SINGULARITIES OF DIRAC–COULOMB PROPAGATORS

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Abstract. In this paper we study singularities of propagators and N-point functions for Dirac fields in a Coulomb potential, possibly with a t-dependent smooth part for $|t| < T < \infty$. We show that the *in* and *out* Dirac–Coulomb vacua are Hadamard states for $r \neq 0$. Furthermore, we prove that the relative charge density of any two Hadamard states is well-defined as a locally integrable function including near $r = 0$. The results are based on a diffractive propagation of singularities theorem for the Dirac–Coulomb system previously obtained by the first and third authors, generalized here to the case of t-dependent potentials.

1. Introduction and main result

1.1. **Introduction.** Second quantization of Dirac fields in external potentials and the construction of perturbative series in interacting Quantum Field Theory require a precise description of singularities of propagators and N-point functions. In related models in relativistic Quantum Mechanics it is often possible to introduce an ultra-violet cutoff that improves the short-distance behavior (see e.g. [17, 38] for the Dirac–Fock model, and [22, 23] and references therein for the Bogoliubov–Dirac–Fock model), but removing the cutoff can then be a very delicate issue. In fully relativistic external field QED one inevitably has to face ultra-violet divergences originated in singularities of Schwartz kernels of operators; see [5, 30, 28, 9] for expository works focused on different formalisms and regimes.

If the external potentials are smooth and possibly depend on time, singularities of propagators are best dealt with by methods of microlocal analysis: these were initially applied in the similar setting of Dirac fields on smooth Lorentzian spin manifolds [26, 36] (cf. [21, 20, 13, 7] for more recent developments) and then reworked for external electromagnetic potentials [30, 41, 43, 44, 18]. As in the case of scalar fields a primary role is played by the Hadamard condition [34], which implies short-distance behavior suitable for renormalization of perturbative series [6, 27].

If the potential is singular at $r = 0$ and one is given a Hadamard state away from $r = 0$, then the constructions are still valid for $r \neq 0$ and in principle one has some well-defined renormalized quantities and perturbative series. However, there are two main problems with this:

(1) It is not clear if a Hadamard state exists at all (or more to the point, it is not known if the natural physical states occurring in this context are Hadamard).
(2) Renormalized quantitities such as the charge density could behave at $r = 0$ bad enough so that the quantum charge is not locally finite.

The latter eventuality would mean infinite charge accumulation near $r = 0$, and in consequence the back-reaction of external electro-magnetic fields with Dirac fields would no longer be negligible, thus undermining the consistency of the theory.

The case of singular potentials is of particular importance in view of their role in modeling atoms, yet it is mathematically much more difficult because of their ability to disrupt regularity properties of propagators. We remark that there has been significant recent progress in studying spectral properties of Dirac–Coulomb operators (see e.g. [14, 17, 15, 16, 11, 12]), but the methods employed so far are not suitable for analyzing local properties of singular Schwartz kernels.

1.2. **Main results.** In the present paper we resolve the two issues (1)–(2) in the case of *Coulomb-like potentials*, possibly with a time-dependent smooth part. Namely, we consider a Dirac–Coulomb Hamiltonian on $\mathbb{R}^3$, i.e. an operator of the form

$$H(t) = \sum_{k=1}^{3} \alpha_k \big(i^{-1}\partial_k + A_k(t) \big) - A_0(t) + m\beta, \tag{1.1}$$

where $m \in \mathbb{R}$, $A_k \in C^\infty(\mathbb{R}^{1,3}) \cap C^\infty_{\rm c}(\mathbb{R}_t; L^\infty(\mathbb{R}^3_{\bar{x}}))$ and the potential A_0 is of the form

$$A_0(t) = \frac{\kappa}{|\bar{x}|} + A_{0,\infty}(t), \quad A_{0,\infty} \in C^\infty(\mathbb{R}^{1,3}) \cap C^\infty_{\rm c}(\mathbb{R}_t; L^\infty(\mathbb{R}^3_{\bar{x}})), \tag{1.2}$$

with $\kappa \neq 0$ a constant. We will suppose in particular that

$$\operatorname{supp} A_k \cup \operatorname{supp} A_{0,\infty} \subset \{ t \in]t_-, t_+[\} \tag{1.3}$$

for some $t_- < t_+$. Above, β, α_k are the 4×4 matrices

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}, \quad k = 1, 2, 3,$$

where $\sigma_k \in M_2(\mathbb{C})$ are the Pauli matrices. Throughout the paper we assume that $|\kappa| < \frac{1}{2}$, in which case $H(t)$ is well-known to be essentially self-adjoint in $L^2(\mathbb{R}^3; \mathbb{C}^4)$. The Dirac–Coulomb equation reads $Du = 0$, where we adopt the convention that

$$D = i\partial_t + H(t).$$

The corresponding Schrödinger evolution operator (which is simply $e^{i(t-s)H}$ if $H(t) \equiv H$ is t-independent) is denoted by $U(t, s)$.

In this setting, quantum states and second quantized fields are obtained from a *density matrix* at some reference time, i.e. an operator $\gamma \in B(L^2(\mathbb{R}^3; \mathbb{C}^4))$ s.t. $0 \leqslant \gamma \leqslant \boldsymbol{1}$. If $\gamma(s)$ is the density matrix at time s, then the density matrix at time t is given by

$$\gamma(t) = U(t, s)\gamma(s)U(s, t).$$

The most important example is when $H(t) \equiv H$ is t-independent. Then the spectral projection $\gamma = \boldsymbol{1}_{]-\infty,0]}(H)$ defines the fundamental physical state, called the *Dirac–Coulomb vacuum*. More generally, if $H(t) \equiv H(t_-)$ is t-independent in the past and $H(t) \equiv H(t_+)$ in the future as assumed in (1.2)–(1.3), there are two natural possibilities. One can either take the Dirac-Coulomb vacuum $\boldsymbol{1}_{]-\infty,0]}(H(t_-))$ in the past, and propagate it to the future, obtaining the trace density $\gamma_{\rm in}(t)$ of the so-called *in*-vacuum, or take $\boldsymbol{1}_{]-\infty,0]}(H(t_+))$ in the future, obtaining the *out*-vacuum. The difference $\gamma_{\rm out}(t) - \gamma_{\rm in}(t)$

is used to compute the charge created by the intermediary t-dependent potential, in fact the trace density

$$\rho_{\gamma_{\rm out},\gamma_{\rm in}}(t,\bar{x}) := \mathrm{Tr}_{\mathbb{C}^4}(\gamma_{\rm out}(t)-\gamma_{\rm in}(t))(\bar{x},\bar{x}) \tag{1.4}$$

is the relative quantum charge density at $(t,\bar{x}) \in \mathbb{R}^{1,3}$. In the absence of a cut-off, $\gamma_{\rm in/out}(t)$ are not trace-class and the trace densities (integrands of the trace, or Schwartz kernels restricted to the diagonal) do not exist, so the only hope for (1.4) to be finite is that the singularities cancel out.

To understand how these singularities evolve in time, it is advantageous to think in terms of space-time quantities (as in QFT on curved spacetimes). Namely, to γ one associates the spatio-temporal *two-point functions* Λ^+ and Λ^-, i.e., the operators

$$\big(\Lambda^- f\big)(t) = \int_{-\infty}^{\infty} U(t,t_0)\gamma(t_0)U(t_0,s)f(s)ds, \quad f \in C_{\rm c}^\infty(\mathbb{R}^{1,3};\mathbb{C}^4),$$

and similarly for Λ^+, with γ replaced by $\mathbf{1}-\gamma$. The name comes from the fact that in QFT terminology, the space-time smeared field operators $C_{\rm c}^\infty(\mathbb{R}^{1,3};\mathbb{C}^4) \ni f \mapsto \hat{\psi}(f), \hat{\psi}^*(f)$ associated to γ satisfy

$$\langle \Omega, \hat{\psi}(f)\hat{\psi}^*(g)\Omega\rangle_{\mathcal{H}} = \langle f, \Lambda^+ g\rangle_{L^2}, \quad \langle \Omega, \hat{\psi}^*(f)\hat{\psi}(g)\Omega\rangle_{\mathcal{H}} = \langle f, \Lambda^- g\rangle_{L^2},$$

where $\mathcal{H}$ is the Hilbert space and $\Omega \in \mathcal{H}$ the vacuum vector in the second quantized theory, see §A.1. The Schwartz kernel of $\Lambda^\pm$ is necessarily singular, but we can hope it is as regular as possible. In the setting with smooth potentials this occurs when $\Lambda^\pm$ satisfy the *Hadamard condition.* This condition can be formulated as follows: for each non-zero $(t_i,\bar{x}_i;\tau_i,\bar{\xi}_i) \in \mathbb{R}^{1,3}\times\mathbb{R}\times\mathbb{R}^3$ with $\pm\tau_i > 0$, $i=1,2$, there exists pseudodifferential operators $B_1, B_2 \in \Psi^0$ elliptic at $(t_1,\bar{x}_1;\tau_1,\bar{\xi}_1)$, $(t_2,\bar{x}_2;\tau_2,\bar{\xi}_2)$ respectively, such that $B_1\Lambda^\pm B_2^*$ is regularizing (i.e., has smooth Schwartz kernel). Thus $\Lambda^\pm$ behave like smoothing operators after restricting localized Fourier transforms in time to $\pm\tau_i > 0$, and since they also satisfy $D\Lambda^\pm = 0$ and $\Lambda^\pm D = 0$, this can be traded for some regularity in the spatial variables.

In the singular setting, we adopt the point of view that the Hadamard condition in the above formulation is still adequate for $r \neq 0$. We say that a density matrix γ is *Hadamard* if the associated two-point functions $\Lambda^\pm$ are Hadamard for $r \neq 0$. Our first main result says that the *in*-vacua (and in analogy, *out*-vacua) are Hadamard in this sense.

Theorem 1.1. *Let $H(t)$ be the Dirac–Coulomb Hamiltonian in an electro-magnetic potential $A_0(t),\dots,A_3(t)$ satisfying (1.1)–(1.3) with $|\kappa| < \frac{1}{2}$, in particular the potential is time-independent for $t \leqslant t_-$. Suppose $0 \notin \mathrm{sp}(H(t_-))$. Then the density matrix*

$$\gamma_{\rm in}(t) := U(t,t_-)\mathbf{1}_{]-\infty,0]}(H(t_-))U(t_-,t), \quad t \in \mathbb{R}, \tag{1.5}$$

of the in*-vacuum is Hadamard.*

In consequence, for $r \neq 0$ all local constructions in perturbative QFT based on *in*-vacua proceed *exactly* as in the non-singular case. In particular, the results on QFT in external potentials summarized in [43] and the earlier work [30] (building on similar results for Dirac fields on globally hyperbolic spacetimes) apply verbatim to this situation, hence the following immediate corollary.

Corollary 1.2. *For any polynomial interaction, the Epstein–Glaser–Brunetti–Fredenhagen perturbative interacting fermionic QFT based on $\gamma_{\rm in}$ is well-defined for $r \neq 0$.*

This result as stated does still not say much about the behavior of renormalized quantities at $r = 0$. However, we get a more precise statement at least for relative charge densities. Our second main result says in fact that renormalizing by subtracting a reference Hadamard density matrix yields a well-defined charge that behaves reasonably well at $r = 0$.

Theorem 1.3. *Suppose $\gamma, \gamma_{\rm ref} \in L^2(\mathbb{R}^3; \mathbb{C}^4)$ are two regular Hadamard density matrices at some arbitrary time $t \in \mathbb{R}$. Then the relative charge density*

$$\rho_{\gamma,\gamma_{\rm ref}}(t, \bar{x}) := \mathrm{Tr}_{\mathbb{C}^4}(\gamma(t) - \gamma_{\rm ref}(t))(\bar{x}, \bar{x}) \in L^1_{\rm loc}(\mathbb{R}^3) \cap C^\infty(\mathbb{R}^3 \setminus \{0\})$$

is well defined, behaves like $O(r^{-2-\epsilon})$ near $r = 0$ and is smooth in t.

Here *regular* means that the associated two-point functions $\Lambda^\pm, \Lambda^\pm_{\rm ref}$ (viewed as operators) preserve conormal regularity (i.e., regularity as measured by acting with $r\partial_r$ and angular derivatives, as opposed to ∂_r and angular derivatives); see Definition 2.13.

We show the regularity condition is satisfied by the *in*- and *out*-vacua, and as they are Hadamard by Theorem 1.1, Theorem 1.3 applies to this case. This implies that the total charge created by turning on and then turning off a smooth time-dependent potential is finite in any bounded region.

1.3. **Method of proof, structure of paper.** The main ingredient of the proof is the propagation of singularities theorem for solutions of the Dirac–Coulomb equation $Du = 0$, obtained by two of us in [3], and generalized here to potentials with time-dependent smooth part.

Propagation of singularities in singular settings has a long history: we mention here the work of Cheeger–Taylor [8] (on wave equations on product cones), Melrose–Wunsch [32] (on more general manifolds with conical singularities), Vasy [40] (manifolds with corners) and Melrose–Vasy–Wunsch [31] (edge singularities). The Dirac–Coulomb equation poses significant challenges as compared to the scalar case (cf. Hintz [24] for a parameter-dependent singular elliptic framework and hyperbolic results adapted in particular to the Dirac–Coulomb operator, Baskin–Booth–Gell-Redman [2] for results on the asymptotic behavior of solutions with microlocal methods, and Hintz [25] for broad existence, uniqueness and regularity results applying to the Dirac–Coulomb setting). On the other hand the generalization to time-dependent potentials and lower a priori regularity requires then only relatively mild modifications of the arguments in [3] which we explain in the proof of Theorem 2.12. The theorem uses Melrose's b-calculus, which permits us to localize singularities arriving at $r = 0$ in time, and to microlocalize them in energy, but not to distinguish among singularities arriving at or leaving from $r = 0$ along rays at different angles; this permits *diffractive* effects.

Instead of dealing directly with Schwartz kernels of operators we use an operator b-wavefront set and show an operator version of propagation of singularities in Theorem 2.18. Its use is then twofold. First, we apply it to prove that if a bi-solution is Hadamard for $r \neq 0$, then this implies a bound on its b-wavefront set at $r = 0$. Second, we show that the corresponding b-wavefront set refinement of the Hadamard condition propagates well. This allows us to propagate regularity of $\gamma_{\rm in}$ and $\gamma_{\rm out}$ from the respective regions where $H(t)$ is time-independent.

Once we establish control of operator b-wavefront sets of space-time quantities, we can use arguments similar to other singular settings [42, 19] combined with a new criterion (Proposition 3.5) to conclude Theorem 1.3. An important prerequisite, however, is the regularity property, that is, we need good enough mapping properties of two-point functions and propagators from $H^{-1}(\mathbb{R}^{1,3};\mathbb{C}^4)$-based b-Sobolev spaces of arbitrary order to $H^1(\mathbb{R}^{1,3};\mathbb{C}^4)$-based b-Sobolev spaces. We show this to boil down to the well-posedness of the Cauchy problem in b-Sobolev spaces of arbitrary order including a good control of negative order regularity; that turns out however to be problematic (we note in particular that the results in [24, 25] do not appear to give the regularity discussed here).The issue is that in our setting, domains of powers of $H(t)$ are t-dependent in a way that makes them of limited use in comparison to the t-independent setting, and their interaction with b-Sobolev space analysis arguments turns out to be subtle. Our strategy is to base the well-posedness theory on Cauchy data in the static region where the use of domains of powers is sound, and to derive energy estimates smeared in time in the non-static region rather than emphasizing Cauchy data there.

The paper is organized as follows.

Section 2 provides the key results on regularity of solutions (in §2.2) and propagation of singularities in the case of t-dependent potentials (in §2.3), also in the operator sense (in §2.4). Section 3 proves the main results on Hadamard two-point functions and gives more precise estimates on their b-wavefront sets. Finally, Appendix A recalls preliminaries on second quantization for Dirac fields needed for the formulation of our results and discusses corollaries for the renormalized quantum current and charge operators.

2. Regularity of solutions and propagation of singularities

2.1. Radial coordinates and blowup. In polar coordinates (r,θ), the singularity at $\{r=0\}\subset\mathbb{R}^3$ is dealt with by replacing $\mathbb{R}^3$ by the blown-up space

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

equipped with the *blowdown map* $b: X\to\mathbb{R}^3$ given by $b:(r,\theta)\mapsto r\theta$. We work on the blown-up spacetime $M=\mathbb{R}_t\times X$, which can also be identified with the blow-up $[\mathbb{R}^{1,3};\mathbb{R}\times\{0\}]$.

Then, X and M are manifolds with boundary, and we denote by $X^\circ=\,]0,\infty[_r\times\mathbb{S}^2_\theta$ and $M^\circ=\mathbb{R}_t\times X^\circ$ their respective interior.

2.2. Dirac–Coulomb propagator. Throughout this section and the rest of the paper, we use the analogous notation $H^1(M;\mathbb{C}^4)$ for the first order Sobolev space in four dimensions, and denote the dual by $H^{-1}(M;\mathbb{C}^4)$. The corresponding spaces with conormality of order $s\in\mathbb{R}$, $s=+\infty$ or $s=-\infty$ are denoted by $H_{\rm b}^{1,s}(M;\mathbb{C}^4)$ and $H_{\rm b}^{-1,s}(M;\mathbb{C}^4)$; see [3, §3.1] for the definition. In brief, s stands for regularity with respect to taking $r\partial_r$, ∂_t, and ∂_θ derivatives. Note that conormality is always measured with respect to $H^1(M;\mathbb{C}^4)$ or its dual, so in particular $H_{\rm b}^{1,0}(M;\mathbb{C}^4)$ equals $H^1(M;\mathbb{C}^4)$ (rather than $H^1_{\rm b}(M;\mathbb{C}^4)$, as the notation could perhaps wrongly suggest). In addition we add a subscript $H^{k,s}_{\rm b,c}(M;\mathbb{C}^4)$, resp. $H^{k,s}_{\mathrm{b,loc}}(M;\mathbb{C}^4)$, to indicate the corresponding compactly supported and local spaces, and often write in short $H^{k,s}_{\mathrm{b,c}}$ and $H^{k,s}_{\mathrm{b,loc}}$ when this creates no risk of confusion (and we abbreviate other spaces similarly).

For each $t\in\mathbb{R}$, $H(t)$ is essentially self-adjoint on $C^\infty_{\mathrm{c}}(X^\circ;\mathbb{C}^4)$ in $L^2(X;\mathbb{C}^4)=L^2(\mathbb{R}^3;\mathbb{C}^4)$. As it differs from the Dirac–Coulomb Hamiltonian by a bounded smooth potential, its domain agrees with Kato's characterization [29] of the domain of the Dirac–Coulomb Hamiltonian. In particular, the domain of $H(t)$ is independent of t and given by $H^1(X;\mathbb{C}^4)$, the closure of $C^\infty_{\mathrm{c}}(X^\circ;\mathbb{C})$ with respect to $\|b_*\cdot\|_{H^1}$, where $\|\cdot\|_{H^1}$ is the usual $H^1(\mathbb{R}^3;\mathbb{C}^4)$ Sobolev norm. Additionally, [3, Lem. 7] says that the norms of $H^1(X;\mathbb{C}^4)$ and $\mathcal{D}$ are equivalent for r bounded.

We use the notation $\langle\lambda\rangle=(1+|\lambda|^2)^{\frac12}$ and define for $s\in\mathbb{R}$

$$\mathcal{D}^s(t)=\mathrm{Dom}\langle H(t)\rangle^s,\quad \mathcal{D}^\infty(t)=\textstyle\bigcap_{s\in\mathbb{R}}\mathcal{D}^s(t),\quad \mathcal{D}^{-\infty}(t)=\textstyle\bigcup_{s\in\mathbb{R}}\mathcal{D}^s(t),$$

where $\mathcal{D}^s(t)$ is equipped with the Hilbert space norm $\|\cdot\|_{\mathcal{D}^s(t)}=\|\langle H(t)\rangle^s\cdot\|$, and then $\mathcal{D}^\infty(t)$ and $\mathcal{D}^{-\infty}(t)$ are Fréchet spaces topologized in the usual way. These spaces are, in general, time-dependent. For all t, [3, Lem. 14] implies that

$$\mathcal{D}^s(t)\cap\mathcal{E}'(X^\circ;\mathbb{C}^4)=H^s_{\mathrm{loc}}(X;\mathbb{C}^4)\cap\mathcal{E}'(X^\circ;\mathbb{C}^4).$$

Because $\mathcal{D}^s(t)$ regularity with large s encodes partial power series expansions of functions at $r=0$, though, the spaces $\mathcal{D}^s(t)$ at different times do not generally agree near the the pole of the potential. We therefore employ these spaces primarily at times $t\leqslant t_-$ for which $A_k,A_{0,\infty}\equiv 0$. For convenience, we will drop the t from the $\mathcal{D}^s(t)$ notation when a time has been fixed; we also omit it (as we have done above) from $\mathcal{D}\equiv\mathcal{D}^1(t)$, which is time independent.

If $A_{0,\infty}=A_j=0$, so that $H(t)$ is time-independent, the spectral theorem implies that there is a unique solution of the Cauchy problem for the homogeneous Dirac equation with initial data in any of the spaces $\mathcal{D}^s$. For time-varying operators, however, this method is unavailable, and we need more flexible tools (although it is useful that solutions via the spectral theorem still exist in the range of times when $A_{0,\infty}=0$).

Lemma 2.1. *For each $t_0\in\mathbb{R}$, consider the Cauchy problem*

$$\begin{cases} Du=f,\\ u|_{t=t_0}=u_0.\end{cases}$$

If $f\in C^0(\mathbb{R};L^2)$ and $u_0\in L^2$, then there is a unique solution $u\in C^0(\mathbb{R};L^2)$. In addition, if $f\in C^1(\mathbb{R};L^2)$ and $u_0\in\mathcal{D}$, then $u\in C^1(\mathbb{R};L^2)\cap C^0(\mathbb{R};\mathcal{D})$. In both cases, u is given by

$$u(t)=U(t,t_0)u_0+\int_{t_0}^t U(t,t_2)f(t_2)\,dt_2, \tag{2.6}$$

where $U(t_1,t_2)\in B(L^2)$ satisfies for all $t,t_1,t_2\in\mathbb{R}$:

$$\begin{aligned} &U(t,t)=\mathbf{1},\quad U(t_1,t)U(t,t_2)=U(t_1,t_2),\\ &\partial_tU(t,t_2)=iH(t)U(t,t_2),\quad \partial_tU(t_1,t)=-U(t_1,t)iH(t),\end{aligned} \tag{2.7}$$

as a $\mathcal{D}$-preserving strongly continuously differentiable family in $B(\mathcal{D},L^2)$.

Proof. This can be shown to follow from general semigroup theory; in particular it suffices to check the hypotheses of [33, §5, Thm. 3.1], [33, §5, Thm. 4.8] and [33, §5, Thm. 5.3]. For each $t \in \mathbb{R}$, $H(t)$ is self-adjoint on the t-independent domains $\mathcal{D}$ in the Hilbert space L^2. It follows that $\{H(t)\}_{t\in\mathbb{R}}$ is a stable family of infinitesimal generators of a C^0-semigroup on L^2 in the terminology of [33, §5, Def. 2.1] (one can easily check it directly, or invoke the more general [33, §5, Thm. 2.4]). Furthermore, for all $u \in \mathcal{D}$, $H(\cdot)u$ is continuously differentiable in L^2, so all the hypotheses are met. $\square$

We now record a useful energy estimate which applies a priori to solutions with higher regularity in t:

Lemma 2.2. *Suppose $u \in C^k(\mathbb{R};\mathcal{D})$. For $[t_1,t_2] \subset \mathbb{R}$, $k \in \mathbb{N}$, and $i = 1$ or $i = 2$, we have the uniform estimate*

$$\left\|\partial_t^k u\right\|_{L^\infty([t_1,t_2];L^2)} \lesssim \sum_{j\leqslant k} \left(\left\|\partial_t^j Du\right\|_{L^1([t_1,t_2];L^2)} + \left\|\partial_t^j u(t_i,\bullet)\right\|_{L^2} \right).$$

Proof. Note that for $k = 0$, the statement follows from Lemma 2.1 above.

Since $\partial_t = -iDu + iHu$, we compute for $k \in \mathbb{N}$, recalling that $H(t)$ is self-adjoint for each t:

$$\begin{aligned} \partial_t \left\|\partial_t^k u\right\|^2 &= 2\,\mathrm{Im}\,\langle \partial_t^k H(t)u, \partial_t^k u\rangle - 2\,\mathrm{Im}\,\langle \partial_t^k Du, \partial_t^k u\rangle \\ &= 2\,\mathrm{Im}\,\langle [\partial_t^k, H(t)]u, \partial_t^k u\rangle - 2\,\mathrm{Im}\,\langle \partial_t^k Du, \partial_t^k u\rangle. \end{aligned}$$

Now $[\partial_t^k, H(t)] = [\partial_t^k, -A_{0,\infty}] + \sum_{\ell=1}^3 \alpha_\ell [\partial_t^k, A_\ell]$ and so $[\partial_t^k, H(t)] = \sum_{j<k} C_j \partial_t^j$, where C_j are uniformly bounded matrix-valued smooth functions. We thus get the bound

$$\partial_t \left\|\partial_t^k u\right\|^2 \lesssim \sum_{j=0}^{k-1} \left\|C_j \partial_t^j u\right\| \left\|\partial_t^k u\right\| + \left\|\partial_t^k Du\right\| \left\|\partial_t^k u\right\|$$

and hence

$$\partial_t \left\|\partial_t^k u\right\| \lesssim \sum_{j=0}^{k-1} \left\|\partial_t^j u\right\| + \left\|\partial_t^k Du\right\|.$$

Integrating from t_i and using induction then finishes the proof. $\square$

We now fix $t_- < t'_- < t''_-$ so that $H(t)$ is t-independent for $t \leqslant t''_-$. We define the homogeneous solution operator T by

$$Tu_0 = U(t,t_-)u_0,$$

where $U(t,s)$ is as in Lemma 2.1. In other words, Tu_0 is the solution of the Cauchy problem posed at t_- with initial data u_0. By Lemma 2.1 we know $T : L^2 \to C^0_{\mathrm{loc}}(\mathbb{R};L^2)$ and $T : \mathcal{D} \to C^0_{\mathrm{loc}}(\mathbb{R};\mathcal{D}) \cap C^1_{\mathrm{loc}}(\mathbb{R};L^2)$.

The rest of this section is devoted to establishing that $T : \mathcal{D}^s(t_-) \to H^{1,s-1}_{\mathrm{b,loc}}$ for all $s \in \mathbb{R}$. We start with the following elliptic lemma, which states that b-regularity of a solution can be verified by controlling its time derivatives (cf. [3, Corollary 3.3]).

Lemma 2.3. *Suppose $k \in \mathbb{Z}$. If $u \in H^k_{\mathrm{loc}}(\mathbb{R};\mathcal{D})$ and $Du \in H^{0,k}_{\mathrm{loc}}$, then $u \in H^{1,k}_{\mathrm{loc}}$.*

(We remark for context that that for $k \in \mathbb{N}$, $H^{1,k}_{\mathrm{b,loc}} \subset H^k_{\mathrm{loc}}(\mathbb{R};\mathcal{D})$, but the reverse inclusion does not hold unless we restrict our attention to solutions of the Dirac equation, as the functions in the space on the left enjoy higher spatial regularity.)

Proof. We begin by noting that $u \in H^{1,-\infty}_{\mathrm{b,loc}}$. Indeed, for $k > 0$, this follows immediately from the inclusion $H^k_{\mathrm{loc}}(\mathbb{R};\mathcal{D}) \subset H^1_{\mathrm{loc}}$, while for $k = 0$, we note that $\partial_t u = -iDu + iH(t)u \in L^2$ and so $u \in H^1$. For $k < 0$, we write $u = \sum_{j \leqslant k+1} \partial_t^j v_j$ for $v_j \in H^1_{\mathrm{loc}}(\mathbb{R}; H^1) \subset H^1_{\mathrm{loc}}$, so that $u \in H^{1,-k-1}_{\mathrm{b,loc}}$.

As the two notions of Sobolev regularity agree away from the singularity, it suffices to work near $r = 0$. In the time-independent case when $k \geqslant 0$, the statement is an immedate consequence of Corollary 33 of [3].[1] The main changes needed in this setting are to extend the results to time-dependent coefficients and to relax the assumption of $u \in H^1$ to $u \in H^{1,-\infty}_{\mathrm{b,loc}}$. We employ the b-pseudodifferential calculus, as described in [3, §3] and the references therein.

Given $u \in H^{1,-m}_{\mathrm{b,loc}}$, we set $v = \Upsilon u$, where $\Upsilon \in \Psi^{-m}_{\mathrm{b}}(M)$ is an invertible, $SO(3)$-invariant, elliptic b-pseudodifferential operator of order $-m$. As Υ is invertible and elliptic, measuring v in $H^{1,k+m}_{\mathrm{b,loc}}$ is equivalent to measuring u in $H^{1,k}_{\mathrm{b,loc}}$ near $r = 0$. The equation satisfied by v is then

$$\widetilde{D}v = \left(D - [D,\Upsilon]\Upsilon^{-1}\right)v = \Upsilon Du.$$

Using now an abbreviated notation for Ψ^k_{b}, a computation in the differential b-calculus shows that

$$\widetilde{D}^2 - D^2 \in \Psi^1_{\mathrm{b}} + \frac{1}{r}\Psi^0_{\mathrm{b}} + \frac{1}{r^2}\Psi^{-1}_{\mathrm{b}} + \Psi^{-1}_{\mathrm{b}}\partial_r^2 + \Psi^{-1}_{\mathrm{b}}\frac{1}{r}\partial_r + \Psi^{-1}_{\mathrm{b}}\frac{1}{r^2}\Delta_\theta.$$

The elliptic estimate [3, Lemma 28, Corollary 33] is based on the real part of the quadratic form $\langle D^2 u, u\rangle$ and in fact holds for a wide class of Klein–Gordon-type operators. Inspection of the proof reveals that all of the components [3, §5.2.2] of the elliptic estimate hold for the time-dependent operator $\widetilde{D}^2$; the key is Lemma 26, which still holds exactly as stated. The remaining estimates in that section treat the remainder terms using only their order, which is unchanged here. This yields an estimate for v in $H^{1,k+m}_{\mathrm{b,loc}}$ and thus an estimate for u in $H^{1,k}_{\mathrm{b,loc}}$, as desired. $\square$

Lemma 2.4. *For $s \geqslant 0$, $T : \mathcal{D}^s(t_-) \to H^{1,s-1}_{\mathrm{b,loc}}$.*

Proof. We first consider $s = k \in \mathbb{N}$. If $u_0 \in \mathcal{D}^k(t_-)$, then we set $v = e^{i(t-t_-)H(t_-)}u_0$ for $t \leqslant t_-$. Because H independent of t in this region, we know $v \in C^k(L^2) \cap C^0(\mathcal{D}^k(t_-))$ there. Moreover, Lemma 2.3 immediately yields $v \in H^{1,k-1}_{\mathrm{b,loc}}$.

Let $\chi(t) \in C^\infty(\mathbb{R})$ satisfy $\chi(t) \equiv 1$ for $t \leqslant t_-$ and $\chi(t) \equiv 0$ for $t > t'_-$. We seek a solution of the form $u = \chi v + w$ to $Du = 0$, i.e., a solution of

$$Dw = [i\partial_t, \chi]v \in H^{1,k-1}_{\mathrm{b,loc}} \tag{2.8}$$

[1]There is a mistake in the statement of Corollary 33 in [3]. The term $\widetilde{G}\eth u$ on the right side of the inequality should be estimated in L^2 rather than in H^1.

with zero initial data. We can of course find an $L^2_{\mathrm{loc}}L^2$ (indeed, C^0L^2) solution w by the above semigroups result, Lemma 2.1; this is all we ask if $k=0$ (as the solution also lies in $H^{-1}_{\mathrm{loc}}(\mathbb{R};\mathcal{D})$), so w.l.o.g. we can now take $k \geqslant 1$. We wish to use the energy estimate, Lemma 2.2, to obtain higher regularity on w, and to this end we regularize w as follows. Let Λ_ϵ be a family of translation invariant, properly-supported pseudodifferential operators of order $-\infty$ on $\mathbb{R}_t$, bounded in $\Psi^0(\mathbb{R})$, and with $\Lambda_\epsilon \to \mathbf{1}$ strongly on H^s for all s as $\epsilon \to 0$. Then $\Lambda_\epsilon w \in C^\infty H^1$, and

$$D\Lambda_\epsilon w = [D,\Lambda_\epsilon]w + \Lambda_\epsilon[i\partial_t,\chi]v. \tag{2.9}$$

Note that since only the zero'th order parts of D are time-dependent, the operators $[D,\Lambda_\epsilon]$ are bounded in $\Psi^{-1}(\mathbb{R})$ (and still smoothing for $\epsilon>0$).

Now we apply the energy estimate to (2.9), which we may do since both $\Lambda_\epsilon w$ and the right-hand side are smooth in t. We know that w is in $L^2_{\mathrm{loc}}L^2$. Inductively assuming $w \in H^{j-1}_{\mathrm{loc}}L^2$ (with $j \leqslant k$), Lemma 2.2 yields

$$\left\|\partial_t^j \Lambda_\epsilon w\right\|_{L^2_{\mathrm{loc}}L^2} \lesssim \left\|[D,\Lambda_\epsilon]w\right\|_{H^j_{\mathrm{loc}}L^2} + \left\|\Lambda_\epsilon[i\partial_t,\chi]v\right\|_{H^j_{\mathrm{loc}}L^2}.$$

As $\epsilon \to 0$, both terms on the RHS are bounded by the inductive assumption and the assumption on v, so $\|\Lambda_\epsilon w\|_{H^j_{\mathrm{loc}}L^2}$ is uniformly bounded as $\epsilon \to 0$, hence has a weak sequential limit in $H^j_{\mathrm{loc}}L^2$. Since $\Lambda_\epsilon w \to w$ in L^2_{loc}, we have inductively obtained $w \in H^k_{\mathrm{loc}}L^2$. As $H(t)w = -i\partial_t w + [i\partial_t,\chi]v \in H^{k-1}_{\mathrm{loc}}L^2$, we also obtain

$$w \in H^{k-1}_{\mathrm{loc}}(\mathbb{R};\mathcal{D}).$$

Now since (2.8) gave

$$Dw \in H^{1,k-1}_{\mathrm{b,loc}} \subset H^{0,k-1}_{\mathrm{b,loc}},$$

Lemma 2.3 yields $u \in H^{1,k-1}_{\mathrm{b,loc}}$ as desired. Interpolation then finishes the proof for general $s \geqslant 0$.

The proof of Lemma 2.4 also establishes the following consequence for the inhomogeneous problem, which we state in time-reversed form in anticipation of our later application of it:

Lemma 2.5. *If $k \geqslant 0$ and $f \in H^k_{\mathrm{loc}}L^2$ is supported in $t \leqslant T$, then there exists $v \in H^k_{\mathrm{loc}}L^2$ with $Dv = f$ and $v=0$ for $t \geqslant T$.*

Proving the analogue of Lemma 2.4 for negative s requires a bit more functional analysis. For a fixed $k \in \mathbb{N}$, we let $T \gg 0$ and set

$$\mathcal{Y} = \{\phi \in \overline{H}^k([t'_-,\infty[;L^2(X)) \mid \operatorname{supp}\phi \subset [t_-,T]\},$$

so that $\mathcal{Y}$ consists of extendible (in t) distributions at t'_- and supported distributions at T. We also let

$$\mathcal{Z} = \overline{H}^k([t'_-,T];L^2(X)),$$

and equip both $\mathcal{Y}$ and $\mathcal{Z}$ with the usual norms.

The following lemma follows immediately from the energy estimate (Lemma 2.2) with $t_2 = T$:

Lemma 2.6. *For all test functions $\phi \in C^\infty_{\mathrm{c}}(\mathbb{R}\times X^\circ) \cap \mathcal{Y}$,*

$$\|\phi\|_{\mathcal{Y}} \lesssim \|D^*\phi\|_{\mathcal{Z}}.$$

Lemma 2.7. *For $k \in \mathbb{N}$, $T : \mathcal{D}^{-k} \to H^{-k-1}_{\mathrm{loc}}(\mathbb{R}; \mathcal{D})$.*

Proof. Let $f \in \mathcal{Y}^*$. For all test functions $\phi \in C^\infty_{\mathrm{c}}(\mathbb{R} \times X^\circ) \cap \mathcal{Y}$, we define

$$F(D^*\phi) = \langle \phi, f \rangle.$$

By Cauchy–Schwarz and Lemma 2.6, F is well-defined and enjoys the estimate

$$|F(D^*\phi)| \lesssim \|D^*\phi\|_{\mathcal{Z}} \, \|f\|_{\mathcal{Y}^*} .$$

We can extend F from the range of D^* on test functions to all of $\mathcal{Z}$ by Hahn–Banach; the Riesz lemma shows that there exists $u \in \mathcal{Z}^*$ so that

$$\langle \phi, f \rangle = F(D^*\phi) = \langle D^*\phi, u \rangle.$$

Thus $Du = f$ distributionally wherever ϕ is allowed to have support, i.e., for $t < T$ as $\phi \in \mathcal{Y}$. Note that we have implicitly obtained weak vanishing of u at the left endpoint t'_- because (locally) $\mathcal{Y}^*$ is in the dual space to a space of extendible distributions and hence is a space of supported distributions. The equation *is* satisfied down to the left endpoint $t = t'_-$ where u vanishes, as the test functions may be supported there.

Thus given any $f \in \mathcal{Y}^*$ there is a solution $u \in \mathcal{Z}^*$ to $Du = f$. We claim this solution is unique. To see this, suppose $u \in \mathcal{Z}^*$ with $Du = 0$. For any test function ψ with compact support in $[t'_-, T[\times X^\circ$, by Lemma 2.5, there exists $v \in H^k_{\mathrm{loc}} L^2$ with $Dv = \psi$ and $v = 0$ for $t \geqslant T$. Owing to the complementary support properties of u, v, with u extendible to vanish for $t \leqslant t'_-$ and v vanishing by construction for $t \geqslant T$, we may integrate by parts to find

$$0 = \langle Du, v \rangle = \langle u, Dv \rangle = \langle u, \psi \rangle.$$

Consequently, u vanishes.

Now fix $u_0 \in \mathcal{D}^{-k}(t_-)$. Let $v = e^{i(t-t_-)H(t_-)} u_0$ be the locally-defined solution near $t = t_-$ of $Dv = 0$ with Cauchy data u_0 given by the spectral theorem. From the spectral-theoretic description, we further have $v \in H^{-k}_{\mathrm{loc}}(] - \infty, t''_-[; L^2)$; we aim to extend it to a global solution in $H^{-k}_{\mathrm{loc}}(\mathbb{R}; L^2)$. Let $\chi(t)$ be a smooth function supported in $] - \infty, t''_-[$ with $\chi \equiv 1$ on a neighborhood of $] - \infty, t'_-]$. We seek a solution u of the form $u = \chi v + w$, with w supported in $[t'_-, \infty[$; such a solution would automatically have the correct initial data as $u = v$ near $t = t_-$. For u to be a solution, we require

$$Dw = -[D, \chi]v = -i\chi'(t)v \in H^{-k}_{\mathrm{c}}(\mathbb{R}; L^2),$$

with $\operatorname{supp} w \subset [t'_-, \infty[$. Our work above shows that such a solution exists, so the map sending Cauchy data to solution extends to

$$T : \mathcal{D}^{-k}(t_-) \to H^{-k}_{\mathrm{loc}}(\mathbb{R}; L^2(X)).$$

Moreover, since $H(t)u = -i\partial_t u \in H^{-k-1}_{\mathrm{loc}}(\mathbb{R}; L^2(X))$, the characterization of the domain of $H(t)$ gives $u \in H^{-k-1}_{\mathrm{loc}}(\mathbb{R}; H^1(X))$, as claimed. $\square$

Proposition 2.8. *For $s \geqslant 0$, $T : \mathcal{D}^{-s}(t_-) \to H^{1,-s-1}_{\mathrm{b,loc}}$.*

Proof. Given $k \in \mathbb{N}$ and $u_0 \in \mathcal{D}^{-k}(t_-)$, let $u = Tu_0$. Lemma 2.7 asserts that $u \in H^{-k-1}_{\mathrm{loc}}(\mathbb{R}; \mathcal{D})$ and Lemma 2.3 that $u \in H^{1,-k-1}_{\mathrm{b,loc}}$. Interpolation in the b-regularity index then finishes the proof. $\square$

2.3. **Propagation of singularities and diffraction.** For each $u \in H^{1,-\infty}_{\mathrm{b,loc}}(M;\mathbb{C}^4)$, resp. $H^{0,-\infty}_{\mathrm{b,loc}}$, we denote by $\mathrm{WF}^{1,\infty}_{\mathrm{b}}(u) \subset {}^{\mathrm{b}}T^*M$, resp. $\mathrm{WF}^{0,\infty}_{\mathrm{b}}(u)$ the wavefront set which microlocalizes infinite order conormal regularity with respect to $H^1(M;\mathbb{C}^4)$, respectively $H^0(M;\mathbb{C}^4)$; see e.g. [3] for a pedagogical introduction. In particular,

$$\mathrm{WF}^{1,\infty}_{\mathrm{b}}(u) = \emptyset \iff u \in H^{1,\infty}_{\mathrm{b}}(M).$$

Let $\Sigma = \{(x,t,\xi,\tau) \in T^*M \mid \tau^2 - \xi^2 = 0\}$ be the characteristic set associated to the Minkowski metric. The *compressed characteristic set* $\dot{\Sigma}$ is the image of Σ under the natural map $T^*M \to {}^{\mathrm{b}}T^*M$. By a *bicharacteristic* we will mean here the image in $\dot{\Sigma} \subset {}^{\mathrm{b}}T^*M$ of a null bicharacteristic for the Minkowski metric.

Let σ, τ, η be the fiber coordinates on ${}^{\mathrm{b}}T^*M$ in which the canonical one-form is

$$\sigma\frac{dr}{r} + \tau dt + \eta \cdot \frac{d\theta}{r}. \tag{2.10}$$

Then

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

Let $\dot{\Sigma}_0$ denote the topological space obtained as the quotient of $\dot{\Sigma}$ by the equivalence relation defined in the coordinates $(r, \theta, t, \sigma, \eta, \tau)$ above by

$$(0, \theta, t, 0, 0, \tau) \sim (0, \theta', t, 0, 0, \tau), \quad \theta, \theta' \in S^2,$$

i.e., identifying the factor of S^2 in the base.

Definition 2.9. A *diffractive bicharacteristic* is either:

(1) a bicharacteristic in ${}^{\mathrm{b}}T^*M^\circ$,
(2) a bicharacteristic starting or ending at $\{r = 0\}$,
(3) a concatenation of two forward, or two backward bicharacteristics, one ending at $\{r = 0\}$ and one starting at $\{r = 0\}$, whose projection to $\dot{\Sigma}_0$ is continuous.

In the case (1) this is simply a null bicharacteristic (in the usual sense) which does not meet $\{r = 0\}$. Note that ${}^{\mathrm{b}}T^*M^\circ$ is naturally identified with T^*M°, and Hörmander's propagation of singularities along null bicharacteristics applies. By equivalence of the wavefront set and b-wavefront set on M°, this means in particular that if $Du = 0$ and $q_1, q_2 \in \dot{\Sigma}$ are connected by a bicharacteristic lying entirely in ${}^{\mathrm{b}}T^*M^\circ$ then

$$q_1 \notin \mathrm{WF}^{1,\infty}_{\mathrm{b}}(u) \implies q_2 \notin \mathrm{WF}^{1,\infty}_{\mathrm{b}}(u).$$

In thinking of the second and third cases, we can distinguish between *incoming* and *outgoing* diffractive bicharacteristics (meaning ones moving *towards*, resp. *away from* $r = 0$ as t increases) by observing that they are contained in

$$\dot{\Sigma}_{\mathrm{in}} := \dot{\Sigma} \cap \{\sigma/\tau > 0 \text{ or } r = 0\} \text{ resp. } \dot{\Sigma}_{\mathrm{out}} := \dot{\Sigma} \cap \{\sigma/\tau < 0 \text{ or } r = 0\}$$

because away from $r = 0$, the sign of σ/τ determines the sign of dr/dt along bicharacteristics. Note that this terminology refers to the time flow on Minkowski space: this agrees with moving along bicharacteristics in the positive energy component $\dot{\Sigma}^+ = \dot{\Sigma} \cap \{\tau > 0\}$, but is the opposite of moving along bicharacteristics in the negative energy component $\dot{\Sigma}^- = \dot{\Sigma} \cap \{\tau < 0\}$.

We use the notation $q = (r, \theta, t, \sigma, \eta, \tau)$, $q' = (r', \theta', t', \sigma', \eta', \tau')$ for points in ${}^{\mathrm{b}}T^*M$ (and ${}^{\mathrm{b}}S^*M$), where the Greek letters indicate fiber coordinates given by (2.10). To take into account the diffraction in the propagation of singularities we first introduce the following terminology, which deals with sets invariant under the same S^2 quotient used above in passing from $\dot{\Sigma}$ to $\dot{\Sigma}_0$.

Definition 2.10. For $q = (r, \theta, t, \sigma, 0, \tau) \in \dot{\Sigma}$ we define its *diffractive spread* as the set

$$S_q := \{q' \in \dot{\Sigma} \mid r' = r,\ \theta' \in \mathbb{S}^2,\ t' = t,\ \operatorname{sgn} \tau' = \operatorname{sgn} \tau,\ \operatorname{sgn} \sigma' = \operatorname{sgn} \sigma,\ \eta' = 0\}.$$

For $q = (r, \theta, t, \sigma, \eta, \tau)$ with $\eta \neq 0$, we simply set $S_q := \{q\}$.

If $\sigma = 0$, then by writing $\operatorname{sgn} \sigma' = \operatorname{sgn} \sigma$ we simply mean $\sigma' = 0$.

On the base manifold, S_q is the orbit of q under spatial rotations around $r = 0$ (in the case $\eta = 0$). In the fibers, S_q consists of incoming or outgoing directions (depending on the nature of q) which lie in the same component $\dot{\Sigma}^{\pm}$ as q.

Definition 2.11. For $q_1, q_2 \in {}^{\mathrm{b}}T^*M$, we write $q_1 \dot{\sim} q_2$ if $q_1, q_2 \in \dot{\Sigma}$ and q_1 is connected with q_2 by a diffractive bicharacteristic.

The continuity enforced in the third part of Definition 2.9 ensures that neither time t nor energy τ jump upon interaction with the spatial origin, but by contrast the relationship of the angular variables of the concatenated bicharacteristics entering and leaving $r = 0$ is unconstrained. Of particular interest for our applications is that the constancy of τ along diffractive bicharacteristics enforces the following: if $q_1 \dot{\sim} q_2$, then q_1 and q_2 lie in the same component $\{\tau > 0\}$ or $\{\tau < 0\}$, i.e. either

$$(q_1, q_2) \in \dot{\Sigma}^+ \times \dot{\Sigma}^+, \text{ or } (q_1, q_2) \in \dot{\Sigma}^- \times \dot{\Sigma}^-.$$

In [3, Thm. 21–22] the first and third authors prove a diffractive propagation of singularities theorem which gives in particular the following statement, generalized here to the time-dependent setting introduced in (1.1)–(1.2).

Theorem 2.12. *Suppose $u \in H^{1,-\infty}_{\mathrm{b,loc}}(M; \mathbb{C}^4)$ satisfies $Du = 0$. Then, $\mathrm{WF}_{\mathrm{b}}^{1,\infty}(u) \subset \dot{\Sigma}$. Furthermore, for all $q_1, q_2 \in \dot{\Sigma}$ such that $q_1 \dot{\sim} q_2$,*

$$S_{q_1} \cap \mathrm{WF}_{\mathrm{b}}^{1,\infty}(u) = \emptyset \implies S_{q_2} \cap \mathrm{WF}_{\mathrm{b}}^{1,\infty}(u) = \emptyset. \tag{2.11}$$

More generally, if $Du = f$ for some $f \in H^{0,-\infty}_{\mathrm{b,loc}}(M; \mathbb{C}^4)$ then (2.11) holds true away from $\mathrm{WF}_{\mathrm{b}}^{0,\infty}(f)$.

Proof. This result follows from Theorems 22 and 23 of [3] in the special case of time independent Hamiltonian $H(t) = H(0)$. The proof in the case of time-dependent Hamiltonian (where we recall that the time dependence is only through the smooth part of the vector potential) requires only fairly minor changes, however; we now describe these changes to the proofs in [3]. Note that we will employ the calculus of b-pseudodifferential operators, as described in [3, §3] and references therein.

The main changes needed in the time dependent case are twofold. Most obviously, one must check that in the presence of time dependent coefficients, the positive commutators employed in [3] remain positive modulo the same types of error terms as before. Additionally, though, the main commutator arguments in [3] are all built around the background regularity assumption $u \in H^1(M;\mathbb{C}^4)$ (or more generally $u \in C(\mathbb{R};\mathcal{D}^{-\infty})$). We claim that a local regularity assumption is sufficient, namely, if the theorem is true for $u \in H^1(M;\mathbb{C}^4)$ then it is also true under the weaker assumption $u \in H^1_{\mathrm{loc}}(M;\mathbb{C}^4)$. In fact, we can find $\chi \in C^\infty_{\mathrm{c}}(M)$ such that $\chi = 1$ on the base projection of the diffractive bicharacteristic segments from q_1 to q_2. Then $\chi u \in H^1(M;\mathbb{C}^4)$ and $P\chi u = f + [P,\chi]u$, with $\operatorname{supp}[P,\chi]u$ disjoint from the region of interest, so we are reduced to applying the $H^1(M;\mathbb{C}^4)$ version of the theorem.

To extend to the more general assumption $u \in H^{1,-\infty}_{\mathrm{b,loc}}(M;\mathbb{C}^4)$ requires no great effort in the time-independent case, as we can simply commute H with powers of of ∂_t (and keep in mind that $\partial_t^k \in \Psi^k_{\mathrm{b}}(M)$) in order to shift regularity up and down on the scale of spaces $H^{1,s}_{\mathrm{b}}(M;\mathbb{C}^4)$. On the other hand, if H is time-dependent, this argument to shift regularity no longer applies as written. We thus need to use a more robust argument, conjugating by an elliptic b-pseudodifferential operator which does not, in general, commute with $H(t)$. We begin by describing this conjugation.

Given $u \in H^{1,-m-1}_{\mathrm{b,loc}}(M;\mathbb{C}^4)$ with $Du = f \in H^{0,-m+1}_{\mathrm{b,loc}}$, we will proceed by proving propagation of singularities for $v = \Upsilon u$, where $\Upsilon \in \Psi^{-m}_{\mathrm{b}}(M)$ is an invertible, SO(3)-invariant, elliptic b-pseudodifferential operator of order $-m$. As Υ is elliptic, measuring $\mathrm{WF}^{1,s}_{\mathrm{b}}(u)$ is equivalent to measuring $\mathrm{WF}^{1,s+m}_{\mathrm{b}}(v)$. The equation satisfied by v is then

$$\widetilde{D}v = \left(D - [D,\Upsilon]\,\Upsilon^{-1}\right) v = \Upsilon f.$$

Establishing propagation of singularities for $\widetilde{D}$ at the level of $H^{1,s-1}_{\mathrm{b,loc}}(M;\mathbb{C}^4)$ for $s \geqslant 0$ provides the statement for (possibly time-dependent) D at the level of $H^{1,s-m-1}_{\mathrm{b,loc}}(M;\mathbb{C}^4)$. Thus, it suffices for us to prove propagation of singularities for the operator $\widetilde{D}$ for a solution lying in $H^1_{\mathrm{loc}}(M;\mathbb{C}^4)$.

As in the proof of Lemma 2.3, a computation in the differential b-calculus verifies that

$$\widetilde{D} - D \in \Psi^0_{\mathrm{b}} + \Psi^{-1}_{\mathrm{b}}\frac{1}{r} + \Psi^{-1}_{\mathrm{b}}\partial_r + \Psi^{-1}_{\mathrm{b}}\left(\frac{1}{r}\beta K\right),$$

where K is Dirac's K-operator, see [3, §2.2].

We now discuss the changes in the proof of the propagation of singularities results [3, Thm. 22–23] necessary to accommodate both the time-varying coefficients and also the need to consider $\widetilde{D}$ rather than D itself. The argument has two main steps: an elliptic estimate and a hyperbolic estimate. The elliptic estimate, discussed in the proof of Lemma 2.3, is based on the real part of the quadratic form $\langle Pu, u\rangle$ and is used in two main ways, both to provide estimates outside the characteristic set and to more generally reduce the problem of estimating an H^1 norm to one of estimating only the L^2 norm of $\partial_t v$. The other main component is the hyperbolic estimate, which is obtained via a positive commutator estimate built out of a microlocalization of $r\partial_r$.

Both pieces require controlling the interactions of r^{-1} and ∂_r with Melrose's b-calculus and the proofs of both pieces hold for $\widetilde{D}$ as well. The elliptic estimate was treated above in Lemma 2.3.

For the hyperbolic estimate, the core arguments are unchanged. Lemma 27 of [3] computes the commutator of D with a b-pseudodifferential operator of order m and is the main change that must be made; there is a new term of the form $\Psi_{\mathrm{b}}^{m-2} r^{-1}\beta K$. On the other hand, similar terms arise already in the application to a specific commutator [3, Lem. 36], where this term is represented as $\mathbf{R}_3$. As this term is treated as an error term and not as a source of positivity, it yields no change in the proof of the hyperbolic estimate. Note that the time dependence of the coefficients, per se, contributes no new types of error terms. □

Note also that if the bicharacteristic segment connecting q_1 and q_2 does not meet $r = 0$, then of course Hörmander's propagation of singularities theorem applies and S_{q_i} can be replaced by q_i, $i = 1, 2$.

2.4. **Operatorial b-wavefront set.** Let us now introduce an operatorial version of the b-wavefront set and discuss its properties, analogously to [42, 19] (in particular the proofs of Lemmas 2.15 and 2.16 below are fully analogous). We first define a class of operators that are suitable for b-wavefront set considerations and propagation of singularities.

Definition 2.13. We say that Λ is *regular* if $\Lambda : H_{\mathrm{b,c}}^{-1,m+1}(M;\mathbb{C}^4) \to H_{\mathrm{b,loc}}^{1,m-1}(M;\mathbb{C}^4)$ continuously for all $m \in \mathbb{R}$.

Definition 2.14. For Λ regular, its *operatorial* b-*wavefront set* is the set $\mathrm{WF}_{\mathrm{b}}'(\Lambda) \subset {}^{\mathrm{b}}S^*M \times {}^{\mathrm{b}}S^*M$ defined as follows: $(q_1, q_2) \notin \mathrm{WF}_{\mathrm{b}}'(\Lambda)$ iff there exist $B_i \in \Psi_{\mathrm{b}}^0(M)$, elliptic at q_i $(i = 1, 2)$, such that

$$B_1 \Lambda B_2^* : H_{\mathrm{b,c}}^{-1,-\infty}(M;\mathbb{C}^4) \to H_{\mathrm{b,loc}}^{1,\infty}(M;\mathbb{C}^4) \tag{2.12}$$

continuously.

Lemma 2.15. *Suppose Λ is regular and $\mathrm{WF}_{\mathrm{b}}'(\Lambda) = \emptyset$. Then $\Lambda : H_{\mathrm{b,c}}^{-1,-\infty}(M;\mathbb{C}^4) \to H_{\mathrm{b,loc}}^{1,\infty}(M;\mathbb{C}^4)$ continuously.*

Lemma 2.16. *If Λ and $\tilde{\Lambda}$ are regular then $\mathrm{WF}_{\mathrm{b}}'(\Lambda + \tilde{\Lambda}) \subset \mathrm{WF}_{\mathrm{b}}'(\Lambda) \cup \mathrm{WF}_{\mathrm{b}}'(\tilde{\Lambda})$.*

Definition 2.17. We say that Λ is a *regular bi-solution* if it is regular and

$$D \circ \Lambda = 0 \text{ on } H_{\mathrm{b,c}}^{-1,-\infty}(M;\mathbb{C}^4), \quad \Lambda \circ D = 0 \text{ on } H_{\mathrm{b,c}}^{1,-\infty}(M;\mathbb{C}^4). \tag{2.13}$$

We will use the following operator version of Theorem 2.12.

Theorem 2.18. *Suppose that Λ is a regular bi-solution. Then $\mathrm{WF}_{\mathrm{b}}'(\Lambda) \subset \dot{\Sigma} \times \dot{\Sigma}$. Furthermore, if $q_1 \in \dot{\Sigma}$ and $\Gamma_2 \subset \dot{\Sigma}$ is closed then for all q_1' s.t. $q_1 \dot{\sim} q_1'$,*

$$(S_{q_1} \times \Gamma_2) \cap \mathrm{WF}_{\mathrm{b}}'(\Lambda) = \emptyset \implies (S_{q_1'} \times \Gamma_2) \cap \mathrm{WF}_{\mathrm{b}}'(\Lambda) = \emptyset. \tag{2.14}$$

Similarly, if $q_2 \in \dot{\Sigma}$ and $\Gamma_1 \subset \dot{\Sigma}$ is closed then for all q_2' s.t. $q_2 \dot{\sim} q_2'$,

$$(\Gamma_1 \times S_{q_2}) \cap \mathrm{WF}_{\mathrm{b}}'(\Lambda) = \emptyset \implies (\Gamma_1 \times S_{q_2'}) \cap \mathrm{WF}_{\mathrm{b}}'(\Lambda) = \emptyset. \tag{2.15}$$

Proof. Let us show (2.14). As the statement is microlocal, without loss of generality we can suppose that the projection of Γ_2 to the base manifold is compact. Suppose $(S_{q_1} \times \Gamma_2) \cap \mathrm{WF}_{\mathrm{b}}'(\Lambda) = \emptyset$. Then there exist compactly supported $B_1, B_2 \in \Psi_{\mathrm{b}}^0(M)$ elliptic on respectively S_{q_1}, Γ_2, such that for any bounded $\mathcal{U} \subset H_{\mathrm{b,c}}^{-1,-\infty}(M;\mathbb{C}^4)$, $B_1 \Lambda B_2^* \mathcal{U}$ is uniformly bounded in $H_{\mathrm{b,loc}}^{1,\infty}(M;\mathbb{C}^4)$. We now apply propagation of singularities to $\Lambda B_2^* v$ for all $v \in \mathcal{U}$ (in the form of the uniform estimate obtained in the proof of Theorem 2.12).

The hypotheses are verified because $\Lambda B_2^* v$ is in $H^{1,-\infty}_{\mathrm{b,loc}}(M;\mathbb{C}^4)$ using that Λ is regular. As a result, for each point of $S_{q_1'}$ we can find $B_1' \in \Psi^0_{\mathrm{b}}(M)$ elliptic at that point, such that $B_1'\Lambda B_2^*\mathcal{U}$ is uniformly bounded in $H^{1,\infty}_{\mathrm{b,loc}}(M;\mathbb{C}^4)$, which shows (2.14).

We now show (2.15). If $(\Gamma_1 \times S_{q_2}) \cap \mathrm{WF}'_{\mathrm{b}}(\Lambda) = \emptyset$ for some compact Γ_1, and all compactly supported $B_1, B_2 \in \Psi^0_{\mathrm{b}}(M)$ elliptic on respectively, Γ_1, S_{q_2}, with sufficiently small microsupport, $B_1\Lambda B_2^* : H^{-1,-\infty}_{\mathrm{b,c}}(M;\mathbb{C}^4) \to H^{1,\infty}_{\mathrm{b,loc}}(M;\mathbb{C}^4)$. By taking adjoints

$$B_2\Lambda^* B_1^* : H^{-1,-\infty}_{\mathrm{b,c}}(M;\mathbb{C}^4) \to H^{1,\infty}_{\mathrm{b,c}}(M;\mathbb{C}^4). \tag{2.16}$$

We apply propagation of singularities to $\Lambda^* B_1^* v$ for v in a bounded subset $\mathcal{U} \subset H^{-1,-\infty}_{\mathrm{b,c}}$ similarly as before, and deduce the existence of B_2' elliptic at any chosen point of $S_{q_2'}$ such that

$$B_2'\Lambda^* B_1^* : H^{-1,-\infty}_{\mathrm{b,c}}(M;\mathbb{C}^4) \to H^{1,\infty}_{\mathrm{b,c}}(M;\mathbb{C}^4).$$

By taking adjoints,

$$B_1\Lambda(B_2')^* : H^{-1,-\infty}_{\mathrm{b,c}}(M;\mathbb{C}^4) \to H^{1,\infty}_{\mathrm{b,c}}(M;\mathbb{C}^4).$$

This implies (2.15). □

3. Singularities of two-point functions

3.1. **Hadamard condition.** Let us first recall one version of the Hadamard condition, formulated here as a regularity condition *away from the* $r = 0$ *singularity* (in fact, we do not expect to control the direct analogue of that condition on the whole of $\mathbb{R}^{1,3}$).

Definition 3.1. We say that a pair of bounded operators $\Lambda^\pm : C^\infty_{\mathrm{c}}(M^\circ;\mathbb{C}^4) \to \mathcal{D}'(M^\circ;\mathbb{C}^4)$ is *Hadamard* if they satisfy (the *Hadamard condition*)

$$\mathrm{WF}'(\Lambda^\pm) \subset \Sigma^\pm \times \Sigma^\pm, \tag{3.17}$$

where WF' is the primed wavefront restricted to $S^*M^\circ \times S^*M^\circ$ and $\Sigma^\pm = \Sigma \cap \{\pm\tau > 0\}$ are the two connected components of the characteristic set Σ.

Note that on $S^*M^\circ \times S^*M^\circ \simeq (T^*M^\circ \setminus o)/\mathbb{R}_+ \times (T^*M^\circ \setminus o)/\mathbb{R}_+$, the above definition of WF' coincides with the standard definition, which refers to the wavefront set of the Schwartz kernel. In contrast, however, it does not say anything about possible singularities located at $o \times T^*M^\circ$ or $T^*M^\circ \times o$. In practice, this type of information is replaced by the regularity assumption $\Lambda^\pm : C^\infty_{\mathrm{c}}(M^\circ;\mathbb{C}^4) \to \mathcal{D}'(M^\circ;\mathbb{C}^4)$.

We stress that in the presence of a singular potential, it is not immediately clear which formulation of the Hadamard condition is adequate, even away from the singularity. Here, we use the Hadamard condition in the form (3.17), following [35, 26]. If the potentials are smooth at $r = 0$ as opposed to having a Coulomb singularity, and if $\Lambda^\pm$ are two-point functions on $\mathbb{R}^{1,3}$ (or on a more general globally hyperbolic spacetime), then condition (3.17) on $\mathbb{R}^{1,3}$ is equivalent to the more precise (and most commonly used) statement

$$\mathrm{WF}'(\Lambda^\pm) \subset (\Sigma^\pm \times \Sigma^\pm) \cap \{(q_1, q_2) \mid q_1 \sim q_2\},$$

where $q_1 \sim q_2$ means that q_1 is connected with q_2 by a bicharacteristic in the usual (non-diffractive) sense. This equivalence needs however not be true in the presence of a

Coulomb singularity because of diffractive bicharacteristics that cross $r = 0$. The correct replacement is given later on in Proposition 3.8.

In practice, to control the Hadamard condition (3.17) we need to consider the operator b-wavefront set on the whole of M.

In what follows we will not distinguish between $\Sigma \cap \{r \neq 0\}$ and $\dot{\Sigma} \cap \{r \neq 0\}$ in the notation (recall that they are identified by a canonical isomorphism).

Proposition 3.2. *If $\Lambda^{\pm}$ is a pair of regular bi-solutions, then it is Hadamard if and only if*

$$\mathrm{WF}'_{\mathrm{b}}(\Lambda^{\pm}) \subset \dot{\Sigma}^{\pm} \times \dot{\Sigma}^{\pm}. \tag{3.18}$$

Proof. For any $q \in \dot{\Sigma}^{\mp} \cap \{r = 0\}$, we can find $q' \in \Sigma^{\mp} \cap \{r \neq 0\}$ such that $q' \dot{\sim} q$. Since $S_{q'} \subset \Sigma^{\mp}$, the Hadamard condition implies

$$(S_{q'} \times (\dot{\Sigma} \cap \{r \neq 0\})) \cap \mathrm{WF}'_{\mathrm{b}}(\Lambda^{\pm}) = \emptyset = (\dot{\Sigma} \cap \{r \neq 0\} \times S_{q'}) \cap \mathrm{WF}'_{\mathrm{b}}(\Lambda^{\pm})$$

By Theorem 2.18 (operator version of propagation of singularities), this yields

$$(\{q\} \times (\dot{\Sigma} \cap \{r \neq 0\})) \cap \mathrm{WF}'_{\mathrm{b}}(\Lambda^{\pm}) = \emptyset = ((\dot{\Sigma} \cap \{r \neq 0\}) \times \{q\}) \cap \mathrm{WF}'_{\mathrm{b}}(\Lambda^{\pm})$$

Let now $(q_1, q_2) \in \dot{\Sigma}^{\mp} \times \dot{\Sigma}^{\mp}$. Then either none of the points q_1, q_2 lie over $r = 0$ (then there is nothing to prove by the Hadamard condition (3.17)), or only q_1 or q_2 lies over $r = 0$ and we can apply the above argument combined with the Hadamard condition to get $(q_1, q_2) \notin \mathrm{WF}'_{\mathrm{b}}(\Lambda^{\pm})$, or else both q_1, q_2 lie over $r = 0$ and then we can apply the argument twice, first to q_1 and then to q_2 to obtain $(q_1, q_2) \notin \mathrm{WF}'_{\mathrm{b}}(\Lambda^{\pm})$. For points not in $\dot{\Sigma} \times \dot{\Sigma}$ it suffices to invoke the elliptic estimate statement in Theorem 2.18. The opposite direction is evident. □

We will show that the differences of regular bi-solutions have a well-defined on-diagonal restriction, and hence a well-defined trace density. We start by recalling an elementary fact about mapping properties of the Mellin transform $\mathcal{M}$, defined here with the normalization

$$(\mathcal{M}f)(\xi) = \int_0^\infty f(r) r^{-i\xi - 1} dr.$$

Lemma 3.3. *If $\mathcal{M}f(\xi)$ is holomorphic and $O(\langle \xi \rangle^{-s})$ in $\operatorname{Im} \xi > -\epsilon$ for some $\epsilon > 0$ and $s > 1$, then $f = O(1)$ near $r = 0$, with*

$$\sup_{r \in]0,1[} |f(r)| \leqslant \frac{1}{2\pi} \int_{-\infty}^{\infty} |\mathcal{M}f(\xi)| d\xi.$$

Proof. We write f as the inverse Mellin transform

$$f(r) = \frac{1}{2\pi} \int_{-\infty}^{\infty} (\mathcal{M}f)(\xi) r^{i\xi} d\xi$$

and bound the integral accordingly. □

Proposition 3.4. *Suppose $\Lambda^{\pm}$ and $\tilde{\Lambda}^{\pm}$ are regular bi-solutions that satisfy the Hadamard condition, and*

$$\Lambda^{+} - \tilde{\Lambda}^{+} = -(\Lambda^{-} - \tilde{\Lambda}^{-}). \tag{3.19}$$

Then $\Lambda^{\pm} - \tilde{\Lambda}^{\pm} : H^{-1,-\infty}_{\mathrm{b,c}}(M; \mathbb{C}^4) \to H^{1,\infty}_{\mathrm{b,loc}}(M; \mathbb{C}^4)$ continuously.

Proof. The b-wave front set of the l.h.s. of (3.19) is contained in $\dot\Sigma^+ \times \dot\Sigma^+$, and the b-wave front set of the RHS is contained in $\dot\Sigma^- \times \dot\Sigma^-$, hence the two are disjoint. Thus, both sides of (3.19) have in fact empty b-wave front set, and thus

$$\Lambda^\pm - \tilde\Lambda^\pm : H^{-1,-\infty}_{\mathrm{b,c}}(M;\mathbb{C}^4) \to H^{1,\infty}_{\mathrm{b,loc}}(M;\mathbb{C}^4) \tag{3.20}$$

is bounded by Lemma 2.15. ☐

Next we show that for the existence of a trace density we need slightly weaker mapping properties than (3.20)

Proposition 3.5. *If $\Lambda : H^{0,-\infty}_{\mathrm{b,c}}(M;\mathbb{C}^4) \to H^{1,\infty}_{\mathrm{b,loc}}(M;\mathbb{C}^4)$ continuously then Λ has a locally integrable trace density.*

Proof. Since the statement is local we can without loss of generality assume that $\Lambda : H^{0,-\infty}_{\mathrm{b,c}} \to H^{1,\infty}_{\mathrm{b,c}}(M;\mathbb{C}^4)$. The b-regularity means that for any N and choices of vector fields $V_1,\ldots,V_N$ with $V_j \in \pi_i^*\mathcal{V}_{\mathrm{b}}(M)$, $i=1,2$ (π_i being the projection on the i-th component of $M\times M$), the operator Λ_V with Schwartz kernel

$$V_1\ldots V_N\Lambda(.,.)$$

still has the property $\Lambda_V : L^2(M;\mathbb{C}^4) \to H^1_{\mathrm{loc}}(M;\mathbb{C}^4)$. Recall that the volume form in our coordinates is $r^2 dt\, dr\, d\theta$. Since $r^s \in L^2_{\mathrm{loc}}(M)$ for $\operatorname{Re} s > -3/2$ and $r^{s'} \in H^{-1}_{\mathrm{loc}}(M)$ for $s' > -5/2$, if we choose any pair of spherical harmonics $Y_\bullet$ on $\mathbb{S}^2$ we obtain

$$\left|\langle \Lambda_V r^s Y_{lm}, r^{s'} Y_{l'm'}\rangle\right| \leqslant C < \infty, \quad \operatorname{Re} s > -3/2,\ \operatorname{Re} s' > -5/2$$

with the constant C uniform in s, s' provided we restrict to strictly smaller half-planes, and also uniform in the orders m, l, m', l' of the spherical harmonics. Thus for $\operatorname{Re} s > -3/2$, $\operatorname{Re} s' > -5/2$,

$$\Big|\int V_1\ldots V_N\Lambda(r_1,r_2,\theta_1,\theta_2) r_1^s r_2^{s'} Y_{lm}(\theta_1) Y_{l'm'}(\theta_2)\, dt_1\, dt_2\, r_1^2 dr_1\, r_2^2 dr_2\, d\theta_1\, d\theta_2\Big| \leqslant C.$$

Now we interpret the integrals in r_1, r_2 as Mellin transforms in r_1, r_2 respectively, denoting these maps as $\mathcal{M}_{(1)}, \mathcal{M}_{(2)}$. Thus our estimate is

$$\Big|\int (\mathcal{M}_{(1)}\mathcal{M}_{(2)} V_1\ldots V_N\Lambda)(is+3i, is'+3i, \theta_1,\theta_2) Y_{lm}(\theta_1) Y_{l'm'}(\theta_2) dt_1\, dt_2\, d\theta_1\, d\theta_2\Big| \leqslant C,$$

again for $\operatorname{Re} s > -3/2$, $\operatorname{Re} s' > -5/2$, and the l.h.s. is holomorphic in s, s' in these half-spaces. Moreover by taking V_j to be vector fields of the form $\partial_{t_1}, \partial_{t_2}, \partial_{\theta_1}, \partial_{\theta_2}$, and integrating by parts so that the θ_1, θ_2 derivatives fall onto the spherical harmonics, the uniform boundedness now shows that for all $N \in \mathbb{N}$, and (t_1, t_2) ranging over a compact set,

$$\Big|\int (\mathcal{M}_{(1)}\mathcal{M}_{(2)}\Lambda)(is+3i, is'+3i, \theta_1,\theta_2) Y_{lm}(\theta_1) Y_{l'm'}(\theta_2) d\theta_1\, d\theta_2\Big| \leqslant C_N \langle l\rangle^{-N} \langle l'\rangle^{-N}$$

(with $l(l+1)$ being the Laplace eigenvalue of Y_{lm}); here we have employed the estimate on the vector fields ∂_{t_1}, ∂_{t_2} to obtain a (locally) uniform estimate in t_1, t_2. Further integration by parts with the b-vector fields V_j chosen to be $r_1\partial_{r_1}$, $r_2\partial_{r_2}$ improves the estimate to

$$
\begin{aligned}
&\Big|\int (\mathcal{M}_{(1)}\mathcal{M}_{(2)}\Lambda)(is+3i, is'+3i, \theta_1, \theta_2) Y_{lm}(\theta_1) Y_{l'm'}(\theta_2) d\theta_1\, d\theta_2\Big| \\
&\qquad \leqslant C_N \langle l\rangle^{-N}\langle l'\rangle^{-N}\langle s\rangle^{-N}\langle s'\rangle^{-N}, \quad \operatorname{Re} s > -3/2,\ \operatorname{Re} s' > -5/2.
\end{aligned}
\tag{3.21}
$$

Applying Lemma 3.3 to the l.h.s. of (3.21) (and recalling that $\mathcal{M}(r^k f)(\xi) = \mathcal{M}f(\xi - ik)$) shows that since for any $\delta > 0$,

$$
\int (\mathcal{M}_{(1)}\mathcal{M}_{(2)} r_1^{3/2+\delta} r_2^{1/2+\delta})\Lambda(\zeta, \zeta', \theta_1, \theta_2) Y_{lm}(\theta) Y_{l'm'}(\theta_2)\, d\theta_1\, d\theta_2
$$

is holomorphic in $\operatorname{Im}\zeta, \operatorname{Im}\zeta' > -\delta$, and bounded by

$$
C_N \langle l\rangle^{-N}\langle l'\rangle^{-N}\langle \zeta\rangle^{-N}\langle \zeta'\rangle^{-N},
$$

then in fact

$$
\int r_1^{3/2+\delta} r_2^{1/2+\delta}\Lambda(t_1, t_2, r_1, r_2, \theta_1, \theta_2) Y_{lm}(\theta_1) Y_{l'm'}(\theta') d\theta\, d\theta' = O(\langle l\rangle^{-N}) O(\langle l'\rangle^{-N})
$$

for all $\delta > 0$. Summing over spherical harmonics (taking N sufficiently large to give convergence) then shows that

$$
\big| r_1^{3/2+\delta} r_2^{1/2+\delta}\Lambda(t_1, t_2, r_1, r_2, \theta_1, \theta_2)\big| \leqslant C.
$$

Restricting to the diagonal gives

$$
\Lambda|_{\mathrm{diag}}(t, r, \theta) = O(r^{-2-2\delta}) \in L^1_{\mathrm{loc}}(\mathrm{diag}; r^2\, dt\, dr\, d\theta)
$$

as asserted, provided we choose $2\delta < 1$. □

We conclude that if $\Lambda^{\pm}$ are a Hadamard pair then they have a well-defined *relative trace density* (relative to some other Hadamard $\tilde{\Lambda}^{\pm}$).

3.2. **Two-point functions.** Let $t_0 \in \mathbb{R}$ be some reference time. In the terminology commonly used for fermions, a *quasi-free state* is determined by its *density matrix*[2] at time t_0, i.e. by a bounded operator γ on $L^2(X; \mathbb{C}^4)$ such that

$$
0 \leqslant \gamma(t_0) \leqslant \mathbf{1}. \tag{3.22}
$$

Its *space-time two-point functions* are the pair of operators $\Lambda^{\pm}$ given by

$$
\begin{aligned}
\Lambda^{-}(t_1, t_2) &= U(t_1, t_0)\gamma(t_0) U(t_0, t_2), \\
\Lambda^{+}(t_1, t_2) &= U(t_1, t_0)(\mathbf{1} - \gamma(t_0)) U(t_0, t_2),
\end{aligned}
\tag{3.23}
$$

where Schwartz kernel notation is used in the time variable only, i.e.

$$
\big(\Lambda^{-} f\big)(t) = \int_{-\infty}^{\infty} U(t, t_0)\gamma(t_0) U(t_0, t_2) f(t_2) dt_2
$$

and similarly for Λ^{+}. They satisfy

$$
\Lambda^{\pm} \geqslant 0, \quad \Lambda^{+} + \Lambda^{-} = S, \tag{3.24}
$$

where S is the operator with time Schwartz kernel $U(t_1, t_2)$.

[2]This is not to be confused with the γ matrices that enters the definition of Dirac operators, see §A.1.

Lemma 3.6. *The operator S is a regular bi-solution, i.e. $S : H^{-1,s+1}_{\mathrm{b,c}}(M;\mathbb{C}^4) \to H^{1,s-1}_{\mathrm{b,loc}}(M;\mathbb{C}^4)$ continuously for all $s \in \mathbb{R}$.*

Proof. Let T be as given in Section 2.2 with $t_- = t_0$. By Lemmas 2.4 and 2.8,

$$T : \mathcal{D}^s \to H^{1,s-1}_{\mathrm{b,loc}}, \quad s \in \mathbb{R}, \tag{3.25}$$

and, dually,

$$T^* : H^{-1,-s+1}_{\mathrm{b,c}} \to \mathcal{D}^{-s}, \quad s \in \mathbb{R}. \tag{3.26}$$

Hence for all $s \in \mathbb{R}$,

$$S = TT^* : H^{-1,s+1}_{\mathrm{b,c}} \to H^{1,s-1}_{\mathrm{b,loc}}.$$

□

In the case when $H(t) \equiv H$ is time-independent, of particular importance are *stationary states*, i.e. those for which $\gamma(t) \equiv \gamma = \chi(H)$ for some Borel function χ with values in $[0,1]$. If $0 \notin \mathrm{sp}(H)$. Then the *Dirac–Coulomb vacuum*, is obtained from the density matrix $\gamma = \mathbf{1}_{]-\infty,0]}(H)$. It is also natural to consider excited states: this corresponds to taking $\mathbf{1}_{]-\infty,\lambda]}(H)$ for some $\lambda \notin \mathrm{sp}(H)$.

More generally, since $H(t)$ is time-independent for $t \leqslant t_-$ and $t \geqslant t_+$ then the *in-state*, resp. *out-state* are defined by taking $\gamma(t_0) = \mathbf{1}_{]-\infty,0]}(H(t_0))$ for some reference time $t_0 \leqslant t_-$, resp. $t_0 \geqslant t_+$.

Proposition 3.7. *Suppose $t_0 \leqslant t_-$ or $t_0 \geqslant t_+$. If $\gamma(t_0) = \chi_-(H)$ for some $\chi_- \in S^0(\mathbb{R};[0,1])$ such that $\chi_- \equiv \mathbf{1}_{]-\infty,0]}$ outside of a neighborhood of 0, then the corresponding pair $\Lambda^\pm$ defined in (3.23) are Hadamard regular bi-solutions.*

Proof. We show regularity for Λ^+; the statement for $\Lambda^- = S - \Lambda^+$ then follows immediately by the previous lemma. Let T be the propagator described in Section 2.2. We write

$$\Lambda^+ = T(\mathbf{1} - \gamma(t_0))T^*,$$

where $T : \mathcal{D}^s \to H^{1,s-1}_{\mathrm{b,loc}}$ and $T^* : H^{-1,s+1}_{\mathrm{b,c}} \to \mathcal{D}^s$ for all $s \in \mathbb{R}$. Because $\gamma(t_0)$ commutes with $H(t_0)$, $\gamma(t_0)$ is bounded $\mathcal{D}^s \to \mathcal{D}^s$ for all $s \in \mathbb{R}$ and so Λ^+ is regular.

That $\Lambda^\pm$ is a bi-solution follows from its representation in terms of the solution operator T. We must therefore only show that $\Lambda^\pm$ is Hadamard. Let $\Lambda^\pm_0$ be $\Lambda^\pm$ restricted to the static region $I \times X$ with I an open interval containing $]-\infty, t_-]$ or $[t_+, \infty[$. First note that $\mathrm{WF}'(\Lambda^\pm_0) \subset \Sigma \times \Sigma$ by elliptic regularity. Furthermore,

$$\tilde{\chi}_\mp(i^{-1}\partial_t)\Lambda^\pm_0 = 0 = \Lambda^\pm_0 \tilde{\chi}_\mp(i^{-1}\partial_t)$$

on $I \times X$ for suitable $\tilde{\chi}_\mp \in S^0(\mathbb{R})$ so that $\tilde{\chi}_\mp(\tau) \equiv 0$ for $\pm\tau \gg 0$ and $\tilde{\chi}_\mp(\tau) \equiv 1$ for $\mp\tau \gg 0$. While $\tilde{\chi}_\mp(i^{-1}\partial_t)$ is not a pseudodifferential operator on M°, it is possible to find a properly supported $A \in \Psi^0(M^\circ)$ so that $A\tilde{\chi}_\mp(i^{-1}\partial_t)$ and $\tilde{\chi}_\mp(i^{-1}\partial_t)A$ are pseudodifferential and elliptic at any chosen point of $\Sigma^\mp$ and hence $\mathrm{WF}'(\Lambda^\pm_0) \subset \Sigma^\pm \times \Sigma$ and $\mathrm{WF}'(\Lambda^\pm_0) \subset \Sigma \times \Sigma^\pm$. Thus, $\mathrm{WF}'(\Lambda^\pm_0) \subset \Sigma^\pm \times \Sigma^\pm$ over $(I \times X^\circ) \times (I \times X^\circ)$. By Proposition 3.2 this implies $\mathrm{WF}'_{\mathrm{b}}(\Lambda^\pm_0) \subset \dot{\Sigma}^\pm \times \dot{\Sigma}^\pm$ over $(I \times X) \times (I \times X)$. Finally, by operator propagation of singularities, i.e., Theorem 2.18, applied to the first and then to the second set of spacetime variables, we conclude $\mathrm{WF}'_{\mathrm{b}}(\Lambda^\pm) \subset \dot{\Sigma}^\pm \times \dot{\Sigma}^\pm$ everywhere. □

In particular this proves Theorem 1.1.

We can also estimate the b-wavefront set of Hadamard two-point functions a bit more precisely.

Proposition 3.8. *If $\Lambda^{\pm}$ are a pair of two-point functions and Hadamard bi-solutions then*

$$\mathrm{WF}_{\mathrm{b}}'(\Lambda^{\pm}) \subset (\dot{\Sigma}^{\pm} \times \dot{\Sigma}^{\pm}) \cap \{(q_1, q_2) \mid q_1 \dot{\sim} q_2\}. \tag{3.27}$$

Proof. Since $\Lambda^{+} + \Lambda^{-} = S$, using Proposition 3.2 Λ^{+} and Λ^{-} have disjoint wavefront sets and we get

$$\mathrm{WF}_{\mathrm{b}}'(\Lambda^{\pm}) \subset (\dot{\Sigma}^{\pm} \times \dot{\Sigma}^{\pm}) \cap \mathrm{WF}_{\mathrm{b}}'(S). \tag{3.28}$$

Recall that $S = S_{+} - S_{-}$ where S_{+} is the retarded, and S_{-} the advanced propagator. By the elliptic regularity statement in Theorem 2.18,

$$\mathrm{WF}_{\mathrm{b}}'(S) \subset \big(\mathrm{WF}_{\mathrm{b}}'(S_{+}) \cup \mathrm{WF}_{\mathrm{b}}'(S_{-})\big) \cap (\dot{\Sigma} \times \dot{\Sigma}). \tag{3.29}$$

Let now q_2 be any point in $\dot{\Sigma}$. Then we claim that for all $q_1 \in \dot{\Sigma}$ such that q_1 is not connected with q_2 by a diffractive bicharacteristic (in particular $q_1 \neq q_2$), $(q_1, q_2) \notin \mathrm{WF}_{\mathrm{b}}'(S_{+})$ and $(q_1, q_2) \notin \mathrm{WF}_{\mathrm{b}}'(S_{-})$.

In fact, if $t_1 < t_2$ this simply follows from support properties of S_{+}. Otherwise, we can take q_1' with $t_1' < t_2$ and $q_1' \dot{\sim} q_1$, then $(S_{q_1'} \times \{q_2\}) \cap \mathrm{WF}_{\mathrm{b}}'(S_{+}) = \emptyset$ by the previous argument, which then implies $(S_{q_1} \times \{q_2\}) \cap \mathrm{WF}_{\mathrm{b}}'(S_{+}) = \emptyset$ by the propagation of singularities statement in Theorem 2.18 (strictly speaking, its obvious generalization microlocalized outside of the diagonal, as S_{+} is not a bi-solution everywhere), in particular $(q_1, q_2) \notin \mathrm{WF}_{\mathrm{b}}'(S_{+})$. The analogous argument applies to S_{-}.

Using (3.29) we conclude that

$$\mathrm{WF}_{\mathrm{b}}'(S) \subset \{(q_1, q_2) \mid q_1 \dot{\sim} q_2\}. \tag{3.30}$$

Plugged into (3.28) this yields (3.27). □

Remark 3.9. Note that here we have proved an estimate (3.30) on the singularities of the Dirac–Coulomb propagator S, but one could wonder if diffraction does actually occur and if one could not replace $q_1 \dot{\sim} q_2$ by $q_1 \sim q_2$. The work [3] conjectures that this is *not* the case (at least in the time-independent case), and diffraction does occur indeed, albeit the resulting extra singularities are $1-\epsilon$ order less severe (with $\epsilon > 0$ arbitrary) in the sense of local Sobolev regularity. From our results we conclude that the diffractive singularities are harmless if one deals only with Hadamard states in the renormalization. On the other hand, diffraction implies a significantly more singular behaviour if one considers states that are not Hadamard (for instance, this issue arises when one subtracts the Dirac or Dirac–Coulomb vacuum in a t-dependent situation). It could also potentially have bad implications for quantities renormalized with the Hadamard parametrix as in [30, 27, 43, 37, 44], though this still has to be studied in more detail.

Appendix A. Second quantization for fermions

A.1. **Fermionic quasi-free states.** In this appendix we briefly recall basics of second quantization in the case of charged fermions following textbook references [1, 39, 10, 4] and explain the implications of our results for the renormalized quantum current and charge density. We use the convention that sesquilinear forms are linear in the second argument.

Given a complex inner product space $\mathcal{V}$ with inner product $\langle\cdot,\cdot\rangle$, the objective of second quantization is to construct a Hilbert space $\mathcal{H}$ and *charged field operators*, i.e. operator-valued anti-linear maps $\mathcal{V} \ni v \mapsto \psi(v) \in B(\mathcal{H})$ which satisfy the *canonical anti-commutation relations* for $\mathcal{V}$, i.e.

$$\begin{aligned} &\{\psi^*(v),\psi^*(w)\} = \{\psi(v),\psi(w)\} = 0, \\ &\{\psi(v),\psi^*(w)\} = \langle v,w\rangle \mathbf{1}_{\mathcal{H}}, \quad v,w\in\mathcal{V}. \end{aligned} \tag{A.1}$$

It is advantageous to view the problem in a representation-theoretic way, and first consider the unital C^*-algebra $\mathrm{CAR}(\mathcal{V})$ which is formally generated by abstract elements $\psi(v)$, $\psi^*(w)$, $v,w\in\mathcal{V}$, satisfying the canonical anti-commutation relations (A.1) (see e.g. [10, §17.2.3] and [10, §2.5] for the precise definition; note that it makes reference to the neutral formalism). Next, one chooses a state ω on $\mathrm{CAR}(\mathcal{V})$, i.e., a positive continuous linear functional of norm 1. Then the *GNS construction* (named after Gelfand, Naimark and Segal) provides a CAR representation associated to ω. More precisely, the GNS construction produces a Hilbert space $\mathcal{H}_\omega$ using the inner product $(A,B)\mapsto\omega(A^*B)$ (the null space is quotiented out to ensure non-degeneracy and then one takes the completion), and it constructs field operators (operator-valued anti-linear maps) $\mathcal{V}\ni v\mapsto\hat\psi(v)\in B(\mathcal{H}_\omega)$ and a distinguished *vacuum vector* $\Omega\in\mathcal{H}_\omega$ such that

$$\omega(\psi(v)\psi^*(w)) = \langle\Omega, \hat\psi(v)\hat\psi^*(w)\Omega\rangle_{\mathcal{H}_\omega}, \quad v,w\in\mathcal{V}.$$

In the sequel we restrict our attention to quasi-free states, defined as follows (we will always tacitly assume them to be gauge-invariant).

Definition A.1. A state ω on $\mathrm{CAR}(\mathcal{V})$ is *gauge-invariant* if and only if

$$\omega(\psi^*(v_1)\cdots\psi^*(v_n)\psi(w_1)\cdots\psi(w_m)) = 0, \quad n\neq m \tag{A.2}$$

for all $v_1,\dots,v_n,w_1,\dots,w_m\in\mathcal{V}$. It is also *quasi-free* if in addition

$$\omega(\psi^*(v_1)\cdots\psi^*(v_n)\psi(w_1)\cdots\psi(w_n)) = \sum_{\sigma\in S_n}\mathrm{sgn}(\sigma)\prod_{j=1}^n \omega(\psi^*(v_j)\psi(w_{\sigma(j)})), \tag{A.3}$$

for all $n\in\mathbb{N}$, $v_1,\dots,v_n,w_1,\dots,w_n\in\mathcal{V}$, where S_n is the set of permutations of $\{1,\dots,n\}$.

Note that the RHS of (A.3) is simply the determinant of $(\omega(\psi^*(v_i)\psi(w_j)))_{ij}$.

Thus, taking also into account the canonical anti-commutation relations (A.1), a quasi-free state ω is uniquely determined by the sesquilinear form $\omega(\psi(v)\psi^*(w))$, $v,w\in\mathcal{V}$. There exists a rather general converse statement; here we only give a special case where $\mathcal{V}$ is assumed to be complete.

Proposition A.2. *Suppose that $\mathcal{V}$ is complete. If $\gamma \in B(\mathcal{V})$ is a density matrix, i.e. satisfies $0 \leqslant \gamma \leqslant \mathbf{1}$, then there exists a unique quasi-free state ω on $\mathrm{CAR}(\mathcal{V})$ such that*

$$\omega(\psi(v)\psi^*(w)) = \langle v, \gamma w\rangle, \quad v, w \in \mathrm{c}V.$$

Now in the context of the Dirac equation in external potentials (possibly with Coulomb singularity as in §1.2), we apply the above proposition in the particular case when we are given a density matrix at some fixed reference time t_0, $\gamma(t_0) \in B(L^2(\mathbb{R}^3;\mathbb{C}^4))$, and we denote by $\mathcal{H}_{t_0}$ the Hilbert space and by $L^2(\mathbb{R}^3;\mathbb{C}^4) \ni v \mapsto \hat\psi_{t_0}(v) \in B(\mathcal{H}_{t_0})$ the field operators obtained by GNS construction for the associated quasi-free state ω_{t_0} on $\mathrm{CAR}(L^2(\mathbb{R}^3;\mathbb{C}^4))$. These have the interpretation of *Cauchy data fields* at $t = t_0$.

For the sake of illustration we give a more direct description of $\hat\psi_{t_0}$ (strictly speaking, a unitarily equivalent CAR representation), under the extra assumption that $\gamma(t_0)$ is a projection. We denote $\mathcal{Z}_{t_0} = \mathrm{Ran}(\mathbf{1} - \gamma(t_0))$. In this case it is possible to obtain $\hat\psi_{t_0}$ as an operator-valued anti-linear map of the form

$$\hat\psi_{t_0}(v) = a((\mathbf{1} - \gamma(t_0))v, 0) + a^*(0, \overline{\gamma(t_0)v}) \in B(\mathcal{H}_{t_0}), \quad v \in L^2(\mathbb{R}^3;\mathbb{C}^4),$$

acting on the *fermionic Fock space*

$$\mathcal{H}_{t_0} = \textstyle\bigoplus_{n=0}^\infty \bigwedge^n(\mathcal{Z}_{t_0} \oplus \overline{\mathcal{Z}_{t_0}})$$

over $\mathcal{Z}_{t_0} \oplus \overline{\mathcal{Z}_{t_0}}$, where $\overline{\mathcal{Z}_{t_0}}$ is the image of $\mathcal{Z}_{t_0}$ by the anti-linear involution denoted by $z \mapsto \bar z$ which maps Cauchy data of solutions to Cauchy data of solutions of a charge reversed Dirac equation (it consists of taking the complex conjugate and then multiplying by $i\beta\alpha_2$). The wedge stands for anti-symmetrized tensor product. Above,

$$\mathcal{Z}_{t_0} \oplus \overline{\mathcal{Z}_{t_0}} \mapsto a(z_1, z_2), a^*(z_1, z_2) \in B(\mathcal{H}_{t_0})$$

are the fermionic annihilation and creation operators on $\mathcal{H}_{t_0}$ (strictly speaking, families of operators), defined by $a^*(z_1, z_2)\Psi = (z_1, z_2) \wedge \Psi$. By convention $\wedge^0(\mathcal{Z}_{t_0} \oplus \overline{\mathcal{Z}_{t_0}}) = \mathbb{C}1$ and then $\Omega := 1 \in \mathcal{H}$ is the vacuum vector. The general construction when $\gamma(t_0)$ is not necessarily a projection requires a further adjustment and is given by the *Araki–Wyss representation*, see e.g. [10, §17.2.3] and [10, §17.2.6].

The fields $\hat\psi_{t_0}$ play the role of Cauchy data of *spacetime fields* $\hat\psi$ constructed as follows. Observe that the Cauchy data fields at an arbitrary time t are given by $\hat\psi_t(v) = \hat\psi_{t_0}(U(t_0, t)v)\Gamma(U(t_0, t))$ corresponding to the density $\gamma(t) = U(t, t_0)\gamma(t_0)U(t_0, t)$, where $U(t_0, t)$ maps Cauchy data at time t to Cauchy data at t_0 and $\Gamma(U(t, t_0))$ is the second quantization of $U(t_0, t)$, i.e. its natural extension as a map between Fock spaces $\mathcal{H}_t \to \mathcal{H}_{t_0}$. For each t, $C^\infty_{\mathrm{c}}(\mathbb{R}^3;\mathbb{C}^4) \ni v \mapsto \hat\psi_t(v)$ is an (anti-linear, operator-valued, vectorial) distribution in the spatial variables, but we can also consider it as a distribution jointly in all space-time variables: this gives rise to the space-time fields $\hat\psi(f)$, i.e.

$$C^\infty_{\mathrm{c}}(\mathbb{R}^{1,3};\mathbb{C}^4) \ni f \mapsto \hat\psi(f)\Psi := \hat\psi_{t_0}((Sf)(t_0))(\Gamma(S)\Psi) \in B(\mathcal{H}), \tag{A.4}$$

where S is the operator with Schwartz kernel $U(t_1, t_2)$ in the time variables and $\Gamma(S)$ is defined by extending the map $\mathcal{Z}_{t_0} \ni z \mapsto (Sz)(t_0)$ to the Fock space $\mathcal{H}_{t_0}$; we define $\mathcal{H} := \Gamma(S)\mathcal{H}_{t_0}$. The space-time fields $\hat\psi$ are the operator-valued solutions of the Dirac equation mentioned in the introduction; when interpreted as distributions they are indeed solutions of $D\hat\psi = 0$.

It is also possible to use the algebraic formalism on the space-time level directly. Namely, we can take $\mathcal{V}$ to be the completion of $C_{\mathrm{c}}^{\infty}(\mathbb{R}^{1,3};\mathbb{C}^4)$ with respect to the inner product

$$f, g \mapsto \langle (Sf)(t_0), (Sg)(t_0)\rangle_{L^2(\mathbb{R}^3;\mathbb{C}^4)}$$

Then ω_{t_0} induces a quasi-free state ω on $\mathrm{CAR}(\mathcal{V})$, and the space-time fields $\hat{\psi}(f)$ can be obtained by taking the GNS representation.

Note that especially when discussing space-time quantities, most of the literature uses the relativistic Dirac–Coulomb equation

$$\big(i^{-1}\gamma^{\mu}(\partial_{\mu} + iA_{\mu}) + m\big)u = 0, \tag{A.5}$$

where $\gamma^0 = \beta$, $\gamma^j = \beta\alpha^j$ are the gamma matrices and we used Einstein summation convention. Note that (A.5) is related to the operator $D = i\partial_t + H(t)$ used here by composition with the γ^0 matrix, so the natural space-time inner product for the operator in (A.5) involves a γ^0 factor, but switching between the two operators is straightforward.

Let now ω_{ref} be another quasi-free state on $\mathrm{CAR}(\mathcal{V})$ associated to some density matrix $\gamma_{\mathrm{ref}}(t)$. We assume that $\gamma(t)$ and $\gamma_{\mathrm{ref}}(t)$ are Hadamard in the terminology of §1.2 (we make the same assumptions on the potentials A_{μ} as in §1.2).

We denote by $x \in \mathbb{R}^{1,3}$ points in spacetime. Using the usual formal notation for distributions, in our conventions the *relative current* is the distribution-valued vector

$$\begin{aligned} j^{\mu}_{\omega,\omega_{\mathrm{ref}}}(x) &= \big(\omega(\psi^*(x)\gamma^0\gamma^{\mu}\psi(y)) - \omega_{\mathrm{ref}}(\psi^*(x)\gamma^0\gamma^{\mu}\psi(y))\big)|_{y=x}, \\ &= \big(\langle \Omega, \hat{\psi}^*(x)\gamma^0\gamma^{\mu}\hat{\psi}(y)\Omega\rangle_{\mathcal{H}} - \omega_{\mathrm{ref}}(\psi^*(x)\gamma^0\gamma^{\mu}\psi(y))\big)|_{y=x}, \end{aligned} \tag{A.6}$$

where $f \mapsto \psi(f)$ are the abstract fields in the C^*-algebra $\mathrm{CAR}(\mathcal{V})$. The relative current plays the role of vacuum expectation value of the quantum version of the classical current

$$j^{\mu}_{u}(x) = u^*(x)\gamma^0\gamma^{\mu}u(x),$$

which becomes ill-defined if one naively inserts a quantum field $\hat{\psi}$ (which is in general a highly singular distribution even if $A_{\mu} \equiv 0$) instead of a smooth solution u. On the other hand, our results imply that

$$j^{\mu}_{\omega,\omega_{\mathrm{ref}}}(x) \in C^{\infty}(\mathbb{R}; L^1_{\mathrm{loc}}(\mathbb{R}^3)) \cap C^{\infty}(\mathbb{R} \times (\mathbb{R}^3 \setminus \{0\})), \quad \mu = 0, \dots, 3,$$

is well-defined.

We illustrate this on the example of the *relative charge density*, i.e. $\rho_{\gamma,\gamma_{\mathrm{ref}}}(x) = j^0_{\omega,\omega_{\mathrm{ref}}}(x)$ (emphasizing the dependence on the density matrices in the notation as in the introduction). Since $(\gamma^0)^2 = I$ it can be written as

$$\begin{aligned} \rho_{\gamma,\gamma_{\mathrm{ref}}}(x) &= \big(\langle \Omega, \hat{\psi}^*(x)\hat{\psi}(y)\Omega\rangle_{\mathcal{H}} - \omega_{\mathrm{ref}}(\psi^*(x)\psi(y))\big)|_{y=x} \\ &= \mathrm{Tr}_{\mathbb{C}^4}\left(\Lambda^-(x,y) - \Lambda^-_{\mathrm{ref}}(x,y)\right)|_{x=y}, \end{aligned}$$

where $\Lambda^-(x,y)$ is the spacetime Schwartz kernel (with values in 4×4 matrices) of the operator

$$\big(\Lambda^- f\big)(t) = \int_{-\infty}^{\infty} U(t,t_0)\gamma(t_0)U(t_0,t_2)f(t_2)dt_2$$

and $\Lambda^-_{\rm ref}$ is defined similarly using $\gamma_{\rm ref}(t_0)$. The on-diagonal restriction is well-defined by Propositions 3.4 and 3.5. Writing $x = (t, \bar{x})$, we get

$$\rho_{\gamma,\gamma_{\rm ref}}(t,\bar{x}) = \mathrm{Tr}_{\mathbb{C}^4}(\gamma(t) - \gamma_{\rm ref}(t))(\bar{x},\bar{x}).$$

In a scattering situation one takes ω and $\omega_{\rm ref}$ to be the *in* and *out* vacuum respectively, and then integrating $\rho_{\gamma,\gamma_{\rm ref}}$ yields the charge created by switching on a time-dependent potential and then turning it off.

A.2. **Wick ordering and quantum current.** Let us now explain in what sense the relative current $j^\mu_{\omega,\omega_{\rm ref}}(x)$ is an expectation value of an operator-valued distribution called the *renormalized* or *Wick-ordered* (with respect to $\omega_{\rm ref}$) *quantum current* $:\!\psi^*\gamma^0\gamma^\mu\psi(x)\!:_{\omega_{\rm ref}}$.

Let $\mathcal{H}_{\rm fin} \subset \mathcal{H}$ be the subspace spanned by vectors of the form

$$\hat{\psi}(f_1)\hat{\psi}(f_2)\cdots\hat{\psi}(f_k)\Omega, \quad k \in \mathbb{N}_0,\ f_1,\ldots,f_k \in C^\infty_{\rm c}(M;\mathbb{C}^4).$$

A standard fact about the GNS representation (called the *cyclicity* of Ω) is that $\mathcal{H}_{\rm fin}$ is dense.

The pointwise products of distributions such as $\hat{\psi}\hat{\psi}^*$, $\hat{\psi}^*\hat{\psi}$, $\hat{\psi}^*\gamma^0\gamma^\mu\hat{\psi}$, etc., are ill-defined and need to be replaced by *Wick squares* $:\!\hat{\psi}\hat{\psi}^*\!:_{\omega_{\rm ref}}$, $:\!\hat{\psi}^*\hat{\psi}\!:_{\omega_{\rm ref}}$, $:\!\hat{\psi}^*\gamma^0\gamma^\mu\hat{\psi}\!:_{\omega_{\rm ref}}$, etc. We focus on explaining the definition of $:\!\hat{\psi}^*\hat{\psi}\!:_{\omega_{\rm ref}}$. First, one introduces the *Wick monomial*

$$:\!\hat{\psi}^*(f)\hat{\psi}(g)\!:_{\omega_{\rm ref}} = \hat{\psi}^*(f)\hat{\psi}(g) - \omega_{\rm ref}\big(\psi^*(f)\psi(g)\big)\mathbf{1}_{\mathcal{H}},$$

or in function-like notation for distributions,

$$:\!\hat{\psi}^*(x)\hat{\psi}(y)\!:_{\omega_{\rm ref}} = \hat{\psi}^*(x)\hat{\psi}(y) - \omega_{\rm ref}\big(\psi^*(x)\psi(y)\big)\mathbf{1}_{\mathcal{H}}. \tag{A.7}$$

Then, $:\!\hat{\psi}^*\hat{\psi}(x)\!:_{\omega_{\rm ref}}$ is defined by restricting $:\!\hat{\psi}^*(x)\hat{\psi}(y)\!:_{\omega_{\rm ref}}$ to the diagonal $x = y$. If well-defined, this gives in particular gives the vacuum expectation value

$$\begin{aligned}\langle\Omega, :\!\hat{\psi}^*\hat{\psi}(x)\!:_{\omega_{\rm ref}}\Omega\rangle_{\mathcal{H}} &= \big(\langle\Omega,\psi^*(x)\psi(y)\Omega\rangle_{\mathcal{H}} - \omega_{\rm ref}(\psi^*(x)\psi(y))\big)|_{y=x}\\ &= \rho_{\gamma,\gamma_{\rm ref}}(x).\end{aligned}$$

Proposition A.3. *Under the hypotheses in §1.2, the Wick square $:\!\hat{\psi}^*\hat{\psi}(x)\!:_{\omega_{\rm ref}}$ is well defined as a locally integrable function on $\mathbb{R}^{1,3}$ with values in quadratic forms on $\mathcal{H}_{\rm fin}$.*

Proof. Let $\Psi \in \mathcal{H}_{\rm fin}$ be of the form $\Psi = \hat{\psi}(f_1)\hat{\psi}(f_2)\cdots\hat{\psi}(f_k)\Omega$. We compute using the quasi-free property

$$\begin{aligned}&\langle\Psi,\hat{\psi}^*(f)\hat{\psi}(g)\Psi\rangle_{\mathcal{H}} = \langle\Omega,\hat{\psi}^*(f_k)\cdots\hat{\psi}^*(f_1)\hat{\psi}^*(f)\hat{\psi}(g)\hat{\psi}(f_1)\cdots\hat{\psi}(f_k)\Omega\rangle_{\mathcal{H}}\\ &= \langle\Omega,\hat{\psi}^*(f)\hat{\psi}(g)\Omega\rangle\|\Psi\|^2_{\mathcal{H}} + \sum_{i,j}\Big(c_{i,j}\langle\Omega,\hat{\psi}^*(f)\hat{\psi}(f_i)\Omega\rangle_{\mathcal{H}}\langle\Omega,\hat{\psi}^*(f_j)\hat{\psi}(g)\Omega\rangle_{\mathcal{H}}\Big),\end{aligned}$$

where $c_{i,j}$ are linear combinations of products of two-point functions not involving f nor g. Thus, mixing function-like and distributional notation,

$$
\begin{aligned}
\langle \Psi, {:}\hat{\psi}^*\hat{\psi}(x){:}_{\omega_{\mathrm{ref}}}\Psi\rangle_{\mathcal{H}} &= \|\Psi\|^2_{\mathcal{H}}\Big(\langle \Omega, \hat{\psi}^*(x)\hat{\psi}(y)\Omega\rangle_{\mathcal{H}} - \omega_{\mathrm{ref}}\big(\psi^*(x)\psi(y)\big)\Big)|_{x=y} \\
&\quad + \sum_{i,j}\Big(c_{i,j}\langle \Omega, \hat{\psi}^*_\mu(x)\hat{\psi}(f_i)\Omega\rangle_{\mathcal{H}}\langle \Omega, \hat{\psi}^*(f_j)\hat{\psi}^\mu(x)\Omega\rangle_{\mathcal{H}}\Big) \\
&= \|\Psi\|^2_{\mathcal{H}}\,\mathrm{Tr}_{\mathbb{C}^4}\big(\Lambda^-(x,y) - \Lambda^-_{\mathrm{ref}}(x,y)\big)|_{x=y} \\
&\quad + \sum_{i,j,a}\Big(c_{i,j}\langle \Omega, \hat{\psi}^*_a(x)\hat{\psi}(f_i)\Omega\rangle_{\mathcal{H}}\langle \Omega, \hat{\psi}^*(f_j)\hat{\psi}^a(x)\Omega\rangle_{\mathcal{H}}\Big)
\end{aligned}
\tag{A.8}
$$

if the restriction to the diagonal and the pointwise product exist. The former is well-defined by Propositions 3.4 and 3.5. The latter is as well since $\langle \Omega, \hat{\psi}^*(x)\hat{\psi}(f_i)\Omega\rangle_{\mathcal{H}} = (\Lambda^+ f_i)(x) \in H^{1,\infty}_{\mathrm{b}}(M;\mathbb{C}^4)$ and similarly $\langle \Omega, \hat{\psi}^*(f_j)\hat{\psi}(x)\Omega\rangle_{\mathcal{H}} \in H^{1,\infty}_{\mathrm{b}}(M;\mathbb{C}^4)$ so their pointwise $\mathbb{C}^4$ inner product exists. Finally, in the case of general Ψ we are easily reduced to computations as above using the gauge invariance condition (A.2). □

The discussion of the renormalized quantum current ${:}\hat{\psi}^*\gamma^0\gamma^\mu\hat{\psi}(x){:}_{\omega_{\mathrm{ref}}}$ is entirely analogous.

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