Section 6 shows that the singularity along the diffracted front is $1-0$ orders smoother than along the propagated one.

2. The Dirac–Coulomb equation

2.1. **Notation.** We use coordinates x^α, $\alpha = 0, \dots, 3$ on $\mathbb{R}^{1,3}$; when referring to spatial coordinates (indices $1, 2, 3$) we use Latin rather than Greek superscripts. When appropriate, we employ the notation $t = x^0$ and use polar coordinates $r \in (0, \infty)$, $\theta \in S^2$ in the spatial variables. Below and in what follows, we use $\mathbf{A}$ to denote an electromagnetic potential with A_μ its components, i.e., $\mathbf{A} = (A_0, A_1, A_2, A_3)$. We are most interested in the case when A_0 has Coulomb-like singularities; in this case we write

$$A_0 = \frac{\mathsf{Z}}{r} + V,$$

where $V \in \mathcal{C}^\infty$.

The Dirac operator on $\mathbb{R}^{1,3}$ is given by

$$\partial\!\!\!/ = \gamma^\alpha \partial_\alpha,$$

where γ^α are the 4×4 matrices

$$\gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix},$$

and

$$\gamma^j = \begin{pmatrix} 0 & \sigma_j \\ -\sigma_j & 0 \end{pmatrix},$$

and σ_j are the Pauli matrices,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The γ matrices satisfy the anticommutation relation[1]

$$\gamma^\alpha \gamma^\beta + \gamma^\beta \gamma^\alpha = -2\eta^{\alpha\beta} \operatorname{Id}_4,$$

where $\eta^{\alpha\beta}$ are the components of the Minkowski metric, i.e.,

$$\eta^{\alpha\beta} = \begin{cases} -1 & \alpha = \beta = 0 \\ 1 & \alpha = \beta \in \{1, 2, 3\} \\ 0 & \alpha \neq \beta \end{cases}.$$

The free Dirac equation then reads

$$(i\partial\!\!\!/ - m)\psi = 0. \tag{1}$$

With an electromagnetic potential $\mathbf{A} = (A_0, A_1, A_2, A_3)$, we replace $\partial\!\!\!/$ by

$$\partial\!\!\!/_{\mathbf{A}} \equiv \gamma^0(\partial_0 + iA_0) + \gamma^j(\partial_j + iA_j);$$

this is the "minimal coupling" convention.

Other notational conventions that we employ are as follows. We use a boldface Greek letter (such as $\boldsymbol{\sigma}$) to denote the associated 3-vector of matrices (such as $(\sigma_1, \sigma_2, \sigma_3)$). We then set

$$\boldsymbol{\Sigma} \equiv \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}. \tag{2}$$

[1]Readers consulting other references should be aware that there are at least two conventions in the literature. Indeed, many physics texts (e.g., Akhiezer and Berestetsky [1] and Rose [36]) ask that the gamma matrices satisfy a *Riemannian* anticommutation relation and then set $x_0 = ict$.

and, in keeping with physics notation, we also write

$$\beta = \gamma^0,$$

and let $\boldsymbol{\alpha}$ be defined by

$$\boldsymbol{\gamma} = \beta\boldsymbol{\alpha},$$

hence

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}.$$

Letting

$$\gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} 0 & \mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix}, \tag{3}$$

we then obtain

$$\boldsymbol{\alpha} = \gamma_5\Sigma.$$

When using spherical coordinates, we will require radial versions of various of the matrix quantities discussed above. To this end, we set

$$\sigma_r = \sum_{j=1}^{3} \frac{\hat{x}_j}{|x|}\sigma_j,\ \alpha_r = \sum_{j=1}^{3} \frac{\hat{x}_j}{|x|}\alpha_j,\ \Sigma_r = \sum_{j=1}^{3} \frac{\hat{x}_j}{|x|}\Sigma_j, \tag{4}$$

2.2. **Spherical spinors and separation.** Let

$$\mathbf{L} = \mathbf{r} \times \mathbf{p},$$

where as usual

$$\mathbf{p} = \begin{pmatrix} i^{-1}\partial_{x^1} \\ i^{-1}\partial_{x^2} \\ i^{-1}\partial_{x^3} \end{pmatrix}.$$

Let

$$\mathbf{J} \equiv \mathbf{L} + \frac{1}{2}\boldsymbol{\Sigma}$$

denote the total angular momentum operators (orbital angular momentum and spin together.) Following Dirac, we also let

$$K = \beta(1 + \boldsymbol{\Sigma} \cdot \mathbf{L}).$$

Lemma 2. *Suppose A_0 is radial and $A_j = 0$. The following operators are mutually commuting:*

$$\not{\partial}_{\mathbf{A}},\ J^2,\ J_3,\ K.$$

Moreover,

$$[\beta, K] = 0.$$

(See e.g. [36], Section 12 for proofs.) In the case where the potential A_0 is exactly radial, we could separate variables explicitly and study the action of $\not{\partial}_{\mathbf{A}}$ on the common eigenfunctions of the remaining operators. Although we do not take this approach, we include a discussion of the eigenfunctions because some of the calculations below are easier to verify on individual eigenspaces. These eigenfunctions are well known to be described blockwise by two component spinor spherical harmonics as follows. Following e.g., [38], we set for $\theta \in S^2$

$$\Omega_{\kappa\mu}(\theta) = \begin{pmatrix} \operatorname{sgn}(-\kappa)\left(\frac{\kappa+1/2-\mu}{2\kappa+1}\right)^{1/2} Y_{l,\mu-1/2}(\theta) \\ \left(\frac{\kappa+1/2+\mu}{2\kappa+1}\right)^{1/2} Y_{l,\mu+1/2}(\theta) \end{pmatrix},$$

where

$$\kappa \in \mathbb{Z}\backslash\{0\}, \tag{5}$$

$$\mu \in \{-|\kappa| + 1/2, \dots, |\kappa| - 1/2\}, \tag{6}$$

$$l = \left|\kappa + \frac{1}{2}\right| - \frac{1}{2}, \tag{7}$$

and where Y_{lm} are the standard spherical harmonics (see [38, (2.1.9)–(2.1.10)] for normalization conventions). Then by [38, (3.2.3)], we obtain

$$(\boldsymbol{\sigma} \cdot \mathbf{L} + 1)\Omega_{\kappa\mu} = -\kappa\Omega_{\kappa\mu},$$

hence

$$K \begin{pmatrix} a\Omega_{\kappa\mu} \\ b\Omega_{\kappa'\mu'} \end{pmatrix} = \begin{pmatrix} -a\kappa\Omega_{\kappa\mu} \\ b\kappa'\Omega_{\kappa'\mu'} \end{pmatrix} \tag{8}$$

and eigenvectors of K are given by the span of

$$\begin{pmatrix} \Omega_{\kappa\mu} \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \Omega_{-\kappa\mu'} \end{pmatrix}, \ \mu, \mu' \in \{-|\kappa| + 1/2, \dots, |\kappa| - 1/2\};$$

the eigenvalue of K on this eigenspace is $-\kappa$. Note that

$$\Sigma_r \begin{pmatrix} a\Omega_{\kappa\mu} \\ b\Omega_{-\kappa\mu'} \end{pmatrix} = \begin{pmatrix} -a\Omega_{-\kappa\mu} \\ -b\Omega_{\kappa\mu'} \end{pmatrix}, \tag{9}$$

where Σ_r is defined in (4) above.

We further record here the relationship between K and Δ_θ:

$$\Delta_\theta = K^2 - \beta K.$$

This follows from the identity (see Rose [36]):

$$(\Sigma \cdot \mathbf{A})(\Sigma \cdot \mathbf{B}) = \mathbf{A} \cdot \mathbf{B} + i\Sigma \cdot (\mathbf{A} \times \mathbf{B}).$$

Applying this to $\Sigma \cdot \mathbf{L}$ yields

$$(\Sigma \cdot \mathbf{L})^2 = \Delta_\theta - \Sigma \cdot \mathbf{L},$$

so that

$$K^2 = (\Sigma \cdot \mathbf{L} + 1)^2 = \Delta_\theta + \Sigma \cdot \mathbf{L} + 1 = \Delta_\theta + \beta K. \tag{10}$$

In particular, note that

$$[\Delta_\theta, K] = [K^2 - \beta K, K] = 0,$$

i.e., K commutes with Δ_θ.

We now describe the separation of variables for a stationary Dirac equation: The massive Dirac equation with an electromagnetic potential $\mathbf{A} = (A_0, A_1, A_2, A_3)$ reads

$$(i\partial\!\!\!/_{\mathbf{A}} - m)\psi \equiv \big(i\big(\gamma^0(\partial_0 + iA_0) + \gamma^j(\partial_j + iA_j)\big) - m\big)\psi = 0,$$

hence multiplying by $\beta \equiv \gamma^0$ we obtain

$$\big(\big(i(\partial_0 + iA_0) + i\beta\gamma^j(\partial_j + iA_j)\big) - m\beta\big)\psi = 0,$$

i.e.,

$$\eth\psi \equiv \big(i(\partial_0 + iA_0) + i\alpha_j(\partial_j + iA_j) - m\beta\big)\psi \equiv i\partial_t\psi - \mathcal{B}\psi = 0, \tag{11}$$

where this is taken as a definition of the operator $\eth$ and

$$\mathcal{B} \equiv \sum_{j=1}^{3} \alpha_j \frac{1}{i}(\partial_j + iA_j) + A_0 + m\beta;$$

here we have, exceptionally, written out the summation explicitly here to remind the reader that it is only over spatial indices $1, 2, 3$.

Thus we are concerned with the unitary group generated by the operator $\mathcal{B}$.

Now we compute, in the notation of [36],

$$\begin{aligned}
\boldsymbol{\alpha} \cdot \frac{1}{i}\nabla &= \boldsymbol{\alpha} \cdot \mathbf{p} \\
&= \gamma^5 \boldsymbol{\Sigma} \cdot \mathbf{p} \\
&= \gamma^5 \boldsymbol{\Sigma}_r \left(\frac{1}{i}\partial_r + \frac{i}{r}\boldsymbol{\Sigma} \cdot \mathbf{L}\right) \\
&= -i\alpha_r \left(\partial_r - \frac{1}{r}(\beta K - \mathrm{Id})\right) \\
&= -i\alpha_r \left(\partial_r + \frac{1}{r} - \frac{1}{r}\beta K\right).
\end{aligned}$$

More detail for the above calculation can be found in Rose [36, p. 158, eq (2.47)].

Thus, finally, in polar coordinates,

$$\mathcal{B} = \big(-i\alpha_r \left(\partial_r + \frac{1}{r} - \frac{1}{r}\beta K\right) + A_0 + \sum \alpha_j A_j + m\beta\big). \tag{12}$$

3. b- and edge-geometry

Owing to the need to microlocalize solutions finely at the potential singularity, it is natural to introduce a new space obtained by *blowup* from our Minkowski space. In the simple case under consideration here, the blowup amounts to substituting the space

$$X \equiv [\mathbb{R}^3; \{0\}] \equiv [0, \infty)_r \times S^2_\theta$$

for the Euclidean space $\mathbb{R}^3$, with the *blowdown map*

$$\mathfrak{b}\colon X \to \mathbb{R}^3$$

being the polar coordinate map $(r,\theta) \to r\theta$; this is a diffeomorphism away from the boundary $r = 0$ (which is referred to as the *front face* of the blowup). We will use the same notation for the blowdown map in the full Minkowski space, where we introduce polar coordinates in spatial variables only, hence set

$$M \equiv [\mathbb{R}^{1,3}; \mathbb{R} \times \{0\}] \equiv \mathbb{R}_t \times X.$$

Both X and M are manifolds with boundary. (That they are noncompact as well will play no essential role in our analysis, owing to the local nature of the propagation of singularities.) We will need to consider two separate calculi of pseudodifferential operators on M, yielding microlocalizations of two different Lie algebras of vector fields. The first, Melrose's *b-calculus* [33], contains as first order operators the vector fields tangent to the boundary of M. The second, Mazzeo's *edge calculus* [26], contains instead the vector fields that are *tangent to the fibers of the blowdown map* as well as to the boundary, hence in particular, we obtain $r\partial_t$ rather than ∂_t in the latter calculus. We describe the important features of these two calculi below.

3.1. b-calculus.

Full technical details on the b-calculus can be found in the book of Melrose [33]; see also the introductory article by Grieser [17].

The space of *b-vector fields*, denoted $\mathcal{V}_{\mathrm{b}}(M)$, is the vector space of vector fields on M tangent to ∂M; they are spanned over $C^\infty(M)$ by the vector fields $r\partial_r$, ∂_t, and ∂_θ. We note that $r\partial_r$ is well-defined, independent of choices of coordinates, modulo $r\mathcal{V}_{\mathrm{b}}(M)$; one may call this the *b-normal vector field* to the boundary. One easily verifies that $\mathcal{V}_{\mathrm{b}}(M)$ forms a Lie algebra. The set of b-differential operators, $\mathrm{Diff}^*_{\mathrm{b}}(M)$, is the universal enveloping algebra of this Lie algebra: it is the filtered algebra consisting of operators of the form

$$A = \sum_{|\alpha|+j+k\leq m} a_{j,k,\alpha}(r,t,\theta)(rD_r)^j D_t^k D_\theta^\alpha \in \mathrm{Diff}^m_{\mathrm{b}}(M) \tag{13}$$

(locally near ∂M) with the coefficients $a_{j,k,\alpha} \in \mathcal{C}^\infty(M)$.

The b-pseudodifferential operators $\Psi^*_{\mathrm{b}}(M)$ are the "microlocalization" of this Lie algebra, formally consisting of (properly supported) operators of the form

$$b(r,t,\theta,rD_r,D_t,D_\theta)$$

with $b(r,t,\theta,\sigma,\tau,\eta)$ a Kohn-Nirenberg symbol.

The space $\mathcal{V}_{\mathrm{b}}(M)$ is in fact the space of sections of a smooth vector bundle over M, the *b-tangent bundle*, denoted ${}^{\mathrm{b}}TM$. The sections of this bundle are of course locally spanned by the vector fields $r\partial_r, \partial_t, \partial_\theta$. The dual bundle to ${}^{\mathrm{b}}TM$ is denoted ${}^{\mathrm{b}}T^*M$ and has sections locally spanned over $\mathcal{C}^\infty(M)$ by the one-forms $dr/r, dt, d\theta$.

The symbols of operators in $\Psi_{\mathrm{b}}^*(M)$ are thus Kohn-Nirenberg symbols defined on ${}^{\mathrm{b}}T^*M$. The principal symbol map, denoted σ_{b}, maps the classical subalgebra of $\Psi_{\mathrm{b}}^m(M)$ to homogeneous functions of order m on ${}^{\mathrm{b}}T^*M$. In the particular case of the subalgebra $\mathrm{Diff}_{\mathrm{b}}^m(M)$, if A is given by (13) we have

$$\sigma_{\mathrm{b}}(A) = \sum_{|\alpha|+j+k=m} a_{j,k,\alpha}(r,t,\theta)\sigma^j\tau^k\eta^\alpha$$

where σ, τ, η are "canonical" fiber coordinates on ${}^{\mathrm{b}}T^*M$ defined by specifying that the canonical one-form be

$$\sigma\frac{dr}{r} + \tau dt + \eta \cdot \frac{d\theta}{r}.$$

As homogeneous functions of a given order on $\mathbb{R}^n \setminus 0$ can be identified with smooth functions on S^{n-1}, we sometimes view σ_{b} as a smooth function on ${}^{\mathrm{b}}S^*M$.

We also identify a subalgebra of $\Psi_{\mathrm{b}}(M)$ that will be essential for the commutator argument in Section 5.

Definition 3. We say $A \in \Psi_{\mathrm{b}}^m(M)$ is *invariant* if it is scalar and invariant under the action of SO(3) on functions, i.e., if A is scalar and $R^{-1}AR = A$ for all $R \in \mathrm{SO}(3)$, where the action of SO(3) on functions is simply $Rf(x) = f(R^{-1}x)$.

Any scalar symbol invariant under the (lifted) action of SO(3) on ${}^{\mathrm{b}}T^*M$ may be quantized to an invariant operator.

Lemma 4. *Invariant operators commute with Δ_θ and K.*

Proof. Let A be invariant. For each $j \in \{1, 2, 3\}$, $[A, L_j] = 0$ since the flowout of L_j is in $SO(3)$. Since $\Delta = \mathbf{L} \cdot \mathbf{L}$ and $K = \beta(1 + \Sigma \cdot \mathbf{L})$ (and A is scalar) we obtain the desired commutation. □

Remark 5. Although invariant operators commute with Δ_θ and K, they *do not commute* with the matrices σ_r (defined in (4)). Because σ_r is independent of r, though, the terms arising from commuting an invariant operator with σ_r will be microsupported away from the characteristic set and so will be handled by the elliptic estimate in the course of the hyperbolic estimate of Section 5.2.3 below.

In addition to the principal symbol map, describing the leading order behavior of elements of $\Psi_{\mathrm{b}}^*(M)$ in terms of the filtration, there is a second map that measures the leading order behavior of the operators at the front face $r = 0$, and which, together with the principal symbol, measures the obstruction to compactness of b-operators. We will refer to this notion below only in the simple case of b-differential operators, where it is simple to describe, and we will work in just spatial variables on X rather than in spacetime. Then this extra symbol, which is operator-valued, is simply the new operator obtained by freezing coefficients of powers of b-vector fields at the boundary. If A is given by

$$\sum_{|\alpha|+j\leq m} a_{j,\alpha}(r,\theta)(rD_r)^j D_\theta^\alpha$$

we thus define the *indicial operator*

$$I(A) = \sum_{|\alpha|+j\leq m} a_{j,\alpha}(0,\theta)(rD_r)^j D_\theta^\alpha.$$

I is a homomorphism. Operators in the range of I, which in terms of r are now simply polynomials in (rD_r), are thus further simplified by Mellin transform in r, hence the same information is contained in the *indicial family*

$$I(A,\sigma) = \sum_{|\alpha|+j\leq m} a_{j,\alpha}(0,\theta)\sigma^j D_\theta^\alpha.$$

The *boundary spectrum* of A is then defined as

$$\operatorname{spec}_{\mathrm{b}}(A) = \{\sigma \in \mathbb{C}\colon I(A,\sigma) \text{ is not invertible on } \mathcal{C}^\infty(S^2)\}.$$

This set plays an important role in establishing the mapping properties of b-operators—see [33, Chapter 5]. It also is a key ingredient in the identification of the domain of the essentially self-adjoint Hamiltonian in Section 4.1 below.

Let $L^2_{\mathrm{b}}(M)$ denote the space of square integrable functions with respect to the *b-density*

$$\frac{dr}{r}\,dt\,d\theta.$$

Note in particular that this space differs from $L^2(M)$, which here denotes the space with the usual metric density, and in particular

$$L^2(M) = r^{-3/2}L^2_{\mathrm{b}}(M).$$

When emphasizing the use of the metric density, we will in fact write

$$L^2_g(M) \equiv L^2(M)$$

for added clarity. We let $H^m_{\mathrm{b}}(M)$ denote the Sobolev space of order m *relative to* $L^2_{\mathrm{b}}(M)$ corresponding to the algebras $\mathrm{Diff}^m_{\mathrm{b}}(M)$ and $\Psi^m_{\mathrm{b}}(M)$. In other words, for $m \geq 0$, fixing $A \in \Psi^m_{\mathrm{b}}(M)$ elliptic, one has $w \in H^m_{\mathrm{b}}(M)$ if $w \in L^2_{\mathrm{b}}(M)$ and $Aw \in L^2_{\mathrm{b}}(M)$; this is independent of the choice of the elliptic A. For m negative, the space is defined by duality. (For m a positive integer, one can alternatively give a characterization in terms of boundedness of elements of $\mathrm{Diff}^m_{\mathrm{b}}(M)$.) Let $H^{m,l}_{\mathrm{b}}(M) = r^l H^m_{\mathrm{b}}(M)$ denote the corresponding weighted spaces. We will also use all these notions on X rather than M, simply omitting the t variable. Sometimes it will be convenient to use the Sobolev spaces defined with respect to the *metric* density rather than the b density we have used here, and to that end we set (on either M or X)

$$H^m_{\mathrm{b},g} \equiv r^{-3/2}H^m_{\mathrm{b}}.$$

Associated to an operator $A \in \Psi_{\mathrm{b}}^m(M)$ is its *microsupport*,

$$\mathrm{WF}_{\mathrm{b}}'(A) \subset {}^{\mathrm{b}}S^*M.$$

This closed subset is the essential support of the total symbol, just as in the usual pseudodifferential calculus, and obeys the usual microlocality property

$$\mathrm{WF}_{\mathrm{b}}'(AB) \subset \mathrm{WF}_{\mathrm{b}}'(A) \cap \mathrm{WF}_{\mathrm{b}}'(B).$$

Conversely, there is a notion of *b-ellipticity* at a point, obtained from the invertibility of the principal symbol. Note that global ellipticity is not sufficient to make an operator Fredholm over a compact set in X; additional decay at $r = 0$ is required to ensure that the remainder term in a parametrix argument is compact.

While there is a notion of wavefront set (lying in ${}^{\mathrm{b}}S^*M$) associated to the b-calculus, we will require a slight variant of this wavefront set in our estimates, hence we postpone discussion of WF_{b} until we have introduced differential-b-pseudodifferential operators.

3.2. **Edge Calculus.** Full technical details on the edge calculus can be found in Mazzeo [26].

The space of *edge-vector fields*, denoted $\mathcal{V}_{\mathrm{e}}(M)$, is the vector space of vector fields on M tangent to ∂M as well as to the fibers of the fibration $\mathfrak{b} : M \to \mathbb{R}^4$; they are spanned over $C^\infty(M)$ by the vector fields $r\partial_r$, $r\partial_t$, and ∂_θ. Like the b vector fields, $\mathcal{V}_{\mathrm{e}}(M)$ forms a Lie algebra. The set of e-differential operators, $\mathrm{Diff}_{\mathrm{e}}^*(M)$, is the universal enveloping algebra of this Lie algebra: it is the filtered algebra consisting of operators of the form

$$A = \sum_{|\alpha|+j+k \leq m} a_{j,k,\alpha}(r, t, \theta)(rD_r)^j (rD_t)^k D_\theta^\alpha \in \mathrm{Diff}_{\mathrm{e}}^m(M) \tag{14}$$

(locally near ∂M) with the coefficients $a_{j,k,\alpha} \in \mathcal{C}^\infty(M)$.

The edge-pseudodifferential operators $\Psi_{\mathrm{e}}^*(M)$ are the "microlocalization" of this Lie algebra, formally consisting of (properly supported) operators of the form

$$b(r, t, \theta, rD_r, rD_t, D_\theta)$$

with $b(r, t, \theta, \xi, \tau, \eta)$ a Kohn-Nirenberg symbol. The (non-canonical) map from total symbols to operators will be denote Op_b.

For the commutator arguments below, we will require a doubly-filtered version of the edge calculus, where we also track variable growth or decay at $r = 0$. In particular, if we set

$$\Psi_{\mathrm{e}}^{m,l}(M) = r^{-l}\Psi_{\mathrm{e}}^m(M),$$

then this is a doubly filtered algebra. We remark that the operators that are residual in the sense of both decay and regularity are

$$\Psi_{\mathrm{e}}^{-\infty,-\infty}(M);$$

the reader is cautioned that different conventions exist in the literature for the sign convention on the l index.

The space $\mathcal{V}_{\mathrm{e}}(M)$ is in fact the space of sections of a smooth vector bundle over M, the *edge tangent bundle*, denoted ${}^{\mathrm{e}}TM$. The sections of this bundle are locally spanned by the vector fields $r\partial_r, r\partial_t, \partial_\theta$. The dual bundle to ${}^{\mathrm{e}}TM$ is denoted ${}^{\mathrm{e}}T^*M$ and has sections locally spanned over $\mathcal{C}^\infty(M)$ by the one-forms $dr/r, dt/r, d\theta$.

The symbols of operators in $\Psi_{\mathrm{b}}^*(M)$ are thus Kohn-Nirenberg symbols defined on ${}^{\mathrm{e}}T^*M$. The principal symbol map, denoted σ_{e}, maps the classical subalgebra of $\Psi_{\mathrm{e}}^{m,l}(M)$ to r^{-l} times homogeneous functions of order m on ${}^{\mathrm{b}}T^*M$. In the particular case of the subalgebra $\mathrm{Diff}_{\mathrm{e}}^{m,l}(M)$, if A is given by (14) we have

$$\sigma_{\mathrm{e}}(r^l A) = r^l \sum_{|\alpha|+j+k=m} a_{j,k,\alpha}(r,t,\theta)\xi^j\lambda^k\zeta^\alpha$$

where ξ, λ, ζ are "canonical" fiber coordinates on ${}^{\mathrm{e}}T^*M$ defined by specifying that the canonical one-form be

$$\xi\frac{dr}{r} + \lambda\frac{dt}{r} + \zeta\cdot d\theta$$

As before we let $L^2_{\mathrm{b}}(M)$ denote the space of square integrable functions with respect to the *b-density*

$$\frac{dr}{r}\,dt\,d\theta.$$

We let $H_{\mathrm{e}}^m(M)$ denote the Sobolev space of order m *relative to* $L^2_{\mathrm{b}}(M)$ corresponding to the algebras $\mathrm{Diff}_{\mathrm{e}}^m(M)$ and $\Psi_{\mathrm{e}}^m(M)$. In other words, for $m \geq 0$, fixing $A \in \Psi_{\mathrm{e}}^m(M)$ elliptic, one has $w \in H_{\mathrm{e}}^m(M)$ if $w \in L^2_{\mathrm{b}}(M)$ and $Aw \in L^2_{\mathrm{b}}(M)$; this is independent of the choice of the elliptic A. For m negative, the space is defined by duality. (For m a positive integer, one can alternatively give a characterization in terms of $\mathrm{Diff}_{\mathrm{e}}^m(M)$.) Let $H_{\mathrm{e}}^{m,l}(M) = r^l H_{\mathrm{e}}^m(M)$ denote the corresponding weighted spaces.

There is a notion of edge microsupport

$$\mathrm{WF}'_{\mathrm{e}}(A) \subset {}^{\mathrm{e}}S^*M,$$

as well as of edge ellipticity satisfying the usual properties.

We recall also that associated to the calculus $\Psi_{\mathrm{e}}^{*,*}(M)$ is associated a notion of Sobolev wavefront set: $\mathrm{WF}_{\mathrm{e}}^{m,l}(w) \subset {}^{\mathrm{e}}S^*M$ is defined only for $w \in H_{\mathrm{e}}^{-\infty,l}$ (since $\Psi_{\mathrm{e}}(M)$ is not commutative to leading order in the decay index); the definition is then $\alpha \notin \mathrm{WF}_{\mathrm{e}}^{m,l}(w)$ if there is $Q \in \Psi_{\mathrm{e}}^{0,0}(M)$ elliptic at α such that $Qw \in H_{\mathrm{e}}^{m,l}(M)$, or equivalently if there is $Q' \in \Psi_{\mathrm{e}}^{m,l}(M)$ elliptic at α such that $Q'w \in L^2_{\mathrm{b}}(M)$. See [32, Section 5] for a fuller list of the properties of the edge calculus and wavefront set.

3.3. **The differential-pseudodifferential** b**-calculus.** The crux of the proof of the diffractive theorem in Section 5 below lies in understanding the interaction between differential operators and the pseudodifferential b-calculus. A crucial ingredient below will be the *Hardy inequality*

Lemma 6. *If $u \in H^1(\mathbb{R}^n)$ with $n \geq 3$, then*

$$\frac{(n-2)^2}{4} \int \frac{|u|^2}{r^2}\, dx \leq \int |\nabla u|^2\, dx.$$

We will use this inequality in $\mathbb{R}^3$, where it reads

$$\|r^{-1}u\| \leq 2\|\partial_r u\|. \tag{15}$$

As the Dirac operator is not a b-operator, it is convenient to measure regularity with respect to the classical Sobolev space H^1, pulled back to X.

Lemma 7. *The pullback $\mathfrak{b}^*(H^1)$ agrees with $\mathcal{D} = r^1 H^1_{\mathrm{b},g} = r^{-1/2} H^1_{\mathrm{b}}$ locally near $r = 0$, and this pullback is injective.*

Proof. We take all functions below to be supported in the unit ball.

The injectivity of the pushforward is assured by the fact that for all $u \in H^1(\mathbb{R}^3)$, if $\chi(r)$ is a cutoff function equal to 1 for $r > 2$ and 0 for $r < 1$, the approximation $\chi(r/\epsilon)u$ converges to u in $H^1(\mathbb{R}^3)$ norm, i.e. elements supported away from the origin are dense in H^1, and it suffices to show that the pushforward is bounded above and below as a Hilbert space map when acting on these distributions. Since $\nabla u \sim (\partial_r u, r^{-1}\partial_\theta u)$, the H^1 norm of u is bounded by the $rH^1_{\mathrm{b},g}$ norm of $\mathfrak{b}^*u$; the Hardy inequality ensures that $\|r^{-1}\mathfrak{b}_*u\|_{L^2}$ is controlled by the H^1 norm of u, which then shows that the $rH^1_{\mathrm{b},g}$ norm of $\mathfrak{b}^*u$ is controlled by the H^1 norm of u. □

In Section 5, we let $H^1(M)$ be the closure in the $H^1(\mathbb{R}^{1+3})$ norm (identified via the blowdown $\mathfrak{b}$) of $\mathcal{C}^\infty_c(M)$. The lemma above can be rephrased as the statement that

$$H^1(M) = \mathfrak{b}^* H^1(\mathbb{R}^{1+3}),$$
$$H^1(X) = \mathfrak{b}^* H^1(\mathbb{R}^3).$$

In this paper we will only be dealing with functions compactly supported in a fixed (large) neighborhood of $x = 0$, and we note that on such functions,

$$\|D_t u\|^2 + \|D_r u\|^2 + \left\|r^{-1}\nabla_\theta u\right\|^2$$

is equivalent to $\|u\|^2_{H^1}$. We will use this equivalence heavily.

To facilitate the accounting of error terms in Section 5, we will use the terminology

$$A \in \mathrm{Diff}^m \Psi^s_{\mathrm{b}}$$

if

$$A = \sum_{j+k \leq m} r^{-j} D_r^k A_{j,k}$$

with $A_{j,k} \in \Psi^s_{\mathrm{b}}$. (Cf. [42, Definition 2.3]; here we allow powers of r^{-1} in addition to differentiations.) For such operators, we write

$$\mathrm{WF}'_{\mathrm{b}} A = \cup_{j,k} \mathrm{WF}'_{\mathrm{b}} A_{j,k}.$$

Vasy [42] made extensive use of these spaces of operators in the setting of manifolds with corners; many of the results below have analogues in that paper.

The following lemma from [30, Lemma 8.6] (cf. also [42, Lemma 2.8]) shows that $\mathrm{Diff}^*\Psi_{\mathrm{b}}^*$ forms an algebra.

Lemma 8. *Let $A \in \Psi_{\mathrm{b}}^m(M)$ and let $a = \sigma_{\mathrm{b}}(A)$. Then*

$$[D_r, A] = B + CD_r,$$

with

$$B \in \Psi_{\mathrm{b}}^m(M), \quad C \in \Psi_{\mathrm{b}}^{m-1}(M),$$
$$\sigma_{\mathrm{b}}(B) = \frac{1}{i}\partial_r a, \quad \sigma_{\mathrm{b}}(C) = \frac{1}{i}\partial_\sigma a;$$

moreover,

$$[r^{-1}, A] = r^{-1}C_R = C_L r^{-1},$$

where $C_\bullet \in \Psi_{\mathrm{b}}^{m-1}(M)$ with

$$\sigma_{\mathrm{b}}(C_\bullet) = \frac{1}{i}\partial_\sigma a.$$

As we will measure b-regularity with respect to H^1, we also need to know that Ψ_{b}^0 is bounded on this space.

Lemma 9. *Given $A \in \Psi_{\mathrm{b}}^0$, there is some $C > 0$ so that for all $u \in H^{\pm 1}$,*

$$\|Au\|_{H^{\pm 1}} \le C\|u\|_{H^{\pm 1}}.$$

Proof. We begin by proving boundedness on H^1. By Lemma 8, $[D_r, A] = S + TD_r$, where $S \in \Psi_{\mathrm{b}}^0$ and $T \in \Psi_{\mathrm{b}}^{-1}$, so that

$$\begin{aligned}\|D_r Au\|_{L^2_g} &\le \|AD_r u\|_{L^2_g} + \|[D_r, A]u\|_{L^2_g} \\ &\le \|AD_r u\|_{L^2_g} + \|Su\|_{L^2_g} + \|TD_r u\|_{L^2_g} \\ &\le C\left(\|D_r u\|_{L^2_g} + \|u\|_{L^2_g}\right) \le C\|u\|_{H^1}.\end{aligned}$$

Similarly, we may use Lemma 8 to write

$$\left[\frac{1}{r}D_\theta, A\right] = \frac{1}{r}\left[D_\theta, A\right] + \left[\frac{1}{r}, A\right] D_\theta = \frac{1}{r}S + T\left(\frac{1}{r}D_\theta\right),$$

where $S \in \Psi_{\mathrm{b}}^0$ and $T \in \Psi_{\mathrm{b}}^{-1}$, so that by the pseudodifferential calculus and the Hardy inequality we may bound

$$\left\|\frac{1}{r}D_\theta Au\right\|_{L^2_g} \le C\|u\|_{H^1}.$$

The boundedness on H^{-1} now follows by duality. □

The previous two lemmas then motivate a definition of H^1 (and H^{-1})-based b-wavefront set.

Definition 10. Let $u \in H^{\pm 1}(M)$. Let $\rho \in {}^{\mathrm{b}}T^*M\backslash o$. We define

$$\rho \notin \mathrm{WF}_{\mathrm{b}}^{\pm 1,m} u$$

if there exists $A \in \Psi_{\mathrm{b}}^m(M)$, elliptic at ρ, such that $Au \in H^{\pm 1}$.

Similarly, for $\rho \in {}^{\mathrm{b}}T^*M\backslash o$, we define

$$\rho \notin \mathrm{WF}_{\mathrm{b}}^{m} u$$

if there exists $A \in \Psi_{\mathrm{b}}^m(M)$, elliptic at ρ, such that $Au \in L^2_g$.

Remark 11. At this moment we provide the reader with two notes of caution: First, observe that we measure b-regularity with respect to L^2_g rather than L^2_{b}; we adopt this convention because it makes applications of the Hardy inequality more straightforward and allows us to avoid introducing the weighted b-calculus. Second, be aware that although $\mathrm{WF}_{\mathrm{b}}^{1,m}$ and $\mathrm{WF}_{\mathrm{e}}^{m,l}$ each have seem to have two superscripts, homologous indices have different meanings in these two objects. Indeed, one should think of $\mathrm{WF}_{\mathrm{b}}^{1,m}$ as having only the index m and therefore measuring Ψ_{b}^m-regularity *with respect to* H^1. On the other hand, $\mathrm{WF}_{\mathrm{e}}^{m,l}$ measures $\Psi_{\mathrm{e}}^{m,l}$-regularity with respect to L^2_{b} and thus has two indices corresponding to those of the edge algebra.

As with other pseudodifferential algebras, it is convenient to know that we can microlocalize our estimates:

Lemma 12. *If $A, G \in \Psi_{\mathrm{b}}^s$ with $\mathrm{WF}'_{\mathrm{b}} A \subseteq \mathrm{ell}\, G$, then for all u with*

$$\mathrm{WF}_{\mathrm{b}}^{\pm 1,s} u \cap \mathrm{WF}'_{\mathrm{b}} G = \emptyset,$$

we may bound

$$\|Au\|_{H^{\pm 1}} \leq C \left(\|Gu\|_{H^{\pm 1}} + \|u\|_{H^{\pm 1}} \right).$$

Proof. The proof is a standard microlocal elliptic parametrix argument: let $E \in \Psi_{\mathrm{b}}^{-s}$ with $\mathrm{WF}'_{\mathrm{b}} E \subseteq \mathrm{WF}'_{\mathrm{b}} G$ so that

$$R = \mathrm{I} - EG \in \Psi_{\mathrm{b}}^0, \quad \mathrm{WF}'_{\mathrm{b}} R \cap \mathrm{WF}'_{\mathrm{b}} A = \emptyset.$$

We may then write

$$Au = A(EG + R)u,$$

so that

$$\|Au\|_{H^{\pm 1}} \leq \|(AE)Gu\|_{H^{\pm 1}} + \|ARu\|_{H^{\pm 1}} \leq C \left(\|Gu\|_{H^{\pm 1}} + \|u\|_{H^{\pm 1}} \right).$$

□

In Section 5, we repeatedly use the algebra properties of $\mathrm{Diff}^* \Psi_{\mathrm{b}}^*$ and the following lemma to allow easy estimates on error terms by doing commutations freely.

Lemma 13. *Suppose $E \in \mathrm{Diff}^1 \Psi_{\mathrm{b}}^{s+r-1} + \Psi_{\mathrm{b}}^{s+r}$. There are pseudodifferential operators $A \in \Psi_{\mathrm{b}}^{s-1}$ and $B \in \Psi_{\mathrm{b}}^r$ with $\mathrm{WF}'_{\mathrm{b}} A \cup \mathrm{WF}'_{\mathrm{b}} B \subseteq \mathrm{WF}'_{\mathrm{b}} E$ so that for all $u \in H^1$ and $v \in L^2$ with $\mathrm{WF}'_{\mathrm{b}} E \cap (\mathrm{WF}_{\mathrm{b}}^{1,s-1} u \cup \mathrm{WF}_{\mathrm{b}}^{1,r-1} v) = \emptyset$,*

$$|\langle Eu, v \rangle| \leq C \left(\|Au\|_{H^1} \|Bv\|_{L^2_g} + \|u\|_{H^1} \|v\|_{L^2_g} \right).$$

Similarly, if $E \in \mathrm{Diff}^2\Psi_{\mathrm{b}}^{s+r-2}+\mathrm{Diff}^1\Psi_{\mathrm{b}}^{s+r-1}+\Psi_{\mathrm{b}}^{s+r}$*, we may find* $A \in \Psi_{\mathrm{b}}^{s-1}$ *and* $B \in \Psi_{\mathrm{b}}^{r-1}$ *so that*

$$|\langle Eu, v\rangle| \leq C\left(\|Au\|_{H^1}\|Bv\|_{H^1} + \|u\|_{H^1}\|v\|_{H^1}\right).$$

Proof. Let $T_{\pm r} \in \Psi_{\mathrm{b}}^{\pm r}$ be elliptic, self-adjoint b-operators which are inverses of one another modulo a smoothing error, so that $T_r T_{-r} = \mathrm{Id} + R$ with $R \in \Psi_{\mathrm{b}}^{-\infty}$. Setting $A = T_{-r}E$ and $B = T_r \in \Psi_{\mathrm{b}}^{r}$ finishes the proof. □

4. Analytic preliminaries

We return to the Dirac–Coulomb equation $(i\partial\!\!\!/_{\mathbf{A}} - m)u = 0$. In this section we discuss several preliminary results needed in the main proofs below.

4.1. Self-adjoint extension.

Recall that

$$M = [\mathbb{R}^{1+3}; \mathbb{R}_t \times 0_x]$$

denotes the blowup of our spacetime at the spatial origin, and

$$X = [\mathbb{R}^3; \times 0]$$

denotes its spatial cross section, with $\mathfrak{b}$ denoting the blowdown map in either case.

We shall abuse notation later on in confusing X with all of $\mathbb{R}^3$, but will begin by distinguishing these two spaces for the purposes of describing domains and Sobolev spaces precisely before proving that the confusion is safe.

We now examine the indicial roots of the formally self-adjoint operator $\mathcal{B}$ (defined in Section 2.1) where[2] $A_0 = \mathsf{Z}/r + V$ and $V, A_j \in \mathcal{C}^\infty$, i.e., the boundary spectrum given by the points of non-invertibility of $I(r\mathcal{B}, \xi)$.

By (12), if σ denotes the dual to rD_r in ${}^{\mathrm{b}}T^*X$,

$$I(r\mathcal{B}, \xi) = \mathsf{Z}\,\mathrm{Id} - i\gamma^5\Sigma_r\big(i\sigma + 1 - \beta K\big).$$

To study the equation $I(r\mathcal{B}, \xi)\psi = 0$ we split

$$\psi = \begin{pmatrix} \psi^u \\ \psi^l \end{pmatrix}$$

into upper and lower spinors, and, as above, expand each in the basis of spherical spinors of the form

$$\begin{pmatrix} \Omega_{\kappa\mu} \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \Omega_{-\kappa\mu'} \end{pmatrix}.$$

Thus, once again using (8), (9), we obtain

$$I(r\mathcal{B}, \xi)\begin{pmatrix} a\Omega_{\kappa\mu} \\ b\Omega_{\kappa'\mu'} \end{pmatrix} = \begin{pmatrix} a\mathsf{Z}\Omega_{\kappa\mu} - (\sigma - i + i\kappa)b\Omega_{\kappa'\mu'} \\ b\mathsf{Z}\Omega_{\kappa'\mu'} - (\sigma - i - i\kappa)a\Omega_{-\kappa\mu} \end{pmatrix}.$$

Hence there is only nullspace when

$$\mathsf{Z}^2 = \kappa^2 + (\sigma - i)^2,$$

[2]More generally, we remark that we can replace the smooth term by a term that is smooth on the blowup of the origin with no change in the arguments of this section.

i.e. when

$$\sigma = i \pm i\sqrt{\kappa^2 - \mathsf{Z}^2}.$$

Because κ takes values in $\mathbb{Z}\backslash\{0\}$, we can explicitly calculate these indicial roots for small values of Z. Indeed, if $|\mathsf{Z}| < \sqrt{3}/2$, we are assured that

$$\operatorname{Im} \operatorname{spec}_{\mathrm{b}}(r\mathcal{B}) \cap [1/2, 3/2] = \emptyset. \tag{16}$$

Now since[3]

$$\mathcal{B} : r^{-1/2} H^1_{\mathrm{b}}(X) \to r^{-3/2} L^2_b(X) = L^2_g(X)$$

is continuous, we certainly find that $r^{-1/2}H^1_{\mathrm{b}}(X)$ is contained in the minimal domain of $\mathcal{B}$. On the other hand, (16) implies by work of Lesch [25, Corollary 1.3.17] (see also Melrose [33, Chapter 5] for a parametrix construction, as well as Gil–Mendoza [16] for a general discussion of self-adjoint extensions of operators of this type) that the maximal and minimal domains must in fact coincide, hence $\mathcal{B}$ is essentially self-adjoint, with domain given by

$$\mathcal{D} = r^{-1/2} H^1_{\mathrm{b}}. \tag{17}$$

(Cf. [22, Theorem V.5.10, Remark V.5.12] for the essential self-adjointness of Dirac operators.)

Having established the self-adjointness of $\mathcal{B}$ with domain $\mathcal{D}$, we now define

$$\mathcal{D}^s = \operatorname{Dom}(\operatorname{Id} + \mathcal{B}^2)^{s/2},$$

with the powers of the operator being defined by the spectral theorem. Note that away from the origin, these simply agree with Sobolev spaces:

Lemma 14. *For all $s \in \mathbb{R}$*

$$\mathcal{D}^s \cap \mathcal{E}'(\mathbb{R}^3\backslash\{0\}) = H^s \cap \mathcal{E}'(\mathbb{R}^3\backslash\{0\}).$$

Proof. For s an even integer, the result follows inductively from the characterization of $\mathcal{D} = \mathcal{D}^1$, which does agree with H^1 away from the origin. Thus for any $\varphi \in \mathcal{C}^\infty_c(\mathbb{R}^3\backslash\{0\})$, whenever $\operatorname{Re} s \in 2\mathbb{N}$,

$$\varphi u \in \mathcal{D}^s \Longleftrightarrow (\operatorname{Id} + \Delta)^s \varphi u \in L^2, \tag{18}$$

since the pure imaginary powers of $(\operatorname{Id} + \mathcal{B}^2)$ and of $(\operatorname{Id} + \Delta^2)$ are both unitary. Then by interpolation and duality (18) holds for all s. □

4.2. **Admissible solutions and energy estimates.**

Definition 15. A solution to $(i\partial\!\!\!/_v - m)u = 0$ is *admissible* if it lies in

$$\mathcal{C}(\mathbb{R}; \mathcal{D}^s)$$

for some $s \in \mathbb{R}$.

[3]Recall that b-Sobolev spaces are by default defined with respect to the b-density rather than the metric density.

In the propagation theorems in this paper, we deal only with admissible solutions. Note that there is a unique admissible fundamental solution, since the initial data $\delta(x-x_0)$ lies in $\mathcal{D}^{-n/2-0}$ by Lemma 14.

Given Cauchy data $u_0 \in \mathcal{D}^s$, there exists a unique admissible solution

$$e^{-it\mathcal{B}}u_0$$

by Stone's theorem; the propagator is of course unitary on $\mathcal{D}^s$ for all $s \in \mathbb{R}$. More generally, we will have use for the following energy estimate:

Lemma 16. *Let u solve $(i\partial\!\!\!/_V - m)u = 0$ on $[t_0, t_1] \times X$ and lie in $\mathcal{C}^\infty(\mathbb{R}; \mathcal{D}^\infty)$. For any operator $Q : \mathcal{C}^\infty(\mathbb{R}; \mathcal{D}^\infty) \to \mathcal{C}^\infty(\mathbb{R}; \mathcal{D}^\infty)$,*

$$\frac{1}{2}\frac{d}{dt}\|Qu\|^2_{\mathcal{D}^s} = \operatorname{Re}\langle i[\mathcal{B}, Q]u, Qu\rangle_{\mathcal{D}^s}$$

Proof. This follows by self-adjointness of $\mathcal{B}$ and the definition of the $\mathcal{D}^s$ norm in terms of its powers. □

For purposes of shifting regularity of solutions up and down conveniently, we now define, for $s \in \mathbb{R}$, $\Theta_s \in \Psi^s(\mathbb{R})$ to be a parametrix for $\langle D_t\rangle^s$ whose Schwartz kernel is properly supported; thus $\Theta_s\Theta_{-s} - \mathrm{Id}$ is a smoothing operator with properly supported Schwartz kernel. We then note by t-translation invariance of the Dirac equation that if $u \in \mathcal{C}(\mathbb{R}; \mathcal{D}^k)$ is a solution to the Dirac equation, then (by ellipticity of the spatial part of the Dirac operator)

$$\Theta_s u \in \mathcal{C}(\mathbb{R}; \mathcal{D}^{k-s}) \cap H^{k-s}_{\mathrm{loc}}$$

is another solution (up to a smooth remainder), and

$$\Theta_{-s}\Theta_s u - u \in \mathcal{C}^\infty(\mathbb{R}; \mathcal{D}^\infty).$$

It is helpful in what follows to be able to pass freely among different notions of solution: viewing a solution as lying in locally $H^s(\mathbb{R} \times \mathbb{R}^3)$ is most natural in dealing with microlocal analysis away from $r = 0$, while the energy spaces $L^2(\mathbb{R}; \mathcal{D}^s)$ or $\mathcal{C}(\mathbb{R}; \mathcal{D}^s)$ are natural from the point of view of global energy estimates.

Lemma 17. *An admissible solution of the Dirac equation in $\mathcal{C}(\mathbb{R}; \mathcal{D}^s)$ lies in $H^s_{loc}(M^\circ)$.*

Proof. For such a solution (with all norms below local ones, for t in a finite interval, and over a compact set in the interior of X)

$$\Theta_s u \in \mathcal{C}(\mathbb{R}; L^2) \subset L^2,$$

hence

$$u \in H^s(\mathbb{R}; L^2) \cap L^2(\mathbb{R}; H^s) \subset H^s,$$

by the local Fourier characterization of Sobolev regularity (and since $|\tau|^s + |\zeta|^s \sim |(\tau, \zeta)|^s$ outside the unit ball). □

4.3. **Reduction to Klein–Gordon.** Some of the arguments below are considerably simplified by considering a related principally scalar second-order operator obtained essentially by squaring the Dirac operator.

Consider a four-spinor solution u to

$$(i\partial\!\!\!/_{\mathbf{A}} - m)u = 0,$$

where $\mathbf{A} = (A_0, A_1, A_2, A_3)$, i.e.,

$$\big(i(\gamma^0(\partial_0 + iA_0) + \gamma^j(\partial_j + i\mathbf{A}_j)) - m\big)u = 0.$$

Applying $(i\partial\!\!\!/_{\mathbf{A}} + m)$ we obtain immediately

$$\begin{aligned}
0 &= (-\partial\!\!\!/_{\mathbf{A}}^2 - m^2)u \\
&= -\big(\gamma^0(\partial_0 + iA_0) + \gamma^j(\partial_j + iA_j)\big)\big(\gamma^0(\partial_0 + iA_0) + \gamma^k(\partial_k + iA_k)\big)u - m^2u \\
&= -\big((\partial_0 + iA_0)^2u - (\partial_j + iA_j)^2u + \gamma^j\gamma^0(i\partial_j(A_0))u + \gamma^j\gamma^k(i\partial_jA_k)u\big) - m^2u \\
&= -(\partial_0 + iA_0)^2u + (\partial_j + iA_j)^2u - m^2u - i\gamma^j\gamma_0\partial_j(A_0)u - i\gamma^j\gamma^k\partial_k(A_k)u - m^2u.
\end{aligned}$$

For A_0 radial,

$$\begin{aligned}
-i\gamma^j\gamma^0\partial_j(A_0) &= i\gamma^0\gamma^j\partial_j(A_0) \\
&= i\gamma^0\gamma_r\partial_r(A_0) \\
&= i\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\begin{pmatrix} 0 & \sigma_r \\ -\sigma_r & 0 \end{pmatrix}\partial_r(A_0) \\
&= i\begin{pmatrix} 0 & \sigma_r \\ \sigma_r & 0 \end{pmatrix}\partial_r(A_0),
\end{aligned}$$

hence, for A_0 radial and $A_j = 0$,

$$-(\partial_0 + iA_0)^2u + \partial_j^2u - m^2u + i\begin{pmatrix} 0 & \sigma_r \\ \sigma_r & 0 \end{pmatrix}\partial_r(A_0)u = 0.$$

More generally, assume $A_j \in \mathcal{C}^\infty$ and

$$A_0 = \frac{\mathsf{Z}}{r} + V,$$

where $V \in \mathcal{C}^\infty$. We now lump the extra terms together as perturbations, and multiply through by γ^0 rewrite the first order equation in a more convenient form as

$$\eth \equiv i(\partial_t + i\frac{\mathsf{Z}}{r} + iV) + i\alpha_r\left(\partial_r + \frac{1}{r} - \frac{1}{r}\beta K\right) - \sum_{j=1}^{3}\alpha_jA_j - m\beta, \tag{19}$$

where we recall that $\beta = \gamma^0$ and $\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}$. The corresponding operator of Klein–Gordon type

$$P \equiv (i\partial\!\!\!/_{\mathbf{A}} + m)(i\partial\!\!\!/_{\mathbf{A}} - m) \tag{20}$$

then satisfies the following hypotheses:

Klein–Gordon Hypotheses. P is a second-order operator of the following form:

$$P = -(\partial_0 + i\frac{\mathsf{Z}}{r})^2 + \sum \partial_j^2 - m^2 - i\frac{\mathsf{Z}}{r^2}\begin{pmatrix} 0 & \sigma_r \\ \sigma_r & 0 \end{pmatrix} + \mathbf{R} \tag{21}$$

with

$$\mathbf{R} = \mathsf{Z}\frac{\mathbf{W}_0}{r} + \mathbf{W}_1^\alpha \partial_\alpha + \mathbf{W}_2 \tag{22}$$

where $\mathbf{W}_\bullet \in \mathcal{C}^\infty(\mathbb{R}^3)$ but are not necessarily scalar.

These assumptions on the operator will suffice for most of our propagation results below.

Note that the term

$$-i\frac{\mathsf{Z}}{r^2}\begin{pmatrix} 0 & \sigma_r \\ \sigma_r & 0 \end{pmatrix}$$

is, in contrast to the other main terms in the equation, formally anti-self-adjoint rather than self-adjoint. This creates significant technical difficulties in the b-propagation arguments, since, while lower order in terms of differentiation, this anti-self-adjoint term is large. If we estimate it in pairings by the Hardy inequality, is larger than the second-order terms in the equation. This obstacle is why we use the first order equation directly in the hyperbolic part of the b-propagation argument below.

The presence of the charge parameter multiplying $\mathbf{W}_0$ is in fact inessential here, as its size will play no role in the analysis of that term.

4.4. **Interior propagation.** In this section, we discuss the propagation *away from* $r = 0$ of singularities (or, dually, of regularity) and also of iterated regularity under the angular test operators D_θ as well as the spacetime scaling vector field

$$R = rD_r + tD_t. \tag{23}$$

First, we remark that away from the potential singularity at the origin, the standard theory of propagation of singularities applies:

Proposition 18. *Let u satisfy $(i\not{\partial}_{\mathbf{A}} - m)u = 0$. Then $\operatorname{WF} u \subset \Sigma \equiv \{\eta^{\alpha\beta}\xi_\alpha\xi_\beta = 0\}$ and is a union of maximally extended integral curves of the Hamilton flow generated by $\eta^{\alpha\beta}\xi^\alpha\xi^\beta$, i.e., lifts of straight lines.*

Here (and here alone) we have used ξ_α to denote the dual cotangent variable to the Minkowski coordinate x^α.

Proof. Applying $(i\not{\partial}_{\mathbf{A}} + m)$ yields $Pu = 0$. Since P is an operator of real principal type (away from the potential singularity), the result follows from the theorem of Hörmander [12]. □

Now we turn to propagation of iterated regularity under R, D_θ. Note that this is a simple case of propagation of *test module regularity*, with

D_θ together with P being generators of a module of operators testing for *coisotropic* regularity relative to the manifold

$$\mathcal{C} \equiv \{\tau^2 = \xi^2,\ \eta = 0\} \subset T^*M^\circ$$

(using coordinates τ, ξ, η dual to t, r, θ respectively) and with D_θ, R, P together testing for regularity relative to the *Lagrangian* submanifold(s)

$$\mathcal{L} \equiv N^*\{t = \pm r\} \subset \mathcal{C}$$

Proposition 19. *Let u be an admissible solution to the Dirac equation.*

Let $p_0 \in \{\sigma(P) = 0\} \subset T^*(M^\circ)$ and let p_1 lie on the maximally extended null bicharacteristic through p_0 in T^*M°.

If $p_0 \notin \mathrm{WF}^s\, D_\theta^\alpha u$ for all $|\alpha| \leq N$ then $p_1 \notin \mathrm{WF}^s\, D_\theta^\alpha u$ for all $|\alpha| \leq N$.

Likewise, if $p_0 \notin \mathrm{WF}^s\, R^j D_\theta^\alpha u$ for all $j + |\alpha| \leq N$ then $p_1 \notin \mathrm{WF}^s\, R^j D_\theta^\alpha u$ for all $j + |\alpha| \leq N$.

Proof. The proof is a standard exercise in propagation of "test module regularity" and is essentially an easier version of the b- and edge-calculus arguments employed below to obtain propagation through the potential singularity, hence we merely sketch it (cf. [30, Proposition 6.11]).

By Taylor's theorem and the symbol calculus, for a solution to $Pu \in \mathcal{C}^\infty$, the regularity hypothesis $p_0 \notin \mathrm{WF}^s\, D_\theta^\alpha u$ for all $|\alpha| \leq N$ is microlocally equivalent to the assertion that for *any* $A_1, \ldots A_N \in \Psi^1(M^\circ)$ with proper support, characteristic on $\mathcal{C}$,

$$A_1 \ldots A_N u \in H^s.$$

Now by [19, Theorem 21.2.4], we may find a homogeneous symplectomorphism Φ, defined on a neighborhood of p_0, mapping from coordinates (y, z, η, ζ) such that $\sigma(P) \circ \Phi = \zeta_1 q$ with q elliptic and $\Phi^{-1}(\mathcal{C}) = \{\zeta = 0\}$. We may also assume $\Phi(p_0) = 0$ and hence $\Phi(p_1)$ lies on the z_1-axis.

We may then quantize Φ to a microlocally unitary FIO T such that $TP = QD_{z_1}T + E$ with $E \in \Psi^{-\infty}$, and where $Q \in \Psi^1$ is elliptic. Then $Pu = 0$ implies $QD_{z_1}Tu \in \mathcal{C}^\infty$, hence $D_{z_1}Tu \in \mathcal{C}^\infty$ by ellipticity. The hypotheses are equivalent to $D_z^\alpha Tu \in H^s$ near $\Phi(p_0)$ for all $|\alpha| \leq N$. Solving the equation $D_{z_1}Tu \in \mathcal{C}^\infty$ then guarantees that the same holds near any $\Phi(p_1)$ along the z_1-axis.

The second part of the result, dealing with Lagrangian regularity, follows via the same kind of proof: here we conjugate instead to a coordinate system (z, ζ) so that the operators P, R, D_θ, whose symbols cut out the Lagrangian $\mathcal{L}$, become multiples of the model operators D_{z_j} and proceed as before. □

5. Diffractive theorem

5.1. **Main theorem.** In this section, we prove the *diffractive theorem*, which tells us that the only wavefront set emanating from the singularity of the potential arises at the time of interaction with a singularity of the solution.

In making our propagation arguments in the b-calculus we will study the Dirac equation directly. It turns out to be simplest to deal with the Klein–Gordon operator P, however, in making the *elliptic* estimates that constrain where the b-wavefront set may lie. We thus employ both equations in turn in proving the diffractive theorem.

In both settings, we deal with large potential terms by employing the Hardy inequality, with the result that our results only hold for $|\mathsf{Z}| < 1/2$.

Definition 20. A *diffractive geodesic* is a geodesic that is either

(1) a lightlike geodesic not passing through $r = 0$, or
(2) a continuous concatenation of two lightlike geodesics, both passing through $t = t_0,\ r = 0$ for some $t_0 \in \mathbb{R}$, hence in polar coordinates a geodesic passing through the origin at time $t = t_0$ with

$$r = |t - t_0|,\ \theta = \begin{cases} \theta_-, & t < t_0 \\ \theta_+, & t > t_0. \end{cases}$$

(*Geodesic* here refers to a geodesic with respect to the Minkowski metric, hence a straight line.) Note that in the latter case, when the geodesic is broken, there is no need for the arriving and departing *spatial directions* of the geodesic to match up as it enters and leaves the origin, though the direction in time must be conserved.

We will abuse notation by using the term *geodesic* interchangeably for the curve in M° and for its lift to T^*M°.

A simple version of the diffractive propagation theorem, making no reference to b-wavefront set, says that the wavefront set of a solution to the Dirac equation is, away from the spatial origin, given by a union of lifts of diffractive geodesics to $T^*\mathbb{R}^3$. To prove the theorem, however, requires proving uniform estimates at the time the geodesic reaches $r = 0$, which requires analysis of the b-wavefront set; Proposition 18 takes care of propagation away from $r = 0$.

In order to describe wavefront sets conveniently, we will use coordinates associated to the canonical one-form

$$\sigma \frac{dr}{r} + \eta \cdot d\theta + \tau\, dt \tag{24}$$

on ${}^{\mathrm{b}}T^*M$. We may canonically identify this cotangent bundle with $T^*\mathbb{R}^4$ away from $r = 0$: this follows from the observation that $\mathfrak{b}$ is a diffeomorphism away from $r = 0$ (identifying $T^*\mathbb{R}^4$and T^*M there) and that the natural map $T^*M \to {}^{\mathrm{b}}T^*M$ is an isomorphism in this region.

In the coordinates given by (24), for the radial geodesics (i.e., integral curves of the Hamilton flow of the metric), $dr/dt = -\sigma/r\tau$, hence the set where σ and τ have the same sign should be viewed as "incoming" toward $r = 0$ under the bicharacteristic flow, while the set where they have opposite signs is outgoing. Thus the following theorem describes propagation into and then back out of the singular point of the Coulomb potential.

Theorem 21. *Let* $\mathbf{A} = (A_0 = \mathsf{Z}/r + V, A_1, A_2, A_3)$ *with* $V, A_j \in \mathcal{C}^\infty(\mathbb{R}^3)$, *and* $|\mathsf{Z}| < 1/2$.

Whenever u *is an admissible solution of*

$$(i\partial\!\!\!/_{\mathbf{A}} - m)u = 0,$$

if

$$\{(r = t_0 - t, \theta, t, \sigma, \tau, \eta = 0)\colon t < t_0, \theta \in S^2, \sigma, \tau \in \mathbb{R}, \tau \gtreqless 0, \sigma \gtreqless 0\} \cap \mathrm{WF}\, u = \emptyset$$

then

$$\{(r = t - t_0, \theta, t, \sigma, \tau, \eta = 0)\colon t > t_0, \theta \in S^2, \sigma, \tau \in \mathbb{R}, \tau \gtreqless 0, \sigma \lesseqgtr 0\} \cap \mathrm{WF}\, u = \emptyset.$$

Thus, no wavefront set *arriving* at $r = 0$ at time $t = t_0$ implies no wavefront set *emanating* from $r = 0$ at time $t = t_0$, and we have established propagation on diffractive geodesics. Moreover the sign of τ is conserved in this interaction.

We will prove Theorem 21 by obtaining a stronger result, uniformly true across $r = 0$, concerning the *propagation of* b-*wavefront set.*

5.2. **Propagation of b-regularity.** The following treatment of the propagation of b-regularity is heavily influenced by the work of Vasy in the context of manifolds with corners [42], which gave in turn a new perspective on previous results of Melrose–Sjöstrand in the boundary case [28], [29].

The main propagation results take place inside the *compressed characteristic set,* which is the appropriate extension of the ordinary characteristic set to the boundary setting. In coordinates associated to the canonical one-form

$$\underline{\tau} dt + \underline{\sigma} dr + \underline{\eta} \cdot d\theta$$

on T^*M, Σ is given by

$$\Sigma = \{(r, \theta, t, \underline{\sigma}, \underline{\eta}, \underline{\tau}) \mid \underline{\tau}^2 - \underline{\sigma}^2 - \frac{1}{r^2}|\underline{\eta}|^2\}.$$

The *compressed characteristic set* $\dot{\Sigma}$, originally due to Melrose–Sjöstrand [28, 29], is the image of the characteristic set under the natural map $T^*M \to {}^{\mathrm{b}}T^*M$. In the coordinates associated to the canonical one-form

$$\tau dt + \sigma \frac{dr}{r} + \eta \cdot d\theta$$

on ${}^{\mathrm{b}}T^*M$, $\dot{\Sigma}$ has the following form over $r = 0$:

$$\dot{\Sigma}|_{r=0} = \{(r = 0, \theta, t, \sigma = 0, \eta = 0, \tau) \mid \theta \in S^2, \tau \neq 0\}.$$

We will obtain Theorem 21 by proving the following more precise statement. Recall from equation (19) that $\eth$ is a Dirac–Coulomb operator with additionally a smooth vector potential, multiplied through by γ^0.

Theorem 22. *Assume* u *is an admissible solution of* $\eth u = 0$*, and assume that* $|\mathsf{Z}| < 1/2$.

For each m, $\mathrm{WF}_{\mathrm{b}}^{1,m} u \subset \dot{\Sigma}$. *Away from* $r = 0$, $\mathrm{WF}_{\mathrm{b}}^{1,m} u$ *is invariant under the bicharacteristic flow.*

Fix $\rho_0 = \{(r = 0, \theta \in S^2, t_0, \sigma = 0, \eta_0 = 0, \tau_0)\} \subset \dot{\Sigma}$ *and let* U *denote a neighborhood of* ρ_0 *in* $\dot{\Sigma}$*. If*

$$U \cap \{\sigma/\tau > 0\} \cap \mathrm{WF}_{\mathrm{b}}^{1,m} u = \emptyset,$$

then

$$\rho_0 \cap \mathrm{WF}_{\mathrm{b}}^{1,m} u = \emptyset.$$

Note that the openness of the complement of $\mathrm{WF}_{\mathrm{b}}^{1,m} u$ means that the theorem yields regularity at the outgoing points (where $\sigma/\tau < 0$) sufficiently near ρ_0.

In fact, we prove a stronger statement for the inhomogeneous problem, in which

$$\mathrm{WF}_{\mathrm{b}}^{1,m} u \subset \dot{\Sigma} \cup \mathrm{WF}_{\mathrm{b}}^{m}(\eth u),$$

and if

$$U \cap \mathrm{WF}_{\mathrm{b}}^{0,m+1}(\eth u) = \emptyset$$

and

$$U \cap \{\sigma/\tau > 0\} \cap \mathrm{WF}_{\mathrm{b}}^{1,m} u = \emptyset,$$

then $\rho_0 \cap \mathrm{WF}_{\mathrm{b}}^{1,m} u = \emptyset$, with analogous statements with the additional factors included.

We also prove a statement about the propagation of coisotropic regularity.

Theorem 23. *The same statements hold with* u *replaced by* $K^\ell u$ *or* $R^\ell u$*, where* K *is Dirac's* K*-operator and* $R = (t - t_0)D_t + rD_r$ *is the scaling vector field. More precisely, for each* ℓ*,* $\mathrm{WF}_{\mathrm{b}}^{1,m}(K^j u)$ *and* $\mathrm{WF}_{\mathrm{b}}^{1,m}(R^j u)$ *are invariant under bicharacteristic flow away from* $r = 0$ *for* $j = 0, \dots, \ell$ *and if*

$$U \cap \{\sigma/\tau > 0\} \cap \mathrm{WF}_{\mathrm{b}}^{1,m}(S^j u) = \emptyset$$

for $S = K$ *or* $S = R$ *and all* $j \leq \ell$*, and* $\rho_0 \cap \mathrm{WF}_{\mathrm{b}}^{m+1}(S^j \eth u)$ *for* $j = 0, \dots, \ell$*, then*

$$\rho_0 \cap \mathrm{WF}_{\mathrm{b}}^{1,m}(S^j u) = \emptyset$$

for all $j \leq \ell$*.*

Remark 24. The statement for K provides a proof of the propagation of Lagrangian regularity through the singularity. It immediately follows that a similar statement (with hypotheses modified as needed) holds for $K^\ell R^k u$; this shows that coisotropic regularity (in the b-sense) also propagates through the singularity.

Since $\mathrm{WF}_{\mathrm{b}}^{1,m}$ is closed, this theorem *implies* Theorem 21 as follows:

Proof of Theorem 21 using Theorem 22. Assuming the hypotheses of Theorem 21, we first can use ordinary propagation of singularities and elliptic regularity over M° to conclude that a neighborhood of

$$\{(r = 0, \theta, t = t_0, \operatorname{sgn}\sigma = \operatorname{sgn}\tau) \colon \theta \in S^2\}$$

over M° is disjoint from the wavefront set, since the backward bicharacteristic flowout of any of these points lies in the region where our hypotheses yield regularity, provided we take a sufficiently small such neighborhood. Without loss of generality, we will focus on the component $\tau < 0$, with the other component to be treated mutatis mutandis.

Now we find that since ordinary and b wavefront sets coincide for $r > 0$, over a neighborhood of $(r = 0, \theta \in S^2, t_0)$, $\mathrm{WF}_{\mathrm{b}}^{1,m} u \cap \{r > 0,\ \operatorname{sgn} \sigma\tau = 1,\ \eta = 0\} = \emptyset$; since $\dot{\Sigma} \cap \{r = 0\} \subset \{\sigma = 0\}$, this suffices to establish the existence of U as in the hypotheses of Theorem 22, where we have taken fixed a sign of τ. Thus Theorem 22 implies that $\rho_0 \cap \mathrm{WF}_{\mathrm{b}}^{1,m} = \emptyset$; since $\mathrm{WF}_{\mathrm{b}}^{1,m}$ is closed, this implies the existence of an open neighborhood of ρ_0 in $\dot{\Sigma}$ that is disjoint from $\mathrm{WF}_{\mathrm{b}}^{1,m} u$, and in particular, there is a such neighborhood in $\dot{\Sigma} \cap \{\sigma > 0, r > 0\}$.

This is then the projection of an open neighborhood in Σ, the usual characteristic set, that is disjoint from $\mathrm{WF}_{\mathrm{b}}^{1,m} u$ and where $\tau\sigma < 0$, and in particular contains a point in every bicharacteristic $(r = t - t_0, t > t_0, \operatorname{sgn} \tau\sigma = -1, \eta = 0)$; this completes the proof of Theorem 21 (since $\mathrm{WF}\, u = \overline{\bigcup_m \mathrm{WF}^m u}$). ☐

We now proceed with the proof of Theorem 22. To this end, we begin with preliminary estimates on commutators, with a crucial role played by commutators between $\Box$ and b-operators that are rotationally symmetric in the space variables.

5.2.1. *b-Commutators.* We record for our use below the form of the commutator of an invariant (defined above in Definition 3) b-pseudodifferential operator with the second order operator P and the first order operator $\eth$.

Lemma 25. *Let $C \in \Psi_{\mathrm{b}}^m(M)$ be invariant, with principal symbol c scalar and real-valued. Then, for P satisfying the Klein-Gordon hypotheses of Section 4.3,*

$$[P, C] = B_0 \frac{1}{r^2} \Delta_\theta + B_1,$$

where

- $B_0 \in \Psi_{\mathrm{b}}^{m-1}$ *and*
- $B_1 \in \mathrm{Diff}^2 \Psi_{\mathrm{b}}^{m-1} + \mathrm{Diff}^1 \Psi_{\mathrm{b}}^m + \Psi_{\mathrm{b}}^{m+1}$.

Both B_0 and B_1 are microsupported in $\mathrm{WF}'_{\mathrm{b}} C$.

Proof. The term containing B_0 arises by commuting C through the $\frac{1}{r^2}\Delta_\theta$ term in P. The remaining terms in P contribute to the B_1 term; as

$$P + \frac{1}{r^2}\Delta_\theta \in \mathrm{Diff}^2 \Psi_b^0,$$

Lemma 8 shows that this commutator lies in $\mathrm{Diff}^2 \Psi_b^{m+1}$. ☐

Lemma 26. *Let $C \in \Psi_{\mathrm{b}}^m(M)$ be invariant, with principal symbol c scalar and real-valued. Then*

(25)
$$\frac{1}{i}[\eth, C] = A_0\left(\alpha_r\left(i\partial_r + \frac{i}{r} - \frac{i}{r}\beta K\right) - \frac{\mathsf{Z}}{r}\right) + B_0 + \alpha_r B_1 + \mathbf{B}_2\frac{1}{r} + \mathbf{B}_3 D_r + \mathbf{B}_4 + \mathbf{B}_5\frac{1}{r} + \mathbf{B}_6 D_r,$$

where

- $A_0 \in \Psi_{\mathrm{b}}^{m-1}(M)$, *with* $\sigma_{\mathrm{b}}(A_\bullet) = -\partial_\sigma(c)$,
- $B_0 \in \Psi_{\mathrm{b}}^m(M)$, *with* $\sigma_{\mathrm{b}}(B_0) = \partial_t(c)$,
- $B_1 \in \Psi_{\mathrm{b}}^m$, *with* $\sigma_{\mathrm{b}}(B_1) = \partial_r(c)$,
- $\mathbf{B}_2 \in \Psi_{\mathrm{b}}^m(M)$, *with* $\operatorname{supp}\sigma_{\mathrm{b}}(\mathbf{B}_2) \subseteq \operatorname{supp}\partial_\eta(c)$,
- $\mathbf{B}_3 \in \Psi_{\mathrm{b}}^{m-1}(M)$, *with* $\operatorname{supp}\sigma_{\mathrm{b}}(\mathbf{B}_3) \subseteq \operatorname{supp}\partial_\eta(c)$,
- $\mathbf{B}_4 \in \Psi_{\mathrm{b}}^{m-1}(M)$, *and*
- $\mathbf{B}_5$, $\mathbf{B}_6 \in \Psi_{\mathrm{b}}^{m-2}(M)$.

Remark 27. Non-scalar pseudodifferential operators are in bold in the expressions above; roman terms are scalar.

Proof. We write
$$\eth = i\partial_t - \frac{\mathsf{Z}}{r} + i\alpha_r\left(\partial_r + \frac{1}{r} - \frac{1}{r}\beta K\right) - \alpha_0 V - \alpha_j A_j,$$
where we use the convention that $\alpha_0 = \mathrm{I}$.

We begin with the angular term. Because α_r and K depend only on the angular variables, their commutators with the invariant operator C are microsupported in the support of $\partial_\eta c$. Writing
$$\frac{1}{i}[-\alpha_r\frac{i}{r}\beta K, C] = -\alpha_r\frac{1}{r}[\beta K, C] - \frac{1}{r}[\alpha_r, C]\beta K - [\frac{1}{r}, C]\alpha_r\beta K,$$
we see that the first two terms give contributions to $\mathbf{B}_2$, while the last term yields the angular part of the A_0 term above. (Indeed, we take this to define the operator A_0.)

We now turn to the terms involving the commutator with $i\partial_t - \frac{\mathsf{Z}}{r}$. The $[\partial_t, C]$ term gives B_0, while the $\frac{\mathsf{Z}}{r}$ term contributes to the A_0 and $\mathbf{B}_5$ terms.

We now consider the term involving $i\alpha_r(\partial_r + \frac{1}{r})$. We observe that because α_r depends only on the angular variables, its commutator with C is microsupported in the support of $\partial_\eta(c)$, yielding a contribution to the $\mathbf{B}_3$ term. Since
$$-\frac{1}{i}[D_r, C] = S + TD_r,$$
where
$$S \in \Psi_{\mathrm{b}}^m, \quad \sigma_{\mathrm{b}}(S) = \partial_r(c),$$
and
$$T \in \Psi_{\mathrm{b}}^{m-1}, \quad \sigma_{\mathrm{b}}(T) = \partial_\sigma(c),$$
we see that the rest of this term yields contributions to the terms involving A_0, B_1, and $\mathbf{B}_6$.

Finally, the commutator of $-\alpha_0 V - \alpha^j \mathbf{A}_j$ with C yields the $\mathbf{B}_4$ term. □

5.2.2. *Elliptic estimate.* The estimates in this section are very close to those in [42, Section 4], hence we will be somewhat brief in the proofs; the main difference here is in the potential terms, which need to be controlled using the Hardy inequality. Unlike in the proof of the hyperbolic estimate in the next section, we work here with the second order equation in order to obtain more direct control over the H^1 norm.

Lemma 28. *If* $|\mathsf{Z}| < 1/2$ *then for all* $u \in H^1$, $\mathrm{WF}_{\mathrm{b}}^{1,m} u \subset \mathrm{WF}_{\mathrm{b}}^{-1,m}(Pu) \cup \dot{\Sigma}$.

Following the treatment in [42, Section 4], we begin with a lemma concerning the quadratic form associated to P. (Cf. Lemma 4.2 of [42].)

In what follows, we split P as

$$P = P_0 + \mathbf{R}$$

with

$$P_0 = -(\partial_0 + i\mathsf{Z}/r)^2 + \sum \partial_j^2 - m^2 - i\frac{\mathsf{Z}}{r^2}\begin{pmatrix} 0 & \sigma_r \\ \sigma_r & 0 \end{pmatrix}.$$

Lemma 29. *Let* $K \subset {}^{\mathrm{b}}S^*M$ *be compact,* $U \subset {}^{\mathrm{b}}S^*M$ *open,* $K \subset U$. *Let* A_λ *be a bounded family of invariant elements in* Ψ_{b}^s *with* $\mathrm{WF}_{\mathrm{b}}' A_\lambda \subset K$ *(in the sense of uniform wavefront set of families), and* $A_\lambda \in \Psi_{\mathrm{b}}^{s-1}$ *for* $\lambda \in (0,1)$. *Then there exist* $G \in \Psi_{\mathrm{b}}^{s-1/2}$, $\widetilde{G} \in \Psi_{\mathrm{b}}^s$, *both microsupported in* U, *and* C_0 *so that for all* $\epsilon > 0$, $\lambda \in (0,1)$, $u \in H^1$ *with* $\mathrm{WF}_{\mathrm{b}}^{1,s-1/2} u \cap U = \emptyset$, $\mathrm{WF}_{\mathrm{b}}^{-1,s}(Pu) \cap U = \emptyset$,

$$\begin{aligned}&\left| \|(D_t + \mathsf{Z}/r)A_\lambda u\|^2 - \|\nabla A_\lambda u\|^2 - m^2\|A_\lambda u\|^2 + \mathrm{Re}\langle \mathbf{R}A_\lambda u, A_\lambda u\rangle \right| \\ &\leq C_0\left(\epsilon\|A_\lambda u\|_{H^1}^2 + \|u\|_{H^1}^2 + \|Gu\|_{H^1}^2 + \epsilon^{-1}\|Pu\|_{H^{-1}}^2 + \epsilon^{-1}\left\|\widetilde{G}Pu\right\|_{H^{-1}}^2\right).\end{aligned}$$

The estimate is uniform *for bounded* Z *(which is not required to be small).*

Remark 30.

- The LHS of the inequality is given by the absolute value of the $\mathrm{Re}\langle PA_\lambda u, A_\lambda u\rangle$; the non-scalar term in P is anti-self-adjoint, hence does not contribute.
- If A_λ commuted with P the G term would not appear; as it is, this term is lower order than A_λ since it arises as a commutator.

Proof. Fix $G, \widetilde{G}$ of the appropriate order, microsupported in U, so that $\sigma_{\mathrm{b}}(G), \sigma_{\mathrm{b}}(\widetilde{G}) \equiv 1$ on K.

The pairing

$$\mathrm{Re}\langle PA_\lambda u, A_\lambda u\rangle$$

is finite for all $\lambda > 0$ by our wavefront set assumption, which implies that $PA_\lambda u \in H^{-1}$ and $A_\lambda u \in H^1$. First write

$$|\mathrm{Re}\,\langle PA_\lambda u, A_\lambda u\rangle| \leq |\langle [P, A_\lambda]u, A_\lambda u\rangle| + |\langle A_\lambda Pu, A_\lambda u\rangle|.$$

We first estimate the term

$$|\langle A_\lambda Pu, A_\lambda u\rangle|.$$

Indeed, we observe that

$$|\langle A_\lambda Pu, A_\lambda u\rangle| \leq \|A_\lambda Pu\|_{H^{-1}}\|A_\lambda u\|_{H^1} \leq \epsilon\|A_\lambda u\|^2_{H^1} + \epsilon^{-1}\|A_\lambda Pu\|^2_{H^{-1}}.$$

Elliptic regularity for $\widetilde{G}$ then shows that

$$|\langle A_\lambda Pu, A_\lambda u\rangle| \leq \epsilon\|A_\lambda u\|^2_{H^1} + C\epsilon^{-1}\left(\|Pu\|^2_{H^{-1}} + \left\|\widetilde{G}Pu\right\|^2_{H^{-1}}\right).$$

We now turn our attention to the commutator term. Indeed, Lemma 25 allows us to write

$$\langle [P, A_\lambda]u, A_\lambda u\rangle = \left\langle \frac{1}{r^2}\Delta_\theta B_0 u, A_\lambda u\right\rangle + \langle B_1 u, A_\lambda u\rangle,$$

where $B_0 \in \Psi_{\mathrm{b}}^{s-1}$ and $B_1 \in \mathrm{Diff}^2\Psi_b^{s-1} + \mathrm{Diff}^1\Psi_b^s + \Psi_b^{s+1}$, both satisfying uniform (in λ) estimates in these spaces.

Lemmas 13 and 12 show that we may bound

$$|\langle [P, A_\lambda]u, A_\lambda u\rangle| \lesssim \|u\|^2_{H^1} + \|Gu\|^2_{H^1},$$

finishing the proof. □

Proof of Lemma 28. (Cf. the proof of [42, Proposition 4.6].) We aim to show that if $\mathrm{WF}'_{\mathrm{b}} A \cap \dot{\Sigma} = \emptyset$ and $\mathrm{WF}_{\mathrm{b}}^{-1,m}(Pu) \cap \mathrm{WF}'_{\mathrm{b}} A = \emptyset$, then $Au \in H^1$. We in fact show this iteratively, assuming by induction that $\mathrm{WF}_{\mathrm{b}}^{1,s-1/2} u$ is disjoint from a(n arbitrarily small neighborhood of) $\mathrm{WF}'_{\mathrm{b}} A$ and then showing $Au \in H^1$. To pass to $s = \infty$, one must guarantee that the supports of the operators in each iteration do not shrink too quickly, but this can be guaranteed as in the end of the proof of [42, Proposition 6.2].

We will use the notation

$$\hat{\sigma} = \frac{\sigma}{|\tau|}, \quad \hat{\eta} = \frac{\eta}{|\tau|}$$

in discussing symbol constructions below.

Since $\mathrm{WF}'_{\mathrm{b}} A \cap \dot{\Sigma} = \emptyset$, without loss of generality (since the lemma is standard over M°), $\hat{\sigma}^2 + |\hat{\eta}|^2 \geq \epsilon^2 > 0$ on $\mathrm{WF}'_{\mathrm{b}} A$; moreover, by a partition of unity in x (again using elliptic regularity over M°), we may take $r < \delta$ over $\mathrm{WF}'_{\mathrm{b}} A$, where we may specify δ independently from ϵ above. Now we let[4]

$$A_\lambda \equiv \mathrm{Op}_b\left((1 + \lambda(\tau^2 + \sigma^2 + |\eta|^2))^{-1}\right) A,$$

so that A_λ is uniformly bounded in Ψ_{b}^s and converges to A in the topology of Ψ_{b}^{s+0}, while for each $\lambda > 0$, $A_\lambda \in \Psi_{\mathrm{b}}^{s-2}$. We may apply Lemma 29 to such

[4]We assume our quantization is arranged so that it yields properly supported operators.

an A, so that for all $\epsilon' > 0$,

(26)

$$- \|(D_t + \mathsf{Z}/r)A_\lambda u\|^2 + \|\nabla A_\lambda u\|^2 + m^2\|A_\lambda u\|^2 - |\langle \mathbf{R} A_\lambda u, A_\lambda u\rangle|$$

(27)

$$\leq C_0 \left(\epsilon' \|A_\lambda u\|^2_{H^1} + \|u\|^2_{H_1} + \|Gu\|^2_{H_1} + (\epsilon')^{-1}\|Pu\|^2_{H^{-1}} + (\epsilon')^{-1}\left\|\widetilde{G}Pu\right\|^2_{H^{-1}} \right).$$

Since $\tau^2 < \epsilon^{-2}(\sigma^2 + |\eta|^2)$ and $r < \delta$ on $\mathrm{WF}_\mathrm{b}' A$, we estimate

$$\begin{aligned}
\|D_t A_\lambda u\|^2 &\leq \left\langle \epsilon^{-2}\operatorname{Op}(\sigma^2 + |\eta|^2)A_\lambda u, A_\lambda u\right\rangle + \|Gu\|^2_{H^1}\\
&= \epsilon^{-2}\left(\|(rD_r)A_\lambda u\|^2 + \|\nabla_\theta A_\lambda u\|^2\right) + \|Gu\|^2_{H^1}\\
&\leq \delta^2\epsilon^{-2}\|\nabla A_\lambda u\|^2 + \|Gu\|^2_{H^1}\\
&\leq C\delta^2\epsilon^{-2}\|A_\lambda u\|^2_{H^1} + \|Gu\|^2_{H^1}.
\end{aligned}$$

Here again $G \in \Psi_\mathrm{b}^{s-1/2}$ is an error term (which we allow to change from line to line as needed); we use it to estimate terms of the form $\|Bu\|^2_{L^2}$ with $B \in \Psi_\mathrm{b}^{s+1/2}$.

We also recall from (15) that

$$\left\|r^{-1}A_\lambda u\right\|^2 \leq 4\|A_\lambda u\|^2_{H^1};$$

thus for any $\epsilon' > 0$,

$$\|(D_t + V)A_\lambda u\|^2 \leq C\delta^2\epsilon^{-2}\|A_\lambda u\|^2_{H^1} + (4+\epsilon')\mathsf{Z}^2\|\nabla A_\lambda u\|^2 + \|Gu\|^2_{H^1}.$$

We also use repeatedly the fact that $\|A_\lambda u\| \leq C\|Gu\|_{H^1}$ together with Cauchy–Schwarz to estimate

$$|\langle \mathbf{R} A_\lambda u, A_\lambda u\rangle| \leq \epsilon'\|A_\lambda u\|^2_{H^1} + C\|Gu\|^2_{H^1}.$$

(The constant on the right side depends on both Z and ϵ'.)

Adding $\|D_t A_\lambda u\|^2 + \|(D_t+V)A_\lambda u\|^2$ to equation (26) now yields

(28)

$$\begin{aligned}
\|D_t A_\lambda u\|^2 + \|\nabla A_\lambda u\|^2 \leq (C\delta^2\epsilon^{-2} + 2\epsilon')\|A_\lambda u\|^2 + (4+\epsilon')\mathsf{Z}^2\|\nabla A_\lambda u\|^2\\
+ C_0\left(\|u\|^2_{H^1} + \|Gu\|^2_{H^1} + (\epsilon')^{-1}\|Pu\|^2_{H^{-1}} + (\epsilon')^{-1}\left\|\widetilde{G}Pu\right\|^2_{H^{-1}}\right).
\end{aligned}$$

Assuming now that $|\mathsf{Z}| < 1/2$, taking ϵ' and δ sufficiently small (and dropping ϵ'-dependence of the constants on the right side), we absorb the $\|\nabla A_\lambda u\|^2$ and $\|A_\lambda u\|^2_{H^1}$ terms on the right into the left side. (For the latter term, we recall that up to $\|A_\lambda u\|^2_{L^2}$, which is controlled by $\|Gu\|^2_{H^1}$, $\|\nabla A_\lambda u\|^2$ is comparable to the squared H^1 norm of $A_\lambda u$.)

We thus obtain

$$\|A_\lambda u\|^2_{H^1} \leq C\left(\|u\|^2_{H^1} + \|Gu\|^2_{H^1} + \|Pu\|^2_{H^{-1}} + \left\|\widetilde{G}Pu\right\|^2_{H^{-1}}\right). \tag{29}$$

The right side is uniformly bounded as $\lambda \downarrow 0$ by our inductive assumption. Now taking $\lambda \to 0$ and employing a standard weak-convergence argument (see, e.g., [42, Lemma 3.7]) shows that $Au \in H^1$. This concludes the proof of Lemma 28. □

We now record two corollaries of the previous lemma; the first is elliptic regularity for $\eth$:

Corollary 31. *If $|\mathsf{Z}| < 1/2$, then for all $u \in H^1$, $\mathrm{WF}_{\mathrm{b}}^{1,m} u \subset \mathrm{WF}_{\mathrm{b}}^m(\eth u) \cup \dot{\Sigma}$.*

More precisely, if $A \in \Psi_{\mathrm{b}}^m$ is properly supported and microsupported near $\rho_0 \notin \dot{\Sigma}$, then there are $G \in \Psi_{\mathrm{b}}^{m-1}$ and $\widetilde{G} \in \Psi_{\mathrm{b}}^m$ also microsupported in $\dot{\Sigma}^c$ so that

$$\|Au\|_{H^1} \leq C \left(\|u\|_{H^1} + \|Gu\|_{H^1} + \left\| \widetilde{G} \eth u \right\|_{L^2} \right).$$

Proof. The final estimate (29) in the proof of Lemma 28 shows that we may bound

$$\|Au\|_{H^1} \leq C \left(\|u\|_{H^1} + \|G_1 u\|_{H^1} + \|Pu\|_{H^{-1}} + \left\| \widetilde{G} P u \right\|_{H^{-1}} \right),$$

for $G_1 \in \Psi_{\mathrm{b}}^{m-1/2}$. We first estimate $\|Pu\|_{H^{-1}}$ and $\left\| \widetilde{G} P u \right\|_{H^{-1}}$ in terms of $\|\eth u\|_{L^2}$.

We recall that we may write $P = \widetilde{L} \eth$, where

$$\widetilde{L} = (i \partial\!\!\!/_{\mathbf{A}} + m) \gamma^0,$$

which maps $L^2 \to H^{-1}$ continuously. We may therefore bound

$$\|Pu\|_{H^{-1}} \leq C \|\eth u\|_{L^2}.$$

Turning to $\left\| \widetilde{G} P u \right\|_{H^{-1}}$, we write

$$\widetilde{G} P u = \widetilde{G} \widetilde{L} \eth u = \widetilde{L} \widetilde{G} \eth u + [\widetilde{G}, \widetilde{L}] \eth u.$$

As $\left\| \widetilde{L} \widetilde{G} \eth u \right\|_{H^{-1}} \leq C \left\| \widetilde{G} \eth u \right\|_{L^2}$, we turn our attention to $[\widetilde{G}, \widetilde{L}]$. As $\widetilde{L} \in r^{-1} \Psi_{\mathrm{b}}^1$, Lemma 8 and basic properties of the b-calculus show that $[\widetilde{G}, \widetilde{L}] \in r^{-1} \Psi_{\mathrm{b}}^m$. Elliptic regularity of (a slightly enlarged) $\widetilde{G}'$ then shows that

$$\left\| [\widetilde{G}, \widetilde{L}] \eth u \right\|_{H^{-1}} \leq C \left(\|\eth u\|_{L^2} + \left\| \widetilde{G}' \eth u \right\|_{L^2} \right).$$

We now repeat the whole argument up to this point with G_1 replacing A; this allows us to replace (at the cost of slightly enlarging the microsupports) the operator $G_1 \in \Psi_{\mathrm{b}}^{m-1/2}$ with $G \in \Psi_{\mathrm{b}}^{m-1}$. □

Remark 32. By iteration, we may replace $G \in \Psi_{\mathrm{b}}^{m-1}$ in the statement of the above corollary by an operator of any order, though we do not need this stronger statement below.

The second corollary has the same proof as Lemma 28 without an estimate on $\|D_t A_\lambda u\|$:

Corollary 33. *If* $|\mathsf{Z}| < 1/2$ *and* $A \in \Psi_{\mathrm{b}}^m$ *is invariant and properly supported, then for* $G \in \Psi_{\mathrm{b}}^{m-1}$ *and* $\widetilde{G} \in \Psi_{\mathrm{b}}^m$ *with* $\mathrm{WF}_{\mathrm{b}}'(A) \subset \operatorname{ell} G \cap \operatorname{ell} \widetilde{G}$*, we have*

$$\|Au\|_{H^1} \leq C\left(\|D_t Au\| + \|Gu\|_{H^1} + \left\|\widetilde{G}\eth u\right\|_{H^1} + \|u\|_{H^1}\right).$$

5.2.3. *Proof of Theorems 22 and 23.* We now turn our attention to the proof of the b-propagation theorems. We first record a consequence of the elliptic estimates of the previous section:

Lemma 34. *Suppose* $u \in H^1$, $\eth u = 0$. *Then*

$$\left(\mathrm{WF}_{\mathrm{b}}^{1,m} u\right)^c = \left\{\rho \in {}^{\mathrm{b}}T^*M\colon \text{ there exists } A \in \Psi_{\mathrm{b}}^{m+1}, \text{ elliptic at } \rho, Au \in L^2\right\}.$$

(Cf. Lemma 6.1 of [42]*.)*

More precisely, if $u \in H^1$ *and* $\rho_0 \notin \mathrm{WF}_{\mathrm{b}}^{m+1}(\eth u)$*, then*

$$\rho_0 \in \mathrm{WF}_{\mathrm{b}}^{1,m} u \text{ if and only if } \rho_0 \in \mathrm{WF}_{\mathrm{b}}^{m+1} u.$$

Proof. Suppose $\rho_0 \notin \mathrm{WF}_{\mathrm{b}}^{1,m} u$. We may use a microlocal partition of unity in the b-calculus to break u into pieces on each of which one of the the operators rD_r D_t, or D_{θ_j} is b-elliptic. If $A \in \Psi_{\mathrm{b}}^{m+1}$ and $G \in \Psi_{\mathrm{b}}^m$ is elliptic on $\mathrm{WF}_{\mathrm{b}}' u$, we thus obtain by microlocal ellipticity

$$\|Au\|^2 \lesssim \|rDrGu\|^2 + \|D_t Gu\|^2 + \|\nabla_\theta Gu\|^2 + \|u\|_{H^1}^2 \lesssim \|Gu\|_{H^1}^2 + \|u\|_{H^1}^2.$$

and we obtain one direction of the lemma.

The other direction of the lemma follows immediately from Corollary 33. □

We now turn to the proof of Theorem 22. Let us first consider the case when $M = 0$ and let U denote a neighborhood of ρ_0 in $\dot{\Sigma}$ with

$$U \cap \{\sigma > 0\} \cap \mathrm{WF}_{\mathrm{b}}^{s+1/2} u = U \cap \mathrm{WF}_{\mathrm{b}}^{s+1/2}(\eth u) = \emptyset.$$

For our inductive hypothesis we assume that $\rho_0 \notin \mathrm{WF}_{\mathrm{b}}^s u$; we aim to show $\rho_0 \notin \mathrm{WF}_{\mathrm{b}}^{s+1/2} u$.

Let $\omega = r^2 + (t - t_0)^2$, and let

$$\phi = -\hat{\sigma} + \frac{1}{\beta^2\delta}\omega.$$

Fix a small neighborhood U of $(t = t_0, x = 0)$ in ${}^{\mathrm{b}}S^*M$ and choose cutoff functions χ_0, χ_1, and χ_2 with the following properties:

- χ_0 is supported in $[0, \infty)$, with $\chi_0(s) = \exp(-1/s)$ for $s > 0$,
- χ_1 is supported in $[0, \infty)$, with $\chi_1(s) = 1$ for $s \geq 1$ and $\chi' \geq 0$, and
- χ_2 is supported in $[-2c_1, 2c_1]$, and is equal to 1 on $[-c_1, c_1]$.

Here c_1 is chosen so that $\hat{\sigma}^2 + \hat{\eta}^2 < c_1 < 2$ in $\dot{\Sigma} \cap U$.

Now set

$$a = |\tau|^{s+1/2}\chi_0(2 - \phi/\delta)\chi_1(2 - \hat{\sigma}/\delta)\chi_2(\hat{\sigma}^2 + |\hat{\eta}|^2)1_{\operatorname{sgn}\tau = \operatorname{sgn}\tau_0} \tag{30}$$

and let A be its quantization to an invariant element of $\Psi_{\mathrm{b}}^{s+1/2}$. Note that

$$\operatorname{supp} a \subset \{|\hat{\sigma}| < 2\delta, \omega < 4\delta^2\beta^2\}, \tag{31}$$

hence the support of a in ${}^{\mathrm{b}}T^*M$ can be taken to be inside any desired neighborhood of ρ_0.

In the following symbol construction and subsequent argument, we will omit a standard regularization argument, described in detail in [42, (6.19) et seq.].

Lemma 35. *For A defined as above,*

(32)
$$i^{-1}[\eth, A^*A] = \tilde{R}\eth - \operatorname{sgn}(\tau_0)Q^*Q + \mathbf{R}_1\frac{1}{r} + \mathbf{R}_2 D_r + \mathbf{R}_3\frac{1}{r}\beta K + \mathbf{R} + B_0 + \alpha_r B_1 + E' + E'',$$

where

- $Q \in \Psi_{\mathrm{b}}^{s+1/2}$ *is invariant and self-adjoint with*
$$\sigma_{\mathrm{b}}(Q) = \sqrt{2}|\tau|^{s+1/2}\delta^{-1/2}(\chi_0'\chi_0)^{1/2}\chi_1\chi_2 1_{\operatorname{sgn}\tau = \operatorname{sgn}\tau_0},$$
- $\tilde{R} \in \Psi_{\mathrm{b}}^{2s}$,
- $\mathbf{R}_j \in \Psi_{\mathrm{b}}^{2s-1}$,
- $\mathbf{R} \in \Psi_{\mathrm{b}}^{2s}$,
- $B_0, B_1 \in \Psi_{\mathrm{b}}^{2s+1}$ *with* $|\sigma_{\mathrm{b}}(B_\bullet)|$ *equal to an order zero symbol times* $C\beta^{-1}\sigma_{\mathrm{b}}(Q)^2$,
- $E' \in \Psi_{\mathrm{b}}^{2s+1}$ *with* $\mathrm{WF}_{\mathrm{b}}' E' \subset \{\delta \le \hat{\sigma} \le 2\delta, \omega \le 4\beta^2\delta\}$, *and*
- $E'' \in \frac{1}{r}\Psi_{\mathrm{b}}^{2s+1} + \mathrm{Diff}^1\Psi_{\mathrm{b}}^{2s} + \Psi_{\mathrm{b}}^{2s+1}$, *with* $\mathrm{WF}_{\mathrm{b}}' E'' \cap \dot{\Sigma} = \emptyset$.

All terms above have microsupport within $\operatorname{supp} a$.

Proof. We apply Lemma 26 and employ the notation therein. The term A_0 arising there has principal symbol $-\partial_\sigma(a^2)$ and arises from $\eth$ being nearly homogeneous in r of degree -1. We may rewrite the A_0 term in (25) as $A_0(\eth + D_t)$, modulo A_0 times smooth lower-order terms (which are then absorbed into $\mathbf{R}$). We now split the symbol of A_0 into three terms: those terms where the derivative falls on χ_0 can be written in the form $\widetilde{Q}^2 D_t$, which we write as the product of $\operatorname{sgn}(\tau_0)$ times squares Q^2 modulo a lower order error we that we absorb into $\mathbf{R}$. Meanwhile, those terms where the σ derivative falls on χ_1 we absorb into E' and those on which it falls on χ_2 we absorb into E''. Thus, modulo further commutators (again absorbed into the error terms $\mathbf{R}, \mathbf{R}_j$) we have written the first term on the RHS of (25) as $\tilde{R}\eth - \operatorname{sgn}(\tau_0)Q^*Q$.

The B_1 term arising in Lemma 26 enjoys the asserted symbol bounds because r derivatives on a^2 may only fall on the χ_0 term, giving

$$2|\tau|^{2s+1}(\chi_0'\chi_0)\chi_1^2\chi_2^2(-2r)(\beta^{-2}\delta^{-2});$$

since $0 \leq r \leq 2\beta\delta$ on the support of a, this term is estimated by a multiple of $\beta^{-1}\delta^{-1}|\tau|^{2s+1}\chi_0'\chi_0\chi_1^2\chi_2^2$, which in turn is a multiple of $\beta^{-1}\sigma_{\mathrm{b}}(Q)^2$. Likewise, the B_0 term in Lemma 26 becomes the B_0 term here and is estimated similarly, as the t derivative may also only hit the χ_0 term.

Finally, the $\mathbf{B}_2$ and $\mathbf{B}_3$ terms from Lemma 26 have symbols proportional to $\partial_\eta(a^2)$, so the derivative must fall on χ_2 and these terms are absorbed into E''. The $\mathbf{B}_5$ term is also absorbed into $\mathbf{R}$. □

We now return to the main argument. We pair $i^{-1}[\eth, A^*A]u$ with u and employ a regularization argument as in the elliptic setting. On the one hand, we may bound

$$|\langle[\eth, A^*A]u, u\rangle| = |\langle Au, A\eth u\rangle - \langle A\eth u, Au\rangle| \leq 2\|Au\|\|A\eth u\| \leq \epsilon\|Au\|^2+\epsilon^{-1}\|A\eth u\|^2.$$

On the other hand, we apply Lemma 35.

The main term is $-\operatorname{sgn}(\tau_0)\langle Q^*Qu, u\rangle = -\operatorname{sgn}(\tau_0)\|Qu\|^2$, which has a definite sign. We may then bound

$$\begin{aligned}\|Qu\|^2 \leq \epsilon\|Au\|^2 + \epsilon^{-1}\|A\eth u\|^2 + \left|\left\langle \widetilde{R}\eth u, u\right\rangle\right| + \left|\left\langle \mathbf{R}_1\frac{1}{r}u, u\right\rangle\right| + |\langle \mathbf{R}_2 D_r u, u\rangle| \\ + \left|\left\langle \mathbf{R}_3\frac{1}{r}\beta K u, u\right\rangle\right| + |\langle \mathbf{R}u, u\rangle| + |\langle B_0 u, u\rangle| + |\langle \alpha_r B_1 u, u\rangle| \\ + \left|\left\langle E'u, u\right\rangle\right| + \left|\left\langle E''u, u\right\rangle\right|.\end{aligned}$$

As $\widetilde{R} \in \Psi_{\mathrm{b}}^{2s}$, the $\left|\left\langle \widetilde{R}\eth u, u\right\rangle\right|$ term is bounded by $\|G_s\eth u\|\|G_s u\|$ for some $G_s \in \Psi_{\mathrm{b}}^s$. Similarly, the terms involving $\mathbf{R}_j$ can be estimated by $\|G_{s-1}u\|_{H^1}\|G_s u\|$ for some $G_{s-1} \in \Psi_{\mathrm{b}}^{s-1}$ and $G_s \in \Psi_{\mathrm{b}}^s$. As $\mathbf{R} \in \Psi_{\mathrm{b}}^{2s}$, the term $\langle \mathbf{R}u, u\rangle$ is bounded by $\|G_s u\|^2$. This leaves the terms involving B_0 and B_1 as well as the E' and E'' terms.

The following lemma allows us to bound the terms involving B_0 and B_1:

Lemma 36. *There exists $G \in \Psi_{\mathrm{b}}^s$ with $\mathrm{WF}_{\mathrm{b}}' G \cap \mathrm{WF}_{\mathrm{b}}^s u = \emptyset$ so that for $j = 0, 1$,*

$$|\langle B_j u, u\rangle| \leq C\beta^{-1}\|Qu\|^2 + C\|Gu\|_{L^2}^2 + C\|u\|_{H^1}^2.$$

Proof of Lemma 36. By the pseudodifferential calculus, we may write $B_j = QC_1C_2Q + R$, where $C_i \in \Psi_{\mathrm{b}}^0$ satisfies $|\sigma_{\mathrm{b}}(C_i)| \leq C\beta^{-1/2}$ and $R \in \Psi_{\mathrm{b}}^{2s}$, and

$$\left(\mathrm{WF}_{\mathrm{b}}' R \cup \mathrm{WF}_{\mathrm{b}}' C_i\right) \cap \mathrm{WF}_{\mathrm{b}}^s u = \emptyset.$$

For any $w \in L^2$ with $\mathrm{WF}_{\mathrm{b}}^0 w \cap \mathrm{WF}_{\mathrm{b}}' C_i = \emptyset$, our symbol estimate gives

$$\|C_i w\|_{L^2} \leq C\beta^{-1/2}\|G_0 w\|_{L^2} + C\|G_0 w\|_{H_{\mathrm{b},g}^{-1}} + C\|w\|_{H_{\mathrm{b},g}^{-N}} \tag{33}$$

for some microlocalizer $G_0 \in \Psi_{\mathrm{b}}^0$ with $\mathrm{WF}_{\mathrm{b}}'(1 - G_0) \cap \mathrm{WF}_{\mathrm{b}}' C_i = \emptyset$. In particular, then, setting $w = Qu$ yields

$$\|C_i Qu\| \leq C\beta^{-1/2}\|Qu\|_{H^1} + C\|Gu\|_{L^2} + C\|u\|_{H^1},$$

for $G = G_0 Q$ as in the statement of the lemma.

An application of Cauchy–Schwarz to $\langle B_j u, u\rangle$ then yields the stated estimate and concludes the proof of Lemma 36. $\square$

The term involving E' is bounded by $\left\|G_{s+1/2}u\right\|^2$, where $G_{s+1/2} \in \Psi_{\mathrm{b}}^{s+1/2}$ has $\mathrm{WF}'_{\mathrm{b}}\, G_{s+1/2} \subset \{\delta \leq \hat{\sigma} \leq 2\delta, \omega \leq 4\beta^2\delta^2\}$. The hypothesis that $U \cap \{\sigma > 0\} \cap \mathrm{WF}'^{1,s-1/2}_{\mathrm{b}}\, u = \emptyset$ implies that this term is finite.

Finally, we estimate the term involving E''. As the microsupport of E'' is contained in the elliptic set of $\eth$, we may use Corollary 31 to bound this term by

$$C\left(\|u\|^2_{H^1} + \|G_{s-1}u\|^2_{H^1} + \left\|\widetilde{G}_s \eth u\right\|^2_{L^2}\right),$$

where $G_{s-1} \in \Psi_{\mathrm{b}}^{s-1}$ and $\widetilde{G}_s \in \Psi_{\mathrm{b}}^{s}$ are microsupported in the elliptic region within U.

Thus,

$$\|Qu\|^2 \leq \epsilon\|Au\|^2 + \epsilon^{-1}\|A\eth u\|^2 + \left\|\widetilde{G}_s\eth u\right\|^2_{L^2} + \text{finite}, \tag{34}$$

where the terms labeled finite have been estimated by our inductive assumptions on u. Since $\sigma_b(A)/\sigma_b(Q) \leq C$, we may absorb the first term on the right into the left side modulo finite terms, provided ϵ is sufficiently small; $\|Qu\|$ is thus bounded. As Q is elliptic at ρ_0, $\rho_0 \notin \mathrm{WF}_{\mathrm{b}}^{s+1/2}\, u$ (and hence, by Lemma 34, not in $\mathrm{WF}_{\mathrm{b}}^{1,s-1/2}\, u$). This completes the proof of Theorem 22.

We now turn to the proof of Theorem 23. The arguments of Section 4.4 imply the propagation result away from the $r = 0$, so we need only prove the result through the singularity. We first describe the commutators of $\eth$ with R and K:

Lemma 37. *The commutators of $\eth$ with R^ℓ K^ℓ are as follows:*

1. *$[\eth, R^\ell]$ can be written as a linear combination of $\eth R^j$ (or, indeed, $R^j\eth$) and $R^j\mathbf{F}_j$ (or $\mathbf{F}_jR^j$), where $j = 0, 1, \ldots, \ell-1$ and $\mathbf{F}_j \in C^\infty$ (but not necessarily scalar).*
2. *$[\eth, K^\ell]$ is a linear combination of terms of the form $K^j\mathbf{B}K^{\ell-1-j}$, where $j = 0, 1, \ldots, \ell-1$ and $\mathbf{B} \in \mathrm{Diff}^1_{\mathrm{b}}$ only differentiates in the angular variables.*

Proof. To prove the first statement, we write $\eth = i\gamma^0\not{\partial}_{\mathsf{Z}/r} + \mathbf{R}$, where $\not{\partial}_{\mathsf{Z}/r}$ is the Dirac operator with potential $\mathbf{A} = (\mathsf{Z}/r, 0, 0, 0)$ and $\mathbf{R} = -\sum_{\mu=0}^3 \alpha_\mu A_\mu$. Because $\not{\partial}_{\mathsf{Z}/r}$ is homogeneous of degree -1 in (t, r), we see that

$$[\eth, R] = \frac{1}{i}(\eth - \mathbf{R}) + [\mathbf{R}, R] = \frac{1}{i}\eth + \mathbf{F}_0.$$

We then observe that

$$[\eth, R^k] = [\eth, R]R^{k-1} + R[\eth, R^{k-1}].$$

The first term on the right is then of the correct form by our calculation of $[\eth, R]$, while the second term is a linear combination of terms of the form

$R\eth R^j$ and $R\mathbf{F}R^j$, where $j = 0, 1, \ldots, k-2$ by the inductive hypothesis. As we can commute R with $\eth$ and $\mathbf{F}_j$ at the cost of lower order terms of the same form, this proves the first statement.

We prove the second statement similarly. Because K commutes with $\not{\partial}_{\mathsf{Z}/r}$ and γ^0, we can see that

$$[\eth, K^\ell] = [\mathbf{R}, K^\ell] = \sum_{j=0}^{\ell-1} K^j [\mathbf{R}, K] K^{\ell-1-j}.$$

As $\mathbf{R}$ is non-scalar, $[\mathbf{R}, K] \in \mathrm{Diff}_{\mathrm{b}}^1$ is only a first order differential operator, but differentiates only in the angular variables. Taking $\mathbf{B} = [\mathbf{R}, K]$ finishes the proof. $\square$

We now proceed inductively to prove Theorem 23; the case $\ell = 0$ is handled above in the proof of Theorem 22. Setting $S = K$ or $S = R$ as appropriate, we proceed using the commutants

$$W_\ell = S^\ell A^* A S^\ell,$$

where A is the commutant employed above. Commuting $\eth$ with W_ℓ yields

$$[\eth, W_\ell] = S^\ell [\eth, A^* A] S^\ell + [\eth, S^\ell] A^* A S^\ell + S^\ell A^* A [\eth, S^\ell]. \tag{35}$$

After applying the operator and pairing with u, the first term yields the same terms in the argument above with $\ell = 0$ (sandwiched between factors of S). Our aim is therefore to absorb or otherwise bound the terms arising from commuting $\eth$ with S^ℓ and pairing with u.

In the case of $S = R$, Lemma 37 allows us to bound the remaining two terms by

$$\epsilon \left\| A R^\ell u \right\|^2 + C\epsilon^{-1} \sum_{j=0}^{\ell-1} \left(\left\| A R^j \eth u \right\|^2 + \left\| A R^j F_j u \right\|^2 \right),$$

$F_j \in \mathcal{C}^\infty$. The first term in this bound can be absorbed into the main term arising from the commutator $[\eth, A^* A]$ in equation (35), while the second term is finite by the hypothesis on $\eth u$. The third term is finite by the inductive hypothesis.

We now consider the case of $S = K$. By Lemma 37, the remaining two terms are bounded by

$$\epsilon \left\| A K^\ell u \right\|^2 + C\epsilon^{-1} \sum_{j=0}^{\ell-1} \left\| A K^j \mathbf{B} K^{\ell-1-j} u \right\|^2.$$

Each of these terms will ultimately be absorbed into the main term by choosing δ sufficiently small using the following lemma:

Lemma 38. *Suppose A is defined as above and $Q \in \Psi_{\mathrm{b}}^{s+1/2}$ is invariant with symbol*

$$\sigma_{\mathrm{b}}(Q) = \sqrt{2} |\tau|^{s+1/2} \delta^{-1/2} (\chi_0' \chi_0)^{1/2} \chi_1 \chi_2 1_{\operatorname{sgn} \tau = \operatorname{sgn} \tau_0}.$$

There exists some C (independent of δ) and some $G \in \Psi_{\mathrm{b}}^{s-1/2}$ so that

$$\|Au\| \leq C\left(\sqrt{\delta}\|Qu\| + \|Gu\| + \|u\|\right).$$

Proof. The proof is nearly identical to the one in Lemma 36; because $\sigma_{\mathrm{b}}(A)$ is a multiple of $\sigma_{\mathrm{b}}(Q)$, we may write $A = CQ + R$, where $C \in \Psi_{\mathrm{b}}^{0}$ has principal symbol

$$\sigma_{\mathrm{b}}(C) = (2 - \phi/\delta)\sqrt{\delta}/\sqrt{2}.$$

Introducing the microlocalizer G as in Lemma 36 finishes the proof. □

We now claim that we can bound $\left\|AK^j\mathbf{B}K^{\ell-1-j}u\right\|$ by $\left\|AK^{\ell}u\right\|$ and terms that are finite by the inductive hypothesis. Given this claim, Lemma 38 then allows us to absorb these terms into the main one by choosing δ sufficiently small, finishing the proof.

The rest of the section is devoted to the proof of the claim. First observe that because $\mathbf{B}$ and K are differential operators acting only in the angular variables, we may replace them by scalar operators in these variables, i.e., we may first bound

$$\left\|AK^j\mathbf{B}K^{\ell-1-j}u\right\| \leq C\sum_{|\alpha|\leq\ell}\|A\partial_\theta^\alpha u\|,$$

where C is independent of u. All but the terms with $|\alpha| = \ell$ are finite by the inductive hypothesis. Because A and ∂_θ^α are scalar operators, we again appeal to the inductive hypothesis so that it suffices to bound $\|\partial_\theta^\alpha Au\|$ for $|\alpha| = \ell$. For $\ell = 2m$ even, it suffices to control $\|\Delta_\theta^m Au\| + \|Au\|$, while for $\ell = 2m+1$, the following lemma shows that it is enough to control $\|K\Delta_\theta^m Au\| + \|Au\|$.

Lemma 39. *There is a constant C so that for any $u \in H^1_{\mathrm{b},g}$,*

$$\|\nabla_\theta u\| \leq C\left(\|Ku\| + \|u\|\right),$$

where the norms are taken with respect to L^2.

Proof. Note that because K contains only angular derivatives, $\|Ku\| \leq C\|\nabla_\theta u\|$. We then use that $\Delta_\theta = K^2 - \beta K$ to see that

$$\begin{aligned}\|\nabla_\theta u\|^2 &= \langle\Delta_\theta u, u\rangle = \left\langle(K^2 - \beta K)u, u\right\rangle \\ &\leq \left\|K^2 u\right\| + \|Ku\|\|u\| \leq C\left(\|Ku\|^2 + \|u\|^2\right).\end{aligned}$$

□

We now rely on Lemma 4 and the following observation: Because $K^2 = \Delta_\theta + \beta K$,

$$K^{2m} = \Delta_\theta^m + \mathcal{L}_{2m}, \quad K^{2m+1} = \Delta_\theta^m K + \mathcal{L}_{2m+1}, \tag{36}$$

where $\mathcal{L}_{2m}$ is a constant linear combination of $\Delta_\theta, \dots, \Delta_\theta^{m-1}$ and $\beta K, \Delta_\theta\beta K, \dots, \Delta_\theta^{m-1}\beta K$, while $\mathcal{L}_{2m+1}$ is a linear combination of $\beta\Delta_\theta, \dots, \beta\Delta_\theta^m$ and $K, \Delta_\theta K, \dots, \Delta_\theta^{m-1}K$.

For $\ell = 2m$, we obtain (using Lemma 4)

$$\|\Delta_\theta^m A u\| = \|A\Delta_\theta^m u\| \leq \left\|AK^{2m}u\right\| + \|A\mathcal{L}_{2m}u\|,$$

where the second term is finite by the inductive hypothesis. Likewise for odd $\ell = 2m+1$,

$$\|\Delta_\theta^m KAu\| = \|AK\Delta_\theta^m u\| \leq \left\|AK^{2m+1}u\right\| + \|A\mathcal{L}_{2m+1}u\|, \tag{37}$$

where again by the inductive hypothesis the last term is finite. This finishes the proof of the claim and thus the proof of Theorem 23.

6. Geometric improvement

In this section we prove the second part of Theorem 1, i.e., we show that the part of the singularity of the fundamental solution lying on the diffracted wave front D and away from the geometrically propagated light cone G is $1-0$ derivatives smoother than the singularity along G.

There are two main steps to this argument. In the first (Section 6.1), we describe the propagation of edge regularity, which allows us to propagate coisotropic regularity along the geometric geodesics under a "non-focusing" condition. In the second part (Section 6.2), we show that we can apply the arguments of the first to a propagator.

6.1. **Propagation of edge regularity.** In this section we establish the propagation of edge regularity. The propagation argument in this setting is somewhat less sensitive to lower-order terms and so we are able to work with the second order operator in this section.

Let P be an operator satisfying the Klein-Gordon Hypotheses in Section 4.3; recall that this means

$$P\psi = -(\partial_0 + i\frac{\mathsf{Z}}{r})^2 + \sum \partial_j^2 - m^2 - i\frac{\mathsf{Z}}{r^2}\begin{pmatrix} 0 & \sigma_r \\ \sigma_r & 0 \end{pmatrix} + \mathbf{R} \tag{38}$$

with

$$\mathbf{R} = \mathsf{Z}\frac{\mathbf{W}_0}{r} + \mathbf{W}_1^\alpha \partial_\alpha + \mathbf{W}_2, \tag{39}$$

where the $\mathbf{W}_\bullet$ coefficients are smooth but non-scalar.

As before, let $X = [\mathbb{R}^3; 0]$ and $M = [\mathbb{R}^{1+3}; \mathbb{R}_t \times \{0\}]$. We now view P as an operator in the *edge* calculus on M :

$$P \in r^{-2}\operatorname{Diff}^2_{\mathrm{e}}(\mathbb{R}\times X)$$

with

$$\sigma_{\mathrm{e}}(P) = \frac{\lambda^2 - \xi^2 - |\zeta|^2_{S^2}}{r^2}.$$

The associated Hamilton vector field is then

$$\mathsf{H} = \frac{2}{r^2}\left(\left(\xi^2 + |\zeta|^2_{S^2}\right)\partial_\xi + \xi\lambda\partial_\lambda + \xi r\partial_r - \lambda r\partial_t\right) - \frac{1}{r^2}\mathsf{H}_{S^2},$$

where H_{S^2} denotes the geodesic flow in $(\theta,\zeta) \in T^*S^2$. Let $\Sigma \subset {}^{\mathrm{e}}S^*(\mathbb{R}\times X)$ denote the characteristic set of P.

Recall that we have defined the edge Sobolev spaces be defined with respect to the b-weight as in [32], [30]. Thus

$$L^2_g = r^{-3/2} H^0_{\mathrm{e}}.$$

Likewise this is the scale on which we measure Sobolev-based edge wavefront set $\mathrm{WF}^*_{\mathrm{e}}$.

We let $\mathcal{M}$ denote the graded module generated by angular derivatives ∇_{S^2}. Let $\mathcal{A}^*$ denote the filtered algebra over $\Psi^0_{\mathrm{e}}(M)$ generated by $\mathcal{M}$. Hence $\mathcal{A}$ is locally generated by the operators D_{θ_j}.

We will additionally be interested in testing for conormal regularity along $N^*(\{t = r + r'\})$. In addition to iterated regularity under vector fields $D_\theta \in \mathcal{M}$, this involves regularity under the operator

$$R = (t - r')D_t + rD_r; \tag{40}$$

cf. (23) where this operator appears with $r' = 0$. We will often take advantage of time-translation invariance and tacitly set $r' = 0$ in computing with this vector field.

The fact that, unlike the D_{θ_j}'s, R is not an edge vector field entails some minor technical complication in what follows.

The commutator properties of P with R and with the generators of $\mathcal{A}$ play an important role in what follows. As we are working in a simpler geometric setting than that of [30], we revert to the simple expedient of using Δ_θ, the angular Laplacian, as a test operator for regularity in $\mathcal{A}$.

Lemma 40. $[P, \Delta_\theta] = Q_0 D_r + Q_1 D_t + r^{-2} Q_2$ *and* $[P, R] = -2iP + \dfrac{1}{r} Q_3$ *where*

$$Q_j \in \mathrm{Diff}^1(S^2), \quad j = 0, 1, 2, \quad \textit{and} \quad Q_3 \in \mathrm{Diff}^1_{\mathrm{e}}(M).$$

Proof. All terms in the model operator $P - \mathbf{R}$ with exact Coulomb potential (see (21)) commute with Δ_θ, except for the matrix valued term

$$-i\frac{\mathsf{Z}}{r^2}\begin{pmatrix} 0 & \sigma_r \\ \sigma_r & 0 \end{pmatrix};$$

commuting this with Δ_θ gives the $r^{-2}Q_2$ term above, while the terms in $\mathbf{R}$ contribute to the remaining error terms in $[P, \Delta_\theta]$.

Additionally, by exact scaling symmetry in t, r

$$[P + m^2 - \mathbf{R}, R] = (-2i)(P + m^2 - \mathbf{R}),$$

hence lumping the remaining terms in the $r^{-1}Q_3$ term gives the desired expression for $[P, R]$. $\square$

As above, let the canonical one form on ${}^{\mathrm{e}}T^*M$ be

$$\lambda \frac{dt}{r} + \xi \frac{dr}{r} + \zeta \cdot d\theta.$$

Let

$$\mathsf{IC}_\pm(t_0, \theta_0) \equiv \big\{t = t_0,\ r = 0,\ \theta = \theta_0,\ \lambda = \pm 1,\ \xi = \pm 1,\ \zeta = 0\big\} \subset {}^{\mathrm{e}}S^*_{\mathbb{R}\times\partial X}(M),$$

$\mathsf{OG}_\pm(t_0,\theta_0) \equiv \big\{t=t_0,\ r=0,\ \theta=\theta_0,\ \lambda=\pm 1,\ \xi=\mp 1,\ \zeta=0\big\} \subset {}^{\mathrm{e}}S^*_{\mathbb{R}\times\partial X}(M).$
These are the endpoint of the closures of bicharacteristic reaching the front face of the blowup (i.e., the origin in the blown-down space) from the interior as time increases ("incoming") resp. as times decreases ("outgoing"). Note indeed that $\mathsf{IC}\cup\mathsf{OG}$ accounts for all the radial points of the edge Hamilton vector field H.

We now let $\mathcal{F}$ denote the backward resp. forward flowouts of boundary points: if $p=\mathsf{IC}_\pm(t_0,\theta_0)$, let

$$\mathcal{F}_I(p) \equiv \big\{t=t_0-r,\ r\in(0,\epsilon),\ \theta=\theta_0,\ \lambda=\pm 1,\ \xi=\pm 1,\ \zeta=0\big\} \subset {}^{\mathrm{e}}S^*(M),$$

and if $p=\mathsf{OG}_\pm(t_0,\theta_0)$, let

$$\mathcal{F}_O(p) \equiv \big\{t=t_0+r,\ r\in(0,\epsilon),\ \theta=\theta_0,\ \lambda=\pm 1,\ \xi=\mp 1,\ \zeta=0\big\} \subset {}^{\mathrm{e}}S^*(M).$$

These are the unique interior bicharacteristics containing the corresponding radial points in their closures.

We now state a theorem about propagation of edge wavefront set, together with module regularity.

Theorem 41. *Suppose $u\in H_{\mathrm{e}}^{-\infty,l}(M)$ solves*

$$Pu=0$$

with P satisfying the Klein-Gordon Hypotheses from §4.3.

(1) *Let $m>l+1$. Set $p=\mathsf{IC}_\pm(t_0,\theta_0)$. If $\mathcal{F}_I(p)\cap \mathrm{WF}_{\mathrm{e}}^m(\Delta_\theta^j u)=\emptyset$ for all $j=0,\dots,k$ then*
$$p\notin \mathrm{WF}_{\mathrm{e}}^{m,l'}(\Delta_\theta^j u)$$
for all $j=0,\dots,k$ and all $l'<l$.

(2) *Let $m<l+1$. Set $p=\mathsf{OG}_\pm(t_0,\theta_0)$. Let U denote a punctured neighborhood of p in ${}^{\mathrm{e}}S^*_{\mathbb{R}\times\partial X}(\mathbb{R}\times X)$. If $U\cap \mathrm{WF}_{\mathrm{e}}^{m,l}\Delta_\theta^j u=\emptyset$ for all $j=0,\dots,k$ then*
$$p\notin \mathrm{WF}_{\mathrm{e}}^{m,l}(\Delta_\theta^j u)$$
for all $j=0,\dots,k$.

(3) *For all m, and $l'\le l$,*
$$\mathrm{WF}_{\mathrm{e}}^{m,l'} u\cap {}^{\mathrm{e}}S^*_{\mathbb{R}\times\partial X}(M)$$
is a union of maximally extended null bicharacteristics.

(4) *Suppose additionally that $R^j u\in H_{\mathrm{e}}^{-\infty,l}$ and that $p\in\mathsf{OG}_\pm(t_0,\theta_0)$ has a neighborhood $U\subset {}^{\mathrm{e}}S^*_{\mathbb{R}\times\partial X}(\mathbb{R}\times X)$ such that $U\cap\mathrm{WF}_{\mathrm{e}}^{m,l}u\subset\mathsf{OG}$. Then for $0\le j'\le j$, $p\notin\mathrm{WF}_{\mathrm{e}}^{M,l}(R^j u)$ for $j\in\mathbb{N}$, provided $M\le m-j$ and $M\le l+1$.*

As shown [32, Section 6], the propagation along null bicharacteristics within ∂M (part (3) above) connects points in IC and points in OG lying over points θ_0,θ_1 that are separated by geodesics of length π with respect to the metric on ∂X. Here ∂X is simply S^2, so this means that the propagation is from a point θ_0 to its antipodal point $\theta_1=-\theta_0$.

The theorem thus says that regularity propagates

(1) From the interior of M into incoming radial points in ∂M (a.k.a. the lift of $r=0$ under blowup) along bicharacteristics, above some threshold regularity dictated by the weight in r
(2) Across ∂M along bicharacteristics, from incoming radial points to antipodal outgoing radial points (instantaneously)
(3) From outgoing radial points back into the interior of M, up to some threshold regularity dictated by the weight in r.

Owing to the limits in regularity in the outgoing part of the theorem (which is typical in radial point problems—cf. [34]), this result does not in fact say that regularity arrives at the boundary, propagates across it, and leaves, at any given Sobolev order. Obtaining regularity (and, ultimately, conormality) at the outgoing wavefront will require subtler arguments involving D_θ and R regularity, hence the need for these factors to propagate through our estimates as well.

Proof. The proof is the same as that of Theorem 8.1 of [32]. We sketch the first part here in order to verify that the passage to a slightly different class of operators under consideration here (with cross term involving $r^{-1}\partial_t$, inverse square potential terms, a principally scalar system with a large anti-self-adjoint 0'th order term) do not vitiate the arguments used there.

Let $p = \mathsf{IC}_\pm(t_0,\theta_0)$. We will begin by sketching the proof of the following propagation result, which gives the first part of the theorem up to the factors in of Δ_θ^k

Propagation Estimate 1. If $m' > l'+1/2$, $u \in H_{\mathrm{e}}^{-\infty,l'}(M)$, $p \notin \mathrm{WF}_{\mathrm{e}}^{m',l'}(u)$, and $\mathcal{F}_I(p) \cap \mathrm{WF}^{m'+1/2}\, u = \emptyset$, then $p \notin \mathrm{WF}_{\mathrm{e}}^{m'+1/2,l'}\, u$.

To establish Propagation Estimate 1 we choose $A \in \Psi_{\mathrm{e}}^{m',l'+1/2}$ such that

$$P^*A^*A - A^*AP = \pm(A')^*(A') \pm \sum B_j^* B_j + E + K + F, \tag{41}$$

where

(1) A, A' are microsupported near p.
(2) $A' \in \Psi_{\mathrm{e}}^{m'+1/2,l'+3/2}$ with $\sigma_{\mathrm{e}}(A') = \sigma_{\mathrm{e}}(A)\cdot(\pm(m'+l'+1/2)\xi)^{1/2}$
(3) $E \in \Psi_{\mathrm{e}}^{2m'+1,2l'+3}$ and $\mathrm{WF}'\, E$ is in an arbitrarily small neighborhood of a single point in $\mathcal{F}_I(p)$.
(4) $K \in \Psi_{\mathrm{e}}^{2m'+1,2l'+3}$ and $\mathrm{WF}'\, K \cap \Sigma = \emptyset$
(5) F is of lower order, lying in $\Psi_{\mathrm{e}}^{2m',2l'+3}$. (Note that it is only the pseudodifferential order that is lower, not the weight.)

Notwithstanding that our convention for b-Sobolev spaces is to base them on L^2_b, the adjoints above are all taken with respect to the inner product on L^2_g, as we will use this inner product (with respect to which P is mostly self-adjoint) in making a pairing argument below.

The operator A is constructed roughly as follows: if $m+l>0$, then $\mathsf{H}(\lambda^m r^l) = (m+l)\xi\lambda^m r^l$, so that if $\chi(s) \equiv 0$ for $s<0$ and $\chi(s) \equiv 1$

for $s \geq 1$, $\mathsf{H}\left(\chi(\pm\lambda)\chi(\pm\xi)(\pm\lambda)^m r^l\right)$ has the same sign as ξ (the $\pm$ used here). We can localize in the θ variable as in the more general treatment in [32, Section 6] by using a function given, in our blown-down Euclidean coordinates $(x, \underline{\xi}) \in T^*\mathbb{R}^3$ by cutting off $-\hat{\underline{\xi}}$ to lie in a small neighborhood of any desired θ_0; such a cutoff manifestly commutes with the Hamilton flow, and is shown in [32] to lift to be a smooth symbol on ${}^{\mathrm{b}}T^*M$. If a geodesic arrives at the origin, then since it is oriented radially, its angle of arrival $\theta \in S^2$ is manifestly $-\hat{\underline{\xi}}$, hence we have achieved an angular localization. Finally, a cutoff in $|\zeta|/|\lambda|$ has the same sign as the signed terms listed above. Thus, the product of these cutoffs localizing in θ, ζ with $\chi(\pm\lambda)\chi(\pm\xi)(\pm\lambda)^m r^l$ may be quantized to give an A with the desired properties – see Lemma 7.1 of [32] for details.

We remark that the system under consideration here may be treated as a scalar equation from the point of view of the positive commutator argument because the principal symbol of P in the edge calculus is scalar. In particular, the anti-self-adjoint term in P,

$$-i\frac{\mathsf{Z}}{r^2}\begin{pmatrix} 0 & \sigma_r \\ \sigma_r & 0 \end{pmatrix},$$

which is large enough to disrupt commutator arguments in the b-calculus, lies in $\Psi_{\mathrm{e}}^{0,2}$, hence in the twisted commutator $P^*A^*A - A^*AP$ gives rise to a term in $\Psi^{2m',2l'+3}$ which may be included in the lower-order error term F above.

Now the propagation argument follows by pairing the equation (41) with u, *using the metric inner product* $r^2\,dr\,d\theta$. The left-hand-side is zero, by integration by parts. Technically, in fact, we require an approximation of A by operators in $\Psi_{\mathrm{e}}^{-\infty,l'+1/2}$ in order to justify this integration by parts—see [32] for details of this approximation process, which involve a family of smoothing operators A_δ with a further parameter approximating A as $\delta \downarrow 0$.

The terms of the right hand side of the pairing are then as follows. The term $\|A'u\|^2_{L^2_g}$ is precisely what we need to control: note that in terms of the b/edge-volume form $dr/r\,dt\,d\theta = r^{-3}dV_g$, this term is of the form

$$\left\| r^{3/2}A' \right\|^2_{L^2_e},$$

hence controls $\mathrm{WF}_{\mathrm{e}}^{m'+1/2,l'}\,u$. The terms $\|Bu\|^2$ have the same sign, and hence may be dropped. The term with E is controlled by our incoming wavefront set hypothesis. The term with K is controlled by microlocal elliptic regularity. And the term with F is controlled by our assumption $p \notin \mathrm{WF}_{\mathrm{e}}^{m',l'}\,u$. This concludes our proof of Propagation Estimate 1.

Now we can employ Propagation Estimate 1 iteratively to obtain the first part of the theorem, in the case $k = 0$. We know a priori that $u \in H_{\mathrm{e}}^{q,l}$ for *some* q; if $q > l + 1/2$ we may immediately iterate the propagation estimate to obtain the result of the theorem. If not, we must artificially lower our l

to some $l' < q - 1/2$ in order to start the iteration. In this case, however, an interpolation argument still recovers the result but ends up with $l' = l - \epsilon$ for any desired $\epsilon > 0$—see Figure 1 of [32] and related discussion.

To include the module regularity in the first part of the theorem, we proceed inductively, employing the same commutant as above and considering the twisted product

$$\begin{aligned} &P^* \Delta_\theta^k A^* A \Delta_\theta^k - \Delta_\theta^k A^* A \Delta_\theta^k P \\ &\quad = [P^*, \Delta_\theta^k] A^* A \Delta_\theta^k - \Delta_\theta^k A^* A [\Delta_\theta^k, P] \\ &\qquad + \Delta_\theta^k \left(P^* A^* A - A^* A P\right) \Delta_\theta^k. \end{aligned} \tag{42}$$

The last term gives rise to similar terms as in the propagation estimate (with u replaced by $\Delta_\theta^k u$) and so allow us to control $\mathrm{WF}_{\mathrm{e}}^{m'+1/2,l'} \Delta_\theta^k u$. Indeed, together with terms that are finite by induction, this term controls $\sum_{|\alpha|\leq 2k} \|D_\theta^\alpha A' u\|^2$ with A' as before. The first two terms on the RHS of (42) can then be absorbed into this main term (modulo inductively finite terms); here we use the fact that while having the same order, these error terms have a smaller r weight.

are controlled by the induction hypothesis (together with the description of $[P, \Delta_\theta]$ given by Lemma 40).

The remaining parts of the theorem follow in an essentially identical way to those of Theorem 8.1 of [32], and similar to the arguments given above. □

6.2. **Global propagation of coisotropic regularity.** Our aim in this section is to apply Theorem 41 to the solution of $(i\partial\!\!\!/_{\mathbf{A}} - m)u = 0$ with initial condition $\psi_0 \delta_y$ and verify that the diffracted wavefront is $1 - 0$ orders smoother than the propagated one.

The sketch of the proof is as follows: For each time, the solution is a distribution u of Sobolev order $-3/2 - 0$. An angularly smoothed version of the solution, $\langle \Delta_\theta \rangle^{-M} u$ (for $M \gg 0$) is, by contrast, a distribution of order $-1/2 - 0$. (In the language below, u has global nonfocusing regularity of order $-1/2 - 0$). Additionally, at a point on the diffracted front away from the propagated light cone, Theorem 41 shows that u has infinite order coisotropic regularity with respect to a *weaker* Sobolev norm, i.e., $D_\theta^\alpha u \in H^k$ for all α, with k fixed. Interpolation of the coisotropic regularity with the angular smoothing effect then shows that in fact u has infinite order coisotropic regularity with respect to the *better space* (up to an ϵ loss) and therefore is locally a distribution of Sobolev order $-1/2 - 0$ enjoying coisotropic regularity. Additionally propagating powers of $R = tD_t + rD_r$ through the evolution then suffices to show that u enjoys Lagrangian regularity with respect to $H^{-1/2-0}$ along the diffracted wave, as desired.

Definition 42. Fix a Hilbert space $\mathcal{H}$ and a set $K \subset {}^{\mathrm{b}}S^*(M)$.

A distribution on $\mathbb{R} \times X$ enjoys *coisotropic regularity* (of order $2N$) with respect to $\mathcal{H}$ on K if there exists a properly supported operator $A \in \Psi_{\mathrm{b}}^0(M)$,

elliptic on K, such that
$$(\mathrm{Id}+\Delta_\theta)^N Au \in \mathcal{H}.$$

A distribution on M is *nonfocusing* with respect to $\mathcal{H}$ on K if there exists a properly supported operator $A \in \Psi_{\mathrm{b}}^0(M^\circ)$, elliptic on K and there exists $N \in \mathbb{N}$ such that
$$Au = (\mathrm{Id}+\Delta_\theta)^N u', \quad u' \in \mathcal{H}.$$

We also make analogous definitions at the level of Cauchy data, i.e., distributions on X: if $\mathcal{H}'$ is a Hilbert space of distributions on X, and $K \subset {}^{\mathrm{b}}S^*X$, a distribution on X enjoys coisotropic regularity (of order $2N$) with respect to $\mathcal{H}$ on K if there exists a properly supported operator $A \in \Psi_{\mathrm{b}}^0(X)$, elliptic on K, such that
$$(\mathrm{Id}+\Delta_\theta)^N Au \in \mathcal{H}.$$

A distribution on X is nonfocusing with respect to $\mathcal{H}'$ on K if there exists a properly supported operator $A \in \Psi_{\mathrm{b}}^0(M)$, elliptic on K and there exists $N \in \mathbb{N}$ such that
$$Au = (\mathrm{Id}+\Delta_\theta)^N u', \quad u' \in \mathcal{H}'.$$

One could of course refine the nonfocusing definition by specifying in the terminology the power N for which it holds, but in practice we will be concerned with the union of this nonfocusing condition over all possible N. In this paper, moreover, we will mainly be concerned with localizing over a particular set in the t variable, but will neither localize in other variables nor microlocalize, hence the subtleties of microlocalizing in the b-calculus are moot.

In practice, it is convenient to take $\mathcal{H}$ to be $L^2_{\mathrm{loc}}(\mathbb{R};\mathcal{D}^s)$ (where we will drop the "loc" from now on as global estimates in time play no role here). This formulation is convenient for duality arguments owing to the sensible behavior of these spaces near the origin, but away from the origin, we remark that nonfocusing with respect to $\mathcal{D}^s$ is in fact equivalent to nonfocusing with respect to H^s.

Note also that we may equivalently test for coisotropic regularity with powers of Dirac's angular operator K instead of powers of Δ_θ : Since
$$K^2 - \beta K = \Delta_\theta,$$
regularity under powers of K up to $2N$ yields regularity under $(\mathrm{Id}+\Delta_\theta)^N$; conversely, regularity under $(\mathrm{Id}+\Delta_\theta)^N$ yields K-regularity by ellipticity of Δ_θ in the angular variables. Likewise the condition of nonfocusing can be recast as lying in the range of sums of powers of K, and we will use this alternative version below.

Lemma 43. *Let*
$$(i\partial\!\!\!/_{\mathbf{A}} - m)u = 0.$$
If for some $\epsilon > 0$, u enjoys coisotropic regularity of order N with respect to $L^2_{loc}(\mathbb{R};\mathcal{D}^s)$ on $(-\epsilon,\epsilon)_t \times X$ then u enjoys coisotropic regularity of order N with respect to $L^2_{loc}(\mathbb{R};\mathcal{D}^s)$ globally on M.

If for some $\epsilon > 0$, u enjoys the nonfocusing condition with respect to $L^2_{loc}(\mathbb{R}; \mathcal{D}^s)$ on $(-\epsilon, \epsilon)_t \times X$ then u enjoys the nonfocusing condition with respect to $L^2_{loc}(\mathbb{R}; \mathcal{D}^s)$ globally on M.

The conditions of coisotropic regularity resp. nonfocusing w.r.t. $L^2_{loc}(\mathbb{R}; \mathcal{D}^s)$ are moreover equivalent to the conditions of coisotropic regularity resp. nonfocusing of the Cauchy data $u(t_0)$ (for any t_0) w.r.t $\mathcal{D}^s$.

Proof. We begin with coisotropic regularity. By Lemma 16,

$$\frac{d}{dt}\left\|K^j u\right\|^2_{\mathcal{D}^s} \lesssim \left|\langle [K^j, \mathcal{B}]u, K^j u\rangle_{\mathcal{D}^s}\right|. \tag{43}$$

By Lemma 37 $[\mathcal{B}, K^j]$ is a linear combination of terms of the form $K^{j'}\mathbf{B}K^{j-1-j'}$, where $j' = 0, 1, \ldots, j-1$ and $\mathbf{B} \in \mathrm{Diff}^1_{\mathrm{b}}$ only differentiates in the angular variables. Thus by Lemma 39 and the following discussion, we may bound

$$\left|\left\langle K^{j'}\mathbf{B}K^{j-1-j'}u, K^j u\right\rangle_{\mathcal{D}^s}\right| \lesssim \sum_{j' \leq j} \left\|K^{j'}u\right\|^2_{\mathcal{D}^s}$$

Thus by Cauchy–Schwarz and Gronwall, (43) yields inductively for all T, j,

$$\sum_{j'=0}^{j} \left\|K^{j'}u(t)\right\|_{\mathcal{D}^s} \leq C_{T,j} \sum_{j'=0}^{j} \left\|K^{j'}u(0)\right\|_{\mathcal{D}^s}, \quad |t| \leq T.$$

This shows that coisotropic regularity of the Cauchy data propagates, and moreover that coisotropic regularity of the Cauchy data implies $L^\infty_{\mathrm{loc}}(\mathbb{R}; \mathcal{D}^s)$ coisotropic regularity of the spacetime solution. Conversely, knowing merely $L^2\mathcal{D}^s$ coisotropic regularity of the spacetimes solution implies that for a.e. t, the Cauchy data $u(t)$ enjoys coisotropic regularity, which then in turn propagates to yield $L^\infty_{\mathrm{loc}}(\mathbb{R}; \mathcal{D}^s)$ spacetime regularity. This finishes the proof of the lemma for coisotropic regularity.

We now turn to nonfocusing. We note that by the coisotropic results, applied backwards in time, if we let $\mathcal{H}$ denote the Hilbert space with squared norm

$$\sum_{j'=0}^{j} \left\|K^{j'}u\right\|^2_{\mathcal{D}^s}, \tag{44}$$

then we have estimated

$$U(t)\mathcal{H} \to L^\infty_{\mathrm{loc}}(\mathbb{R}; \mathcal{H}). \tag{45}$$

In particular, for fixed t, $U(-t)$ is bounded $\mathcal{H} \to \mathcal{H}$. Thus (by unitarity on $\mathcal{D}^s$,) $U(-t) = U(t)^* : \mathcal{H}^* \to \mathcal{H}^*$, with dual spaces taken with respect to $\mathcal{D}^s$ inner product. By the Riesz lemma,

$$\mathcal{H}^* = \sum_{j'=0}^{j} K^{j'}\mathcal{D}^s. \tag{46}$$

This is just the space of Cauchy data nonfocusing with respect to $\mathcal{D}^s$, hence the nonfocusing of Cauchy data is preserved under propagation. Moreover, uniformity in t of the maps $\mathcal{H} \to \mathcal{H}$ show the uniformity in t of the dual maps, hence yield the equivalence with nonfocusing with respect to $L^2_{\text{loc}}(\mathbb{R}; \mathcal{D}^s)$ as above in the coisotropic regularity case. $\square$

In order to show conormal regularity of the diffracted wavefront, it is useful to have a refinement of Lemma 43 that additionally allows powers of the scaling operator R.

Lemma 44. *Let*

$$(i\not{\partial}_{\mathbf{A}} - m)u = 0.$$

Fix $k \in \mathbb{N}$. If for some $\epsilon > 0$, $u, Ru, \dots, R^k u$ enjoy coisotropic regularity of order N with respect to $L^2_{loc}(\mathbb{R}; \mathcal{D}^s)$ on $(-\epsilon, \epsilon)_t \times X$ then $u, Ru, \dots, R^k u$ enjoy coisotropic regularity of order N with respect to $L^2_{loc}(\mathbb{R}; \mathcal{D}^s)$ globally on M.

If for some $\epsilon > 0$, $u, \dots, R^k u$ enjoy the nonfocusing condition with respect to $L^2_{loc}(\mathbb{R}; \mathcal{D}^s)$ on $(-\epsilon, \epsilon)_t \times X$ then $u, \dots, R^k u$ enjoy the nonfocusing condition with respect to $L^2_{loc}(\mathbb{R}; \mathcal{D}^s)$ globally on M.

The conditions of coisotropic regularity resp. nonfocusing w.r.t. $L^2_{loc}(\mathbb{R}; \mathcal{D}^s)$ for $R^j u$ are moreover equivalent to the conditions of coisotropic regularity resp. nonfocusing of the Cauchy data $\widetilde{R}^j u(t_0)$, where $\widetilde{R} = -t\mathcal{B} + rD_r$ (for any $t \in \mathbb{R}$) w.r.t $\mathcal{D}^s$.

Proof. To obtain the propagation of coisotropic regularity of order N, we recall from Lemma 37 that

$$\eth R^k u = \sum_{k'=0}^{k-1} \mathcal{C}^\infty R^{k'} u \tag{47}$$

(with the $\mathcal{C}^\infty$ terms non-scalar). Thus, if $\mathcal{H}$ is defined as in (44), and if we inductively assume that $u, \dots, R^{j-1} u$ enjoy coisotropic regularity, i.e., lie in $L^\infty_{\text{loc}}(\mathbb{R}; \mathcal{H})$, then

$$\eth R^j u = \sum_{j'=0}^{j-1} \mathcal{C}^\infty R^{j'} u \in L^\infty(\mathbb{R}; \mathcal{H}).$$

Moreover if we assume that $R^j u$ has coisotropic regularity initially, then it has initial data in $\mathcal{H}$. Duhamel's theorem (employed with values in $\mathcal{H}$) and (45) then imply that

$$R^j u \in L^\infty(\mathbb{R}; \mathcal{H})$$

as well; this inductively shows propagation of coisotropic regularity for $R^j u$.

The equivalence with the Cauchy data statement simply follows from the fact that

$$Ru = \widetilde{R} u$$

for solutions of the Dirac equation.

To obtain the propagation of nonfocusing for $R^j u$, where we have to dualize in powers of K but not in powers of R, we apply the same argument as above but with solutions in $L^\infty(\mathbb{R};\mathcal{H}^*)$ rather than $L^\infty(\mathbb{R};\mathcal{H})$: we inductively show that $R^j u \in L^\infty_{\text{loc}}(\mathbb{R};\mathcal{H}^*)$ for each $j \in \mathbb{N}$.

□

Lemma 45. *Fix a 4–spinor ψ_0 and a point $x_0 \in \mathbb{R}^3$. Then the solution u to the Dirac equation with initial data*

$$\delta(x - x_0)\psi_0$$

is in $\mathcal{C}(\mathbb{R};\mathcal{D}^{-3/2-0})$, and enjoys nonfocusing (on all of M°) with respect to $\mathcal{D}^{-1/2-0}$.

Proof. This is essentially a vector-valued version of [32, Lemma 16.1, Proposition 16.2]. We first note that by energy conservation (see §4.2), $u \in \mathcal{C}(\mathbb{R};\mathcal{D}^{-3/2-0})$ since $\delta \in H^{-3/2-0}$. On the other hand, given any k, for N large,

$$(\mathrm{Id} + \Delta_\theta)^{-N}\delta(r - r_0)\delta(\theta - \theta_0) \in \mathcal{C}^k(S^2; H^{-1/2-0}(\mathbb{R}_+)),$$

hence taking $k \gg 0$ yields

$$(\mathrm{Id} + \Delta_\theta)^{-N} u(0) \in \mathcal{D}^{-1/2-0}.$$

This suffices to establish nonfocusing at $t = 0$ and hence globally in time, by Lemma 43. □

Finally, we consider the regularity of the solution on the strictly diffracted wavefront $\mathsf{D}\backslash\mathsf{G}$. Let u denote the solution with initial data $\delta(x - x_0)\psi_0$, where $x_0 = (r_0, \theta_0)$ in polar coordinates. For $t_0 > r_0$, consider any point $(r = t_0 - r_0, \theta)$ with $\theta \neq -\theta_0$ and let U be a neighborhood of this point in X° disjoint from $\pi(\mathsf{G}) = \{|x - x_0| = t\}$ for $t \in I \equiv (t_0 - \epsilon, t_0 + \epsilon)$. By Lemma 45, u is nonfocusing in $T^*(I \times U)$ (or, indeed, globally) relative to $L^2\mathcal{D}^{-1/2-0}$. On the other hand, we now apply the edge propagation theorem (Theorem 41) to the solution $\Theta_{-3/2+\epsilon}u$, which lies in $\mathcal{C}^0(\mathbb{R};\mathcal{D}^0)$, hence in particular, say, in $L^2_{\text{loc}}(M)$. Thus the edge regularity hypotheses of the edge propagation theorem are satisfied (with $l = 0$), and we conclude, also using Proposition 19 for propagation into $r > 0$, that for some fixed M, for all $k \in \mathbb{N}$, $\mathrm{WF}^M(\Delta_\theta^k \Theta_{-3/2-\epsilon}u) \cap T^*(M^\circ)$ is disjoint from the strictly diffractive flowout from the origin

$$N^*\{r = t - r_0\} \cap \{\theta \neq -\theta_0\}.$$

In particular, then, since no points in $T^*(I \times U)$ are geometrically related to the initial singularity, u (which differs from $\Theta_{3/2+\epsilon}(\Theta_{-3/2-\epsilon}u)$ by a smooth error) enjoys *coisotropic regularity of every order* relative to some Sobolev space $H^{M'}$ on $I \times U$. By an interpolation argument [30, Section 13], a distribution that is nonfocusing relative to H^s and enjoys infinite order coisotropic regularity relative to some fixed H^k in fact lies in H^{s-0}, hence u enjoys this regularity over $I \times U$ (and it moreover also enjoys iterated regularity under

K relative to these spaces). This proves that the fundamental solution u lies in $H^{-1/2-0}$ near $\mathsf{D}\backslash\mathsf{G}$ and moreover that $\Delta_\theta^k u$ enjoys the same regularity for all k.

Finally, we show that the diffracted wave is a conormal singularity. To begin, we further analyze the singularity of the fundamental solution for short time: since $Pu = 0$ with $P = \Box$ modulo lower order terms, we have energy estimates for u for short time, and the parametrix construction [20, Theorem 29.1.1] applies, and shows that $u \in \mathcal{C}(\mathbb{R}; \mathcal{D}^{-3/2-0})$ is conormal to $|x - x_0| = |t|$ whenever $|t| < |x_0|$. (Beyond this range of times, the support reaches the singularity of the potential, which cannot be treated as a perturbation any longer). Consequently, as $N \to \infty$, the angular smoothing of u,

$$(\mathrm{Id} + \Delta_\theta)^{-N} u,$$

approximates a sum of conormal distributions in $H^{-1/2-0}$ at the hypersurfaces $r = r_0 \pm t$. Since $R \equiv (t - r_0)D_t + rD_r$ is tangent to $\{r = r_0 - t\}$, for $t \in (0, r_0)$ the regularity of this latter piece of the solution is unaffected by the iterated application of R. Thus for each $j \in \mathbb{N}$, $R^j u$ satisfies the nonfocusing condition relative to $\mathcal{D}^{-1/2-0}$ for $t \in (0, r_0)$, microlocally away from the outgoing spherical wave $N^*\{r = r_0 + t\}$. (See [32, Lemma 16.1] for details of this computation.) Note that we may microlocalize our solution away from the outgoing spherical wave without changing the diffracted wave (by the b propagation theorem), hence we may ignore this part of the solution.

By Lemma 44, the nonfocusing condition persists for all $t \in \mathbb{R}$. On the other hand, Theorem 41 implies that along the strictly diffracted wavefront (and for r small), for every $j \in \mathbb{N}$, $R^j u$ enjoys coisotropic regularity with respect to some fixed (but j-dependent) Sobolev space $H^{-M(j)}$. Once again, by interpolation, we then have $R^j u \in H^{-1/2-0}$ along the strictly diffracted wavefront for every j, and this, along with the coisotropic regularity and the equation $Pu = 0$, establishes conormal regularity along the Lagrangian $\mathsf{D} = N^*\{r = t - r_0\}$ at points $\theta \neq -\theta_0$ (i.e., away from G).

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