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ABSTRACT

A recently proposed approach for avoiding the ultraviolet divergence of Hamiltonians with particle creation is based on interior-boundary conditions (IBCs). The approach works well in the non-relativistic case, i.e., for the Laplacian operator. Here, we study how the approach can be applied to Dirac operators. While this has successfully been done already in one space dimension, and more generally for codimension-1 boundaries, the situation of point sources in three dimensions corresponds to a codimension-3 boundary. One would expect that, for such a boundary, Dirac operators do not allow for boundary conditions because they are known not to allow for point interactions in 3D, which also correspond to a boundary condition. Indeed, we confirm this expectation here by proving that there is no self-adjoint operator on a (truncated) Fock space that would correspond to a Dirac operator with an IBC at configurations with a particle at the origin. However, we also present a positive result showing that there are self-adjoint operators with an IBC (on the boundary consisting of configurations with a particle at the origin) that are away from those configurations, given by a Dirac operator plus a sufficiently strong Coulomb potential.

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I. INTRODUCTION

Hamiltonians for quantum theories with particle creation and annihilation are often plagued by ultraviolet divergence.^{1–3} For defining such a Hamiltonian in a rigorous way, one might employ an ultraviolet cutoff corresponding to smearing out the source of particle creation over a positive volume, or in some cases, one can obtain a renormalized Hamiltonian by taking a limit of the cutoff Hamiltonian in which the volume of the source tends to zero.^{4–7} Another more recent approach is based on interior-boundary conditions (IBCs)^{8,9} and yields directly (i.e., without taking a limit) a Hamiltonian suitable for a point source. Here, the wave function ψ is a function on the configuration space

$$\mathcal{Q} = \bigcup_{N=0}^{\infty} \mathcal{Q}_1^N \quad (1)$$

of a variable number of particles that can move in the one-particle space \mathcal{Q}_1 , for example

$$\mathcal{Q}_1 = \mathbb{R}^3 \setminus \{\mathbf{0}\} \quad (2)$$

if particles can be created at a point source fixed at the origin $\mathbf{0} \in \mathbb{R}^3$. In this example, the boundary $\partial\mathcal{Q}$ of \mathcal{Q} consists of configurations with at least one particle at the origin,

$$\partial\mathcal{Q} = \bigcup_{N=0}^{\infty} \partial(\mathcal{Q}_1^N) = \bigcup_{N=0}^{\infty} \{(\mathbf{x}_1, \dots, \mathbf{x}_N) \in (\mathbb{R}^3)^N : \mathbf{x}_i = \mathbf{0} \text{ for some } i \in \{1, \dots, N\}\}. \quad (3)$$

The IBC is a condition on ψ relating values on the boundary and values in the interior, more precisely, relating the values on two configurations q, q' that differ by the creation (respectively, annihilation) of a particle at the origin,

$$q = (\mathbf{x}_1, \dots, \mathbf{x}_i = \mathbf{0}, \dots, \mathbf{x}_N) \in \partial\mathcal{Q}_1^N \quad (4a)$$

and

$$q' = (\mathbf{x}_1, \dots, \mathbf{x}_{i-1}, \mathbf{x}_{i+1}, \dots, \mathbf{x}_N) \in \mathcal{Q}_1^{N-1}. \quad (4b)$$

As shown by Lampart *et al.*,¹⁰ a Hamiltonian with particle creation at the origin can be defined rigorously in this way in the non-relativistic case without UV divergence or the need for renormalization. Our goal here is to examine in what way and to what extent this approach can be extended to the Dirac equation.

There are already two works about IBCs for the Dirac equation: Schmidt *et al.*¹¹ explored what IBCs for the Dirac equation can look like on a codimension-1 boundary. However, in our case, boundary (3) has codimension 3. Lienert and Nickel¹² developed a quantum field theory (QFT) model in one space dimension using Dirac particles and an IBC that allows two particles to merge into one or one particle to split in two. In contrast, we consider here space dimension 3.

We present here a negative result and a positive one. The negative result (Theorem 1) asserts, roughly speaking, that in three space dimensions, there exists no self-adjoint Hamiltonian for the configuration space as in (1)–(3) (or even the truncated one allowing only $N = 0$ and $N = 1$) that acts like the free Dirac Hamiltonian away from the boundary but involves particle creation. Put differently, the free Dirac equation cannot be combined with IBCs in three dimensions. The fact is analogous to the known impossibility of point interaction (δ potentials) for the Dirac equation in three dimensions (see, e.g., Refs. 13–15, Theorem 1.1), in particular, since the point interaction is described by a boundary condition,^{16,34} and for an external field that acts nontrivially only at $\mathbf{0} \in \mathbb{R}^3$, the relevant boundary for this boundary condition is precisely (3), or one sector thereof. Our proof of Theorem 1 makes use of the impossibility theorems for point interaction to deduce the impossibility of IBCs in this situation. We formulate some variants of Theorem 1 as Theorems 3 and 4.

The positive result (Theorem 6) concerns a way in which, nevertheless, a self-adjoint Hamiltonian with particle creation can be rigorously defined by means of an IBC and the Dirac equation for the configuration space as in (1)–(3); it is based on adding a potential. Specifically, we show in Theorem 6 that if a Coulomb potential of sufficient strength, centered at the origin and acting on each of the particles in the model, is added to the action of the Hamiltonian away from the boundary, then a self-adjoint version of the Hamiltonian exists that involves an IBC and leads to particle creation and annihilation at the origin, analogously to the non-relativistic case with the Laplacian operator. The IBC is analogous to the known IBCs for codimension-1 boundaries.¹¹ We formulate the result for a truncated Fock space with only the $N = 0$ and $N = 1$ sectors.

The results are formulated in detail in Sec. II. They can be expressed as statements about self-adjoint extensions. That is because, when considering a truncated Fock space ($N \leq N_{\max}$) and configuration space, for functions ψ that vanish in a neighborhood of the boundary in the top sector N_{\max} and also vanish in all lower sectors, we know how the desired Hamiltonian should act: in the same way as the Dirac operator H^{free} of N_{\max} particles (respectively, with a Coulomb potential). Let D° be the space of these functions (not dense). Thus, the desired Hamiltonian H is a self-adjoint extension of a (symmetric but not closed) operator $H^\circ = H|_{D^\circ} = H^{\text{free}}|_{D^\circ}$. (By the way, when we say “self-adjoint,” we always mean that the operator is densely defined.) The no-go result (Theorem 1) will show that H° has only one self-adjoint extension, viz., H^{free} ; that means that it is not possible to implement particle creation and annihilation at just one point $\mathbf{0}$, using IBCs or otherwise. Theorem 6 will take H° to include a suitable Coulomb potential and provide a self-adjoint extension (even several ones) featuring particle creation and annihilation. It remains to be seen whether and how IBCs can be employed in more realistic models of relativistic QFTs.

The IBC Hamiltonians provided by Theorem 6 are neither translation invariant nor rotation invariant, but that was only to be expected: the model cannot be translation invariant, given that the source is fixed at the origin, and the emission of a spin- $\frac{1}{2}$ particle by a spinless source cannot conserve angular momentum and, thus, cannot be rotation invariant. (An alternative proof is given in Sec. II D.)¹⁷

Here are further comments on the literature. Some forms of interior-boundary conditions were considered, not necessarily with the UV problem in mind, early on by Moshinsky.^{18–20} Self-adjoint Hamiltonians based on IBCs and the Laplacian were first rigorously defined by Thomas²¹ and Yafaev.²² Lampart *et al.*¹⁰ extended these results to the full Fock space and showed that the non-relativistic IBC Hamiltonian agrees, up to addition of a constant, with the one obtained through UV cutoff and renormalization. Lampart and Schmidt²³ further extended the proofs to moving sources in two space dimensions, and Lampart,²⁴ in three dimensions. Keppeler and Sieber²⁵ studied the one-dimensional non-relativistic case. Bohmian trajectories for IBC Hamiltonians were defined and studied in Refs. 26, 27 and 40. Other kinds of boundary conditions come up in the study of detection times (see Ref. 35). Further studies of IBC Hamiltonians and their properties include Refs. 28–33.

In Sec. II, we describe our results. In Sec. III, we collect the proofs.

II. RESULTS

For comparison, it will be useful to recapitulate some aspects of the non-relativistic case in three dimensions with a single point source fixed at the origin.¹⁰ For simplicity, we consider a truncated Fock space of spinless particles,

$$\mathcal{H}_{\text{nr}} := \bigoplus_{N=0}^{N_{\text{max}}} \mathcal{H}_{\text{nr}}^{(N)} := \bigoplus_{N=0}^{N_{\text{max}}} S_{\pm} L^2(\mathbb{R}^3, \mathbb{C})^{\otimes N} \quad (5)$$

with \oplus the orthogonal sum of Hilbert spaces and $S_{\pm} \cdots$ the image of the symmetrization operator S_+ or anti-symmetrization operator S_- (subscript nr is for “non-relativistic case”). There is a five-parameter family of IBC Hamiltonians; some members of this family can be regarded as involving an external zero-range potential at the origin in addition to the particle source; there is a two-parameter subfamily that can be regarded as involving no such potential, i.e., as being a pure particle source. The remaining parameters are the energy E_0 that must be expended for creating a particle and the strength g of particle creation. Let us fix values $E_0 > 0$ and $g \in \mathbb{C} \setminus \{0\}$ and call the corresponding operator H_{nr} . H_{nr} is a self-adjoint operator in \mathcal{H}_{nr} ; let D_{nr} denote its domain of self-adjointness. Functions $\psi = (\psi^{(0)}, \dots, \psi^{(N_{\text{max}})})$ in D_{nr} satisfy the IBC

$$\lim_{r \searrow 0} r \psi^{(N+1)}(\mathbf{x}_1, \dots, \mathbf{x}_N, r\boldsymbol{\omega}) = -\frac{gm}{2\pi\hbar^2\sqrt{N+1}} \psi^{(N)}(\mathbf{x}_1, \dots, \mathbf{x}_N) \quad (6)$$

(suitably understood, and with $r \searrow 0$ meaning the limit from the right) for $N = 0, \dots, N_{\text{max}} - 1$ and every unit vector $\boldsymbol{\omega} \in \mathbb{R}^3$. Another operator to compare to is the free Hamiltonian $H_{\text{nr}}^{\text{free}}$, which acts on functions ψ from its domain

$$D_{\text{nr}}^{\text{free}} := \bigoplus_{N=0}^{N_{\text{max}}} S_{\pm} H^2(\mathbb{R}^{3N}, \mathbb{C}) \quad (7)$$

(with H^2 the second Sobolev space) according to

$$H_{\text{nr}}^{\text{free}} \psi^{(N)} = \sum_{j=1}^N H_{1\text{nr},j} \psi^{(N)} \quad (8)$$

with $H_{1\text{nr},j}$ the one-particle Hamiltonian

$$H_{1\text{nr}} = E_0 - \frac{\hbar^2}{2m} \Delta \quad (9)$$

acting on particle j .

Now, we want to express that away from the boundary, H_{nr} acts like $H_{\text{nr}}^{\text{free}}$. However, the IBC enforces that if $\psi^{(N)} \neq 0$ for some $N \geq 0$, then every higher sector, $\psi^{(N')}$ with $N' > N$, must be nonzero (and, in fact, unbounded) in a neighborhood of the boundary $\partial\mathcal{Q}_1^{N'}$. In contrast, ψ can lie in D_{nr} if $\psi^{(N_{\text{max}})}$ vanishes in a neighborhood of the boundary and $\psi^{(N)} = 0$ for all $N < N_{\text{max}}$; in fact, ψ will lie in D_{nr} if $\psi^{(N_{\text{max}})} \in C_c^\infty(\mathcal{Q}_1^{N_{\text{max}}}, \mathbb{C})$ (where C_c^∞ means smooth functions with compact support) and $\psi^{(N)} = 0$ for all $N < N_{\text{max}}$,

$$D_{\text{nr}} \supset D_{\text{nr}}^\circ := \{0\} \oplus \cdots \oplus \{0\} \oplus C_c^\infty(\mathcal{Q}_1^{N_{\text{max}}}, \mathbb{C}). \quad (10)$$

Note that since $\mathbf{0}$ was excluded from \mathcal{Q}_1 , “compact support” entails that the support stays away from the boundary. The symbol \oplus , when applied to sets that are not Hilbert spaces, should be understood as the Cartesian product, resulting in a subset of \mathcal{H}_{nr} . On D_{nr}° , H_{nr} acts like the free Hamiltonian,

$$H_{\text{nr}} \Big|_{D_{\text{nr}}^\circ} = H_{\text{nr}}^{\text{free}} \Big|_{D_{\text{nr}}^\circ} =: H_{\text{nr}}^\circ. \quad (11)$$

That is both $(H_{\text{nr}}, D_{\text{nr}})$ and $(H_{\text{nr}}^{\text{free}}, D_{\text{nr}}^{\text{free}})$ are self-adjoint extensions of $(H_{\text{nr}}^\circ, D_{\text{nr}}^\circ)$. Note that D_{nr}° is not a *dense* subspace of \mathcal{H}_{nr} (whereas D_{nr} and $D_{\text{nr}}^{\text{free}}$ are). The condition that $(H_{\text{nr}}, D_{\text{nr}})$ is an extension of $(H_{\text{nr}}^\circ, D_{\text{nr}}^\circ)$ expresses that in the highest sector, particle creation can occur only at the origin. In passing, we remark that Yafaev²² showed for $N_{\text{max}} = 1$ that all self-adjoint extensions of $(H_{\text{nr}}^\circ, D_{\text{nr}}^\circ)$ belong to the five-parameter family of IBC Hamiltonians (which includes, as a subfamily, the Hamiltonians without particle creation but with point interaction at the origin).

A. No-go theorem

Now, we turn to the Dirac case. We define the truncated Fock space

$$\mathcal{H} := \bigoplus_{N=0}^{N_{\max}} \mathcal{H}^{(N)} := \bigoplus_{N=0}^{N_{\max}} S_{\pm} L^2(\mathbb{R}^3, \mathbb{C}^4). \quad (12)$$

(Although spin- $\frac{1}{2}$ particles are fermions in nature, we cover here also the mathematical case of Dirac particles that are bosons.) The one-particle Hamiltonian is the Dirac Hamiltonian

$$H_1 = -i\hbar c \boldsymbol{\alpha} \cdot \nabla + mc^2 \beta \quad (13)$$

with mass $m \geq 0$, which is self-adjoint on $D_1 = H^1(\mathbb{R}^3, \mathbb{C}^4)$ (first Sobolev space). Let H_N^{free} be the free N -particle Hamiltonian, which acts according to

$$H_N^{\text{free}} \psi = \sum_{j=1}^N H_{1j} \psi, \quad (14)$$

$D(H_N^{\text{free}})$ its domain of self-adjointness in $L^2(\mathbb{R}^{3N}, (\mathbb{C}^4)^{\otimes N})$, and

$$H^{\text{free}} \psi^{(N)} = H_N^{\text{free}} \psi^{(N)} \quad (15)$$

on the domain

$$D^{\text{free}} = \bigoplus_{N=0}^{N_{\max}} S_{\pm} D(H_N^{\text{free}}). \quad (16)$$

H^{free} is self-adjoint and is the (truncated) “second quantization” of H_1 in \mathcal{H} .

The desired IBC Hamiltonian (H, D) , or, in fact, any Hamiltonian that agrees with H^{free} except for particle creation and annihilation at the origin, must be a self-adjoint extension of (H°, D°) with

$$D^{\circ} = \{0\} \oplus \dots \oplus \{0\} \oplus S_{\pm} C_c^{\infty}(\mathcal{Q}_1^{N_{\max}}, (\mathbb{C}^4)^{\otimes N_{\max}}) \quad (17)$$

and

$$H^{\circ} := H^{\text{free}} \Big|_{D^{\circ}}. \quad (18)$$

Let $\mathcal{H}^{(<N_{\max})} := \mathcal{H}^{(0)} \oplus \dots \oplus \mathcal{H}^{(N_{\max}-1)}$.

Theorem 1. *Let $N_{\max} > 0$. For every self-adjoint extension (H, D) of (H°, D°) , the highest sector decouples from the other sectors; that is, H is block diagonal with respect to the decomposition $\mathcal{H} = \mathcal{H}^{(<N_{\max})} \oplus \mathcal{H}^{(N_{\max})}$.*

We give all proofs in Sec. III. To paraphrase the conclusion of Theorem 1, the time evolution generated by H involves no exchange between $\psi^{(N_{\max})}$ and the other sectors; no particle creation or annihilation occurs toward or from the N_{\max} -sector; in particular, $\|\psi^{(N_{\max})}\|$ is time independent. So, Theorem 1 implies that there is no IBC Hamiltonian for the Dirac equation in three space dimensions, as long as no further element such as potentials, space–time curvature, or other particles is introduced.

Theorem 1 is obtained by combining two theorems, Theorem 2 and Theorem 3. The former is a specialized form of a theorem of Svendsen.¹⁴

Theorem 2. *Let $N \geq 1$ and $M \subset \mathbb{R}^{3N}$ the union of finitely many C^{∞} submanifolds of equal codimension c . Let $H_{\setminus M}$ be the restriction of H_N^{free} to $C_c^{\infty}(\mathbb{R}^{3N} \setminus M, (\mathbb{C}^4)^{\otimes N})$. Then, $H_{\setminus M}$ is essentially self-adjoint in $L^2(\mathbb{R}^{3N}, (\mathbb{C}^4)^{\otimes N})$ if and only if $c \geq 2$. In particular, the restriction of H_N^{free} to $C_c^{\infty}(\mathcal{Q}_1^N, (\mathbb{C}^4)^{\otimes N})$ is essentially self-adjoint, and its restriction to $S_{\pm} C_c^{\infty}(\mathcal{Q}_1^N, (\mathbb{C}^4)^{\otimes N})$ is essentially self-adjoint in $S_{\pm} L^2(\mathbb{R}^{3N}, (\mathbb{C}^4)^{\otimes N})$.*

The last sentence follows by taking

$$M = \{(\mathbf{x}_1, \dots, \mathbf{x}_N) \in \mathbb{R}^{3N} : \mathbf{x}_i = \mathbf{0} \text{ for some } i\} \quad (19a)$$

$$= \bigcup_{i=1}^N \{(\mathbf{x}_1, \dots, \mathbf{x}_N) \in \mathbb{R}^{3N} : \mathbf{x}_i = \mathbf{0}\}, \quad (19b)$$

so $c = 3$ and $\mathbb{R}^{3N} \setminus M = \mathcal{Q}_1^N$. This theorem excludes point interaction for the free Dirac equation in three space dimensions. Note, however, that Theorem 1 is not a direct corollary of Theorem 2 because our Hilbert space \mathcal{H} is not $L^2(\mathbb{R}^{3N}, \mathbb{C}^k)$ but contains further sectors, and D° is not dense. What we need is the following statement, a kind of generalization of Theorem 1.

Theorem 3. Let $N_{\max} > 0$, let (\tilde{H}, \tilde{D}) be essentially self-adjoint in $\mathcal{H}^{(N_{\max})}$, and let now

$$D^\circ := \{0\} \oplus \dots \oplus \{0\} \oplus \tilde{D} \subset \mathcal{H} \quad (20)$$

and $H^\circ : D^\circ \rightarrow \mathcal{H}$ be given by

$$H^\circ(0, \dots, 0, \psi^{(N_{\max})}) := (0, \dots, 0, \tilde{H}\psi^{(N_{\max})}). \quad (21)$$

For every self-adjoint extension (H, D) of (H°, D°) , the highest sector decouples from the other sectors; in fact, with respect to the decomposition $\mathcal{H} = \mathcal{H}^{(<N_{\max})} \oplus \mathcal{H}^{(N_{\max})}$, $D = D^{(<N_{\max})} \oplus D^{(N_{\max})}$ and H is block diagonal with blocks $H^{(<N_{\max})}$ and $H^{(N_{\max})}$, where $(H^{(N_{\max})}, D^{(N_{\max})})$ is the unique self-adjoint extension of (\tilde{H}, \tilde{D}) .

B. Hamiltonians with Coulomb potential

In this section and Sec. II C, we focus on the case of two sectors, i.e., $N_{\max} = 1$. Our positive result is about examples of Dirac Hamiltonians in 3D with particle creation by means of IBCs. These Hamiltonians are based on the one-particle Hamiltonian

$$H_1 = -i\hbar\boldsymbol{\alpha} \cdot \nabla + mc^2\beta + \frac{v}{|\mathbf{x}|}, \quad v := \hbar q, \quad (22)$$

which consists of the free Dirac Hamiltonian plus a Coulomb potential of strength q (i.e., q is the product of the charge at \mathbf{x} and the charge at the origin). We will show in Theorem 6 that for $\sqrt{3}/2 < |q| < 1$, there exist IBC Hamiltonians. We conjecture that also for $|q| \geq 1$, IBC Hamiltonians exist. On the other hand, the following theorem, a generalization of Theorem 1 in the case $N_{\max} = 1$, shows that for $|q| \leq \sqrt{3}/2$, no IBC Hamiltonian exists.

Theorem 4. Let $\mathcal{H} = \mathbb{C} \oplus L^2(\mathbb{R}^3, \mathbb{C}^4)$, $D^\circ = \{0\} \oplus C_c^\infty(\mathcal{Q}_1, \mathbb{C}^4)$, and let H° act on $\psi = (0, \psi^{(1)}) \in D^\circ$ like H_1 as in (22),

$$H^\circ\psi = (0, H_1\psi^{(1)}) \quad (23)$$

with $|q| \leq \sqrt{3}/2$. For every self-adjoint extension (H, D) of (H°, D°) , the two sectors decouple; that is H is block diagonal. In fact, $D = \mathbb{C} \oplus D(\overline{H_1})$ with $\overline{H_1}$ the closure of H_1 , and for $\psi \in D$,

$$H\psi = (E_{00}\psi^{(0)}, \overline{H_1}\psi^{(1)}) \quad (24)$$

with some constant $E_{00} \in \mathbb{R}$.

It is known (e.g., Ref. 36, Proposition A1) that for $|q| < \sqrt{3}/2$, $D(\overline{H_1}) = H^1(\mathbb{R}^3, \mathbb{C}^4)$ (first Sobolev space), whereas for $|q| = \sqrt{3}/2$, the domain is bigger than the first Sobolev space. Theorem 4 follows by means of Theorem 3 from the following known theorem (Ref. 37, Theorem 6.9).³⁸

Theorem 5. In $L^2(\mathbb{R}^3, \mathbb{C}^4)$, the operator H_1 as in (22) is essentially self-adjoint on $C_c^\infty(\mathcal{Q}_1, \mathbb{C}^4)$ if and only if $|q| \leq \sqrt{3}/2$.

Remark 1. It is also known¹⁵ that

$$H_1 = -i\hbar\boldsymbol{\alpha} \cdot \nabla + mc^2\beta + V(\mathbf{x}) \quad (25)$$

with a matrix-valued potential V such that each component V_{ij} satisfies the bound

$$|V_{ij}(\mathbf{x})| \leq q \frac{c\hbar}{|\mathbf{x}|} + b \tag{26}$$

with constants $b > 0$ and $0 < q \leq 1/2$ is essentially self-adjoint. By Theorem 3, Theorem 4 still applies if (22) is replaced by (25) and (26) with $0 < q \leq 1/2$.

Cassano and Pizzichillo³⁹ improved upon (26) in the case of general Coulomb-type potentials

$$V(\mathbf{x}) = \frac{1}{|\mathbf{x}|} \left(v + \mu\beta + \lambda \left(-i\boldsymbol{\alpha} \cdot \frac{\mathbf{x}}{|\mathbf{x}|} \beta \right) \right) =: V_{\text{el}}(\mathbf{x}) + V_{\text{sc}}(\mathbf{x}) + V_{\text{am}}(\mathbf{x}), \tag{27}$$

but allowing for an additional *scalar* and *anomalous magnetic* contribution. More precisely, by exploiting the behavior of functions in the domain at the origin, they showed that H_1 in (25) with V given by (27) is essentially self-adjoint if and only if

$$\min_{k \in \mathbb{Z} \setminus \{0\}} ((c\hbar k + \lambda)^2 + \mu^2 - v^2) \geq \left(\frac{c\hbar}{2} \right)^2,$$

which reproduces Theorem 5 for $\mu = \lambda = 0$.

C. Existence of IBC Hamiltonian

It will be helpful again to consider first the non-relativistic IBC Hamiltonian $(H_{\text{nr}}, D_{\text{nr}})$, now for $N_{\text{max}} = 1$, so $\mathcal{H}_{\text{nr}} = \mathbb{C} \oplus L^2(\mathbb{R}^3, \mathbb{C})$. We report a few facts:¹⁰ for every $\psi \in D_{\text{nr}}$, the upper sector is of the form

$$\psi^{(1)}(\mathbf{x}) = c_{-1}|\mathbf{x}|^{-1} + c_0|\mathbf{x}|^0 + o(|\mathbf{x}|^0) \tag{28}$$

as $\mathbf{x} \rightarrow \mathbf{0}$, with (uniquely defined) “short distance coefficients” $c_{-1}, c_0 \in \mathbb{C}$. $\psi \in D_{\text{nr}}$ satisfies the IBC (6), which can be written in the form

$$c_{-1} = g \psi^{(0)}, \tag{29}$$

and the Hamiltonian acts on ψ like

$$(H_{\text{nr}}\psi)^{(0)} = g^* c_0, \tag{30a}$$

$$(H_{\text{nr}}\psi)^{(1)}(\mathbf{x}) = \left(E_0 - \frac{\hbar^2}{2m} \Delta \right) \psi^{(1)}(\mathbf{x}) \quad \text{for } \mathbf{x} \neq \mathbf{0}. \tag{30b}$$

[At $\mathbf{x} = \mathbf{0}$, $\Delta\psi^{(1)}$, when understood in the distributional sense, includes a delta distribution stemming from the $|\mathbf{x}|^{-1}$ contribution in (28).]

Now, we turn again to the Dirac case with

$$\mathcal{H} = \mathbb{C} \oplus L^2(\mathbb{R}^3, \mathbb{C}^4) \tag{31}$$

and one-particle operator H_1 as in (22). In the following, we take H_1 to be an operator on the domain

$$D_1 = C_c^\infty(Q_1, \mathbb{C}^4) \subset L^2(\mathbb{R}^3, \mathbb{C}^4) \tag{32}$$

with adjoint (H_1^*, D_1^*) in $L^2(\mathbb{R}^3, \mathbb{C}^4)$.

The notation

$$\Phi_{m_j, \kappa_j}^\pm \tag{33}$$

is common for certain functions that form an orthonormal basis of $L^2(\mathbb{S}^2, \mathbb{C}^4)$ (where \mathbb{S}^2 means the unit sphere in \mathbb{R}^3) and are simultaneous eigenvectors of J^2, K, J_3 with $\mathbf{J} = \mathbf{L} + \mathbf{S}$ the total angular momentum and $K = \beta(2\mathbf{S} \cdot \mathbf{L} + 1)$ the “spin-orbit operator.” Their explicit definition in terms of spherical harmonics can be found in, e.g., Ref. 15, p. 126. The symbols m_j and κ_j are the traditional names of their indices.

Theorem 6. Let $\mathcal{H} = \mathbb{C} \oplus L^2(\mathbb{R}^3, \mathbb{C}^4)$, $D^\circ = \{0\} \oplus C_c^\infty(Q_1, \mathbb{C}^4)$, and H° be given by (23) with $\sqrt{3}/2 < |q| < 1$. Set $B := \sqrt{1 - q^2}$, and note that $0 < B < 1/2$. Choose $g \in \mathbb{C} \setminus \{0\}$ and

$$(\tilde{m}_j, \tilde{\kappa}_j) \in \mathcal{A} := \left\{ \left(-\frac{1}{2}, -1 \right), \left(-\frac{1}{2}, 1 \right), \left(\frac{1}{2}, -1 \right), \left(\frac{1}{2}, 1 \right) \right\}. \quad (34)$$

Then, there is a self-adjoint extension (H, D) of (H°, D°) with the following properties:

1. Particle creation occurs; i.e., the two sectors do not decouple [H is not block diagonal in the decomposition (31)].
2. For every $\psi \in D$, the upper sector is of the form

$$\psi^{(1)}(\mathbf{x}) = c_- f_{\tilde{m}_j, \tilde{\kappa}_j}^- \left(\frac{\mathbf{x}}{|\mathbf{x}|} \right) |\mathbf{x}|^{-1-B} + \sum_{(m_j, \kappa_j) \in \mathcal{A}} c_{+m_j, \kappa_j} f_{m_j, \kappa_j}^+ \left(\frac{\mathbf{x}}{|\mathbf{x}|} \right) |\mathbf{x}|^{-1+B} + o(|\mathbf{x}|^{-1/2}) \quad (35)$$

as $\mathbf{x} \rightarrow \mathbf{0}$ with (uniquely defined) short distance coefficients $c_-, c_{+m_j, \kappa_j} \in \mathbb{C}$ and particular functions $f_{m_j, \kappa_j}^\pm : \mathbb{S}^2 \rightarrow \mathbb{C}^4$ given by

$$f_{m_j, \kappa_j}^+ = (1 + q - B)\Phi_{m_j, \kappa_j}^+ - (1 + q + B)\Phi_{m_j, \kappa_j}^-, \quad (36a)$$

$$f_{m_j, \kappa_j}^- = (1 + q + B)\Phi_{m_j, \kappa_j}^+ - (1 + q - B)\Phi_{m_j, \kappa_j}^-. \quad (36b)$$

3. Every $\psi \in D$ obeys the IBC

$$c_- = g \psi^{(0)}, \quad (37)$$

and H acts on $\psi \in D$ according to

$$(H\psi)^{(0)} = g^* 4B(1 + q) c_{+m_j, \tilde{\kappa}_j}, \quad (38a)$$

$$(H\psi)^{(1)}(\mathbf{x}) = \left(-i\hbar \boldsymbol{\alpha} \cdot \nabla + mc^2 \beta + \frac{q}{|\mathbf{x}|} \right) \psi^{(1)}(\mathbf{x}) \quad (\mathbf{x} \neq \mathbf{0}). \quad (38b)$$

Equivalently, the IBC (37) could be written as

$$\lim_{r \searrow 0} r^{1+B} \psi^{(1)}(r\boldsymbol{\omega}) = g f_{\tilde{m}_j, \tilde{\kappa}_j}^- (\boldsymbol{\omega}) \psi^{(0)} \quad (39)$$

for every $\boldsymbol{\omega} \in \mathbb{S}^2$.

Remark 2. It seems plausible that an analogous IBC Hamiltonian can be set up for $N_{\max} > 1$ by applying the same terms on each particle sector.

Remark 3. The IBC Hamiltonian described in Theorem 6 belongs to a whole family of IBC Hamiltonians in which (37) and (38a) are replaced by

$$a_1 c_- + a_2 c_{+m_j, \tilde{\kappa}_j} = g \psi^{(0)} \quad (40)$$

and

$$(H\psi)^{(0)} = g^* (a_3 c_- + a_4 c_{+m_j, \tilde{\kappa}_j}), \quad (41)$$

respectively, with real constants a_1, \dots, a_4 satisfying

$$a_1 a_4 - a_2 a_3 = 4B(1 + q). \quad (42)$$

As we will show in the Proof of Theorem 6, each of these choices defines a self-adjoint operator. The Hamiltonian defined through (37) and (38a) corresponds to $a_1 = 1, a_2 = 0, a_3 = 0$, and $a_4 = 4B(1 + q)$.

Remark 4. In our construction of H , one angular momentum sector of $L^2(\mathbb{R}^3, \mathbb{C}^4)$, indexed by $(\tilde{m}_j, \tilde{\kappa}_j)$, gets coupled to the 0-particle sector. If we took the 0-particle sector to have more than one dimension, say $\mathcal{H}^{(0)} = \mathbb{C}^4$ instead of \mathbb{C} , then we could couple several angu-

lar momentum sectors listed in (34) to several mutually orthogonal subspaces of the 0-particle sector $\mathcal{H}^{(0)}$. However, this mathematical possibility does not seem physically natural.

Remark 5. It would be interesting to investigate also the case $|q| \geq 1$. We expect that IBC Hamiltonians exist also in that case because h_{m_j, κ_j} (an angular momentum block of H_1 , see Sec. III) is known to have multiple self-adjoint extensions also in that case. However, we do not have a proof.

Remark 6. It is also of interest to define a $|\psi|^2$ -distributed jump process for the Bohmian configuration in analogy to the processes defined in Ref. 26 for non-relativistic IBC Hamiltonians. This issue is addressed in a separate work.⁴⁰

D. Rotational symmetry

The Hamiltonian H provided by Theorem 6 is not rotationally symmetric, for example, because the subspace $\mathcal{H}_{\vec{m}_j, \vec{\kappa}_j}$ that plays a special role for H is not invariant under J_1 or J_2 , and, thus, not under the action of the rotation group (more precisely, of its covering group). One might think of coupling all four angular momentum sectors $\mathcal{H}_{m_j, \kappa_j}$ with $(m_j, \kappa_j) \in \mathcal{A}$ to the 0-particle sector in a symmetric way, but actually, that does not help.

Theorem 7. *Let \mathcal{H} and (H°, D°) be as in Theorems 4 and 6 with any $q \in \mathbb{R}$. None of the self-adjoint extensions of (H°, D°) with particle creation is rotationally symmetric.⁴¹*

The proof is based on the following fact that we also prove in Sec. III.

Lemma 1. *The only vector in $L^2(\mathbb{R}^3, \mathbb{C}^4)$ invariant under rotations [i.e., under the representation of the covering group of $SO(3)$] is the zero vector.*

III. PROOFS

Proof of Theorem 1. Let $\tilde{D} = S_\pm C_c^\infty(\mathcal{Q}_1^{N_{\max}}, (\mathbb{C}^4)^{\otimes N_{\max}})$ and \tilde{H} the restriction of H_N^{free} to \tilde{D} . By Theorem 2, (\tilde{H}, \tilde{D}) is essentially self-adjoint in $\mathcal{H}^{(N_{\max})}$. Now, Theorem 3 yields the statement of Theorem 1. \square

Proof of Theorem 3. As a shorthand notation, we write

$$\mathcal{H}^\leftarrow := \mathcal{H}^{(\leftarrow N_{\max})}, \quad \mathcal{H}^\rightarrow := \mathcal{H}^{(N_{\max})}, \tag{43}$$

and correspondingly, $H^\leftarrow, D^\leftarrow, H^\rightarrow,$ and D^\rightarrow . Let $\Gamma(A)$ denote the graph of an operator $[A, D(A)]$ and $\overline{\Gamma(A)}$ its closure in $\mathcal{H} \oplus \mathcal{H}$, which is the graph of the closure of A , $\Gamma(\overline{A})$. Since \tilde{H} is essentially self-adjoint, its closure $\overline{\tilde{H}}$ is its self-adjoint extension H^\rightarrow . Since (H°, D°) is symmetric (and \tilde{H} is densely defined), it is closable with closure $[\overline{H^\circ}, D(\overline{H^\circ})]$, and we get that

$$\Gamma(H) = \overline{\Gamma(\tilde{H})} \supset \overline{\Gamma(H^\circ)} = \left\{ \begin{pmatrix} 0 \\ f \\ 0 \\ \tilde{H}f \end{pmatrix} : f \in \tilde{D} \right\} = \left\{ \begin{pmatrix} 0 \\ f \\ 0 \\ g \end{pmatrix} : \begin{pmatrix} f \\ g \end{pmatrix} \in \overline{\Gamma(\tilde{H})} \right\} \tag{44a}$$

$$= \left\{ \begin{pmatrix} 0 \\ f \\ 0 \\ g \end{pmatrix} : \begin{pmatrix} f \\ g \end{pmatrix} \in \Gamma(H^\rightarrow) \right\} = \left\{ \begin{pmatrix} 0 \\ f \\ 0 \\ H^\rightarrow f \end{pmatrix} : f \in D^\rightarrow \right\}, \tag{44b}$$

where 0 means the zero of \mathcal{H}^\leftarrow . In particular,

$$D \supset D(\overline{H^\circ}) = \{0\} \oplus D^\rightarrow. \tag{45}$$

Now, define the “adjoint domain” of the not densely defined operator $\overline{H^\circ}$ as

$$D^*(\overline{H^\circ}) = \{ \phi \in \mathcal{H} : \exists \eta \in \mathcal{H} \forall \psi \in D(\overline{H^\circ}) : \langle \phi | \overline{H^\circ} \psi \rangle_{\mathcal{H}} = \langle \eta | \psi \rangle_{\mathcal{H}} \} \quad (46)$$

and note that

$$D \subset D^*(\overline{H^\circ}). \quad (47)$$

By (45), ψ in (46) is of the form $(0, f)$ with $f \in D^-$, so (writing $\phi^- = g$ and $\eta^- = h$)

$$D^*(\overline{H^\circ}) = \mathcal{H}^< \oplus \{ g \in \mathcal{H}^- : \exists h \in \mathcal{H}^- \forall f \in D^- : \langle g | H^- f \rangle_{\mathcal{H}^-} = \langle h | f \rangle_{\mathcal{H}^-} \} \quad (48a)$$

$$= \mathcal{H}^< \oplus D^- \quad (48b)$$

by self-adjointness of H^- . We, thus, obtain the chain of inclusions

$$\{0\} \oplus D^- \subset D \subset \mathcal{H}^< \oplus D^-. \quad (49)$$

This entails further that

$$D = D^< \oplus D^- \text{ with } D^< := \left\{ \psi^< : \begin{pmatrix} \psi^< \\ \psi^- \end{pmatrix} \in D \right\}. \quad (50)$$

Indeed, writing vectors now as rows, for any $(\psi^<, \psi^-) \in D$, we have that $\psi^< \in D^<$ by definition of $D^<$ and $\psi^- \in D^-$ by (49), so $(\psi^<, \psi^-) \in D^< \oplus D^-$. Conversely, if $\psi^< \in D^<$ and $\psi^- \in D^-$, then by definition of $D^<$, there is $\phi^- \in \mathcal{H}^-$ such that $(\psi^<, \phi^-) \in D$, but then, $\phi^- \in D^-$ by (49), so $\psi^- - \phi^- \in D^-$ since D^- is a subspace, so $(0, \psi^- - \phi^-) \in D$ by (49), so $(\psi^<, \psi^-) = (\psi^<, \phi^-) + (0, \psi^- - \phi^-) \in D$ since D is a subspace.

Now, we turn to the action of the operator H and claim that for every $\phi = (\phi^<, \phi^-) \in D^< \oplus D^-$,

$$(H\phi)^- = H^- \phi^- \quad (51)$$

regardless of the choice of $\phi^< \in D^<$. Indeed, from (47), we obtain that

$$\begin{aligned} \forall \begin{pmatrix} \phi^< \\ \phi^- \end{pmatrix} = \phi \in D \quad \exists \begin{pmatrix} \eta^< \\ \eta^- \end{pmatrix} = \eta \in \mathcal{H} \quad \forall \begin{pmatrix} \psi^< \\ \psi^- \end{pmatrix} = \psi \in D(\overline{H^\circ}) : \\ \langle (H\phi)^- | \psi^- \rangle_{\mathcal{H}^-} \stackrel{\psi^<=0}{=} \langle H\phi | \psi \rangle_{\mathcal{H}} \stackrel{H \text{ s.a.}}{=} \langle \phi | H\psi \rangle_{\mathcal{H}} \\ \stackrel{\overline{H^\circ} \subset H}{=} \langle \phi | \overline{H^\circ} \psi \rangle_{\mathcal{H}} \stackrel{46}{=} \langle \eta | \psi \rangle_{\mathcal{H}} \stackrel{\psi^<=0}{=} \langle \eta^- | \psi^- \rangle_{\mathcal{H}^-} \stackrel{48a}{=} \langle \phi^- | H^- \psi^- \rangle_{\mathcal{H}^-} \\ \stackrel{H^- \text{ s.a.}}{=} \langle H^- \phi^- | \psi^- \rangle_{\mathcal{H}^-}. \end{aligned} \quad (52)$$

By (45), $\langle (H\phi)^- | f \rangle_{\mathcal{H}^-} = \langle H^- \phi^- | f \rangle_{\mathcal{H}^-}$ for every $f \in D^-$. Since D^- is dense, (51) follows.

Now, it follows further from (51) that there is an operator $H^< : D^< \rightarrow \mathcal{H}^<$ such that

$$(H\phi)^< = H^< \phi^< \quad (53)$$

regardless of ϕ^- . Indeed, by setting $\phi^- = 0$, we obtain from (51) that $(H(\phi^<, 0))^< = 0$ and define

$$H \begin{pmatrix} \phi^< \\ 0 \end{pmatrix} = \begin{pmatrix} H^< \phi^< \\ 0 \end{pmatrix}. \quad (54)$$

From (44), it follows that

$$H \begin{pmatrix} 0 \\ \phi^- \end{pmatrix} = \begin{pmatrix} 0 \\ H^- \phi^- \end{pmatrix}. \quad (55)$$

Thus,

$$H \begin{pmatrix} \phi^< \\ \phi^= \end{pmatrix} = H \begin{pmatrix} \phi^< \\ 0 \end{pmatrix} + H \begin{pmatrix} 0 \\ \phi^= \end{pmatrix} = \begin{pmatrix} H^< \phi^< \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ H^= \phi^= \end{pmatrix} = \begin{pmatrix} H^< \phi^< \\ H^= \phi^= \end{pmatrix} \quad (56)$$

for all $\phi \in D = D^< \oplus D^=$; that is H is block diagonal. This completes the proof. \square

Proof of Theorem 4. Use Theorems 3 and 5 with $N_{\max} = 1$, $\tilde{H} = H_1$ as in (22), $\tilde{D} = C_c^\infty(\mathbb{R}^3 \setminus \{\mathbf{0}\}, \mathbb{C}^4)$. Since $\mathcal{H}^< = \mathbb{C}$, the only possibilities for $D^<$ are $D^< = \{0\}$ and $D^< = \mathbb{C}$, and since D is dense, only $D^< = \mathbb{C}$ remains. In particular, $H^<$ is multiplication by some real constant E_{00} . \square

Proof of Theorem 6. We begin by reviewing the well known decomposition of Hilbert space $\mathcal{H}^{(1)} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ in terms of the functions Φ_{m_j, κ_j}^\pm . By passing to spherical coordinates and denoting with $d^2\omega$ the surface measure of the unit sphere S^2 , we obtain the canonical isomorphism

$$U : \mathcal{H}^{(1)} \rightarrow L^2((0, \infty), \mathbb{C}, dr) \otimes L^2(S^2, \mathbb{C}^4, d^2\omega) \quad (57)$$

by setting, for each $\psi \in \mathcal{H}^{(1)}$,

$$(U\psi)(r, \omega) = r\psi(r\omega). \quad (58)$$

Under this transformation, the Dirac–Coulomb operator H_1 as in (22) takes the form (Ref. 15, p. 125)

$$UH_1U^\dagger = -i\alpha_r \left(\partial_r + \frac{1}{r} - \frac{1}{r}\beta K \right) + m\beta + \frac{q}{r}, \quad (59)$$

where $\alpha_r = \mathbf{e}_r \cdot \boldsymbol{\alpha}$ is the radial component of $\boldsymbol{\alpha}$ and $K = \beta(2\mathbf{S} \cdot \mathbf{L} + 1)$ is the spin–orbit operator consisting of the spin operator $\mathbf{S} = -\frac{i}{4}\boldsymbol{\alpha} \times \boldsymbol{\alpha}$ and the angular momentum operator $\mathbf{L} = \mathbf{x} \times (-i\nabla)$. Denoting with $\mathbf{J} = \mathbf{L} + \mathbf{S}$ the total angular momentum, one can show¹⁵ that K commutes with \mathbf{J}^2 and with the third component J_3 of \mathbf{J} . The functions Φ_{m_j, κ_j}^\pm form a joint eigenbasis of \mathbf{J}^2, K , and J_3 with eigenvalues $j(j+1), \kappa_j$, and m_j , respectively, thus providing the following orthogonal decomposition:

$$L^2(S^2, \mathbb{C}^4, d\Omega) = \bigoplus_{j \in \mathbb{N}_0 + \frac{1}{2}} \bigoplus_{m_j = -j}^j \bigoplus_{\kappa_j = \pm(j + \frac{1}{2})} \mathcal{H}_{m_j, \kappa_j} \quad (60)$$

with

$$\mathcal{H}_{m_j, \kappa_j} = \text{span}(\Phi_{m_j, \kappa_j}^+, \Phi_{m_j, \kappa_j}^-). \quad (61)$$

In this basis, we have that (Ref. 15, Lemma 4.13)

$$\alpha_r = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad i\alpha_r\beta = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \quad (62)$$

and we quote the following fact.

Lemma 2. (Ref. 15, Theorem 4.14). U as in (58) maps $C_c^\infty(\mathcal{Q}_1, \mathbb{C}^4)$ to (but not onto)

$$\bigoplus_{j, m_j, \kappa_j} C_c^\infty((0, \infty), \mathbb{C}^2) \otimes \mathcal{H}_{m_j, \kappa_j}, \quad (63)$$

and (the closure of) H_1 is unitarily equivalent to (the closure of) UH_1U^\dagger , which is block diagonal with respect to (63) with blocks

$$h_{m_j, \kappa_j} = \begin{pmatrix} m + \frac{q}{r} & -\partial_r + \frac{\kappa_j}{r} \\ \partial_r + \frac{\kappa_j}{r} & -m + \frac{q}{r} \end{pmatrix}. \quad (64)$$

In the following, we will say “angular momentum sector” to $\mathcal{H}_{m_j, \kappa_j}$. Our construction of the IBC Hamiltonian H proceeds for each angular momentum sector separately. For one sector, the one chosen in (34), we will couple $h_{\tilde{m}_j, \tilde{\kappa}_j}$ to the 0-particle sector of our mini-Fock space \mathcal{H} ; all other angular momentum sectors will decouple. That is, H will be block diagonal relative to the sum decomposition

$$\mathcal{H} \cong \widehat{\mathcal{H}} \oplus \bigoplus_{(j, m_j, \kappa_j) \neq (\tilde{j}, \tilde{m}_j, \tilde{\kappa}_j)} L^2((0, \infty)) \otimes \mathcal{H}_{m_j, \kappa_j} \tag{65}$$

(note that j is determined by κ_j through $j = |\kappa_j| - \frac{1}{2}$), but not relative to

$$\widehat{\mathcal{H}} = \mathcal{H}^{(0)} \oplus L^2((0, \infty)) \otimes \mathcal{H}_{\tilde{m}_j, \tilde{\kappa}_j}. \tag{66}$$

To this end, we need a self-adjoint extension for every h_{m_j, κ_j} with $(m_j, \kappa_j) \neq (\tilde{m}_j, \tilde{\kappa}_j)$.

Lemma 3 (Refs. 42 and 43, Propositions 1.2 and 2.2–2.4). The operator $[h_{m_j, \kappa_j}, C_c^\infty((0, \infty)) \otimes \mathcal{H}_{m_j, \kappa_j}]$ is essentially self-adjoint if and only if $q^2 \leq \kappa_j^2 - \frac{1}{4}$. As a consequence, for $\sqrt{3}/2 < |q| < 1$, the only angular momentum sectors for which h_{m_j, κ_j} is not essentially self-adjoint are those mentioned in (34). Furthermore, for $\sqrt{3}/2 < |q| < 1$, those sectors that are not essentially self-adjoint possess, among an infinitude of self-adjoint extensions, a distinguished one, $h_{D_{m_j, \kappa_j}}$ that is uniquely characterized by the property that for all functions ϕ in the domain, kinetic and potential energy are separately finite, $\|h_{D_{m_j, \kappa_j}} - \frac{q}{r}|^{1/2}\phi\| < \infty$ and $\|(\frac{|q|}{r})^{1/2}\phi\| < \infty$. Functions ϕ in the domain of the distinguished extension obey the asymptotics

$$\phi(r, \omega) = c_{+m_j, \kappa_j} f_{B_{m_j, \kappa_j}}^+(\omega) r^B + o(r^{1/2}) \tag{67}$$

as $r \searrow 0$.

For the three sectors in \mathcal{A} mentioned in (34) but different from $(\tilde{m}_j, \tilde{\kappa}_j)$, we choose the distinguished extension, and for those not mentioned there (i.e., with $|\kappa_j| \geq 2$), the extension is unique. These extensions can be combined to form an extension of H° on all summands but the first in (65). So, it remains to construct the block \widehat{H} of H acting in $\widehat{\mathcal{H}}$, which is where the coupling between particle sectors takes place. Correspondingly,

$$D := \widehat{D} \oplus D_{\text{distinguished}} \subset \widehat{\mathcal{H}} \oplus \widehat{\mathcal{H}}^\perp = \mathcal{H} \tag{68}$$

with \widehat{D} to be determined. For brevity, we set

$$\mathcal{K} := \mathcal{H}_{\tilde{m}_j, \tilde{\kappa}_j} \text{ and } h := h_{\tilde{m}_j, \tilde{\kappa}_j}. \tag{69}$$

We regard h as defined on $C_c^\infty((0, \infty)) \otimes \mathcal{H}$. Another known fact is the following.

Lemma 4 (Ref. 43, Theorem 2.6). Every function ϕ in the domain $D(h^)$ of the adjoint h^* of h obeys, as $r \searrow 0$, the asymptotics⁴⁴*

$$\phi(r, \omega) = c_- f_{\tilde{m}_j, \tilde{\kappa}_j}^-(\omega) r^{-B} + c_+ f_{\tilde{m}_j, \tilde{\kappa}_j}^+(\omega) r^B + o(r^{1/2}) \tag{70}$$

with f^\pm as in (36); the coefficients $c_-, c_+ = c_{+\tilde{m}_j, \tilde{\kappa}_j} \in \mathbb{C}$ are uniquely determined by ϕ , and all combinations $(c_-, c_+) \in \mathbb{C}^2$ occur for some ϕ .

For higher angular momentum sectors ($|\kappa_j| \geq 2$), functions in the domain of the unique self-adjoint extension of h_{m_j, κ_j} are $o(r^{1/2})$ [because the extension is $\overline{h_{m_j, \kappa_j}}$, and the domain of that contains only $o(r^{1/2})$ functions by Ref. 43, Proposition 2.4] and, thus, contribute only $o(|\mathbf{x}|^{-1/2})$ in (35).

We will directly consider the more general form (40) of the IBC, which contains (37) as a special case. We define the domain \widehat{D} of \widehat{H} as follows, containing functions satisfying the IBC (40)

$$\widehat{D} := \left\{ (\psi^{(0)}, \psi^{(1)}) \in \widehat{\mathcal{H}} : \psi^{(1)} \in D(h^*) \text{ and (40)} \right\}. \tag{71}$$

We define the action of \widehat{H} [according to (38b) and (41)] as

$$(\widehat{H}\psi)^{(0)} = g^* (a_3 c_- + a_4 c_{+\tilde{m}_j, \tilde{\kappa}_j}), \tag{72a}$$

$$(\widehat{H}\psi)^{(1)} = h^* \psi^{(1)}. \tag{72b}$$

\widehat{D} is dense in \mathcal{H} because (i) in $D(h^*)$, there exist functions with arbitrary values of c_- and c_+ , so for $\psi \in \widehat{D}$, any desired complex number can occur as $\psi^{(0)}$; (ii) since $D(h) = C_c^\infty((0, \infty)) \otimes \mathcal{H}$ is contained in $D(h^*)$ and dense in $L^2((0, \infty)) \otimes \mathcal{H}$, the set $\{(\psi^{(0)}, \psi^{(1)} + \phi) : \phi \in D(h)\} \subset \widehat{D}$ is dense in $\{\psi^{(0)}\} \oplus L^2((0, \infty)) \otimes \mathcal{H}$. Together, (i) and (ii) imply that \widehat{D} is dense.

We now prove that \widehat{H} is a symmetric operator on \widehat{D} . Let $\psi \in \widehat{D}$ with short distance coefficients c_- and c_+ , and $\phi \in \widehat{D}$ with short distance coefficients d_- and d_+ . Then,

$$\begin{aligned} & \langle \phi, H\psi \rangle_{\mathcal{H}} - \langle H\phi, \psi \rangle_{\mathcal{H}} \\ &= \langle \phi^{(0)}, g^*(a_3 c_- + a_4 c_+) \rangle_{\mathbb{C}} + \langle \phi^{(1)}, h^* \psi^{(1)} \rangle_{L^2((0, \infty), \mathcal{H})} \\ & \quad - \langle g^*(a_3 d_- + a_4 d_+), \psi^{(0)} \rangle_{\mathbb{C}} - \langle h^* \phi^{(1)}, \psi^{(1)} \rangle_{L^2((0, \infty), \mathcal{H})} \end{aligned} \tag{73}$$

$$\begin{aligned} &= \langle a_1 d_- + a_2 d_+, a_3 c_- + a_4 c_+ \rangle_{\mathbb{C}} - \langle a_3 d_- + a_4 d_+, a_1 c_- + a_2 c_+ \rangle_{\mathbb{C}} \\ & \quad + \langle \phi^{(1)}, h^* \psi^{(1)} \rangle_{L^2((0, \infty), \mathcal{H})} - \langle h^* \phi^{(1)}, \psi^{(1)} \rangle_{L^2((0, \infty), \mathcal{H})}. \end{aligned} \tag{74}$$

Now, note that h^* can be written as $h^* = -i\alpha_r \partial_r + M(r)$, where $M(r)$ is a Hermitian operator $\mathcal{H} \rightarrow \mathcal{H}$ for each $r > 0$. Thus, the last two terms of (74) can be written as

$$\begin{aligned} & \langle \phi^{(1)}, h^* \psi^{(1)} \rangle_{L^2((0, \infty), \mathcal{H})} - \langle h^* \phi^{(1)}, \psi^{(1)} \rangle_{L^2((0, \infty), \mathcal{H})} \\ &= \int_0^\infty dr \left[\langle \phi^{(1)}(r), (-i\alpha_r) \partial_r \psi^{(1)}(r) \rangle_{\mathcal{H}} + \langle \partial_r \phi^{(1)}(r), (-i\alpha_r) \psi^{(1)}(r) \rangle_{\mathcal{H}} \right] \end{aligned} \tag{75}$$

$$= \int_0^\infty dr \partial_r \langle \phi^{(1)}(r), (-i\alpha_r) \psi^{(1)}(r) \rangle_{\mathcal{H}} \tag{76}$$

$$= \lim_{r \searrow 0} \langle \phi^{(1)}(r), (+i\alpha_r) \psi^{(1)}(r) \rangle_{\mathcal{H}} \tag{77}$$

$$= \lim_{r \searrow 0} \langle d_- f^- r^{-B} + d_+ f^+ r^B + o(r^{1/2}), c_- (i\alpha_r) f^- r^{-B} + c_+ (i\alpha_r) f^+ r^B + o(r^{1/2}) \rangle_{\mathcal{H}} \tag{78}$$

$$\begin{aligned} &= \lim_{r \searrow 0} \left[d_-^* c_- \langle f^-, i\alpha_r f^- \rangle_{\mathcal{H}} r^{-2B} \right. \\ & \quad \left. + (d_-^* c_+ \langle f^-, i\alpha_r f^+ \rangle_{\mathcal{H}} + d_+^* c_- \langle f^+, i\alpha_r f^- \rangle_{\mathcal{H}}) r^0 + o(r^0) \right]. \end{aligned} \tag{79}$$

Since in the orthonormal basis $\Phi^\pm = \Phi_{\vec{m}_i \vec{k}_j}^\pm$ of \mathcal{H} , the explicit form of α_r is given by (62), any vector $v = x\Phi^+ + y\Phi^- \in \mathcal{H}$ with coefficients $x, y \in \mathbb{C}$ has

$$\langle v, i\alpha_r v \rangle_{\mathcal{H}} = (x^* \ y^*) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = x^* y - y^* x = 2 \operatorname{Im}(x^* y). \tag{80}$$

Since by (36), f^\pm has real coefficients relative to Φ^\pm , we have that

$$\langle f^\pm, i\alpha_r f^\pm \rangle_{\mathcal{H}} = 0. \tag{81}$$

Thus, the r^{-2B} term in (79) vanishes. Moreover, by (36) and (62) again,

$$\langle f^-, i\alpha_r f^+ \rangle_{\mathcal{H}} = -4B(1 + q), \quad \langle f^+, i\alpha_r f^- \rangle_{\mathcal{H}} = 4B(1 + q). \tag{82}$$

Thus,

$$\begin{aligned} & \langle \phi^{(1)}, h^* \psi^{(1)} \rangle_{L^2((0, \infty), \mathcal{H})} - \langle h^* \phi^{(1)}, \psi^{(1)} \rangle_{L^2((0, \infty), \mathcal{H})} \\ &= d_+^* c_- 4B(1 + q) - d_-^* c_+ 4B(1 + q). \end{aligned} \tag{83}$$

Therefore, putting together (74) and (83),

$$\begin{aligned} \langle \phi, H\psi \rangle_{\mathcal{H}} - \langle H\phi, \psi \rangle_{\mathcal{H}} &= a_1 a_3 d_-^* c_- + a_2 a_3 d_+^* c_- + a_1 a_4 d_-^* c_+ + a_2 a_4 d_+^* c_+ \\ &\quad - a_1 a_3 d_-^* c_- - a_2 a_3 d_+^* c_+ - a_1 a_4 d_+^* c_- - a_2 a_4 d_+^* c_+ \\ &\quad + (d_+^* c_- - d_-^* c_+) 4B(1+q) \end{aligned} \tag{84}$$

$$= (d_+^* c_- - d_-^* c_+) (-a_1 a_4 + a_2 a_3 + 4B(1+q)) \tag{85}$$

$$= 0 \tag{86}$$

if (42) holds.

In order to see that \widehat{H} is also self-adjoint, it remains to verify that $\widehat{D} = D(\widehat{H}^*)$. To this end, we first note that

$$\widehat{D} \subseteq D(\widehat{H}^*) \subseteq \mathbb{C} \oplus D(h^*). \tag{87}$$

Any given $\phi \in \mathbb{C} \oplus D(h^*)$ lies in $D(\widehat{H}^*)$ if and only if there is $\eta \in \widehat{\mathcal{H}}$ such that for every $\psi \in \widehat{D}$,

$$\langle \eta, \psi \rangle_{\widehat{\mathcal{H}}} = \langle \phi, \widehat{H}\psi \rangle_{\widehat{\mathcal{H}}}. \tag{88}$$

If we write again c_-, c_+ for the short-distance coefficients of $\psi^{(1)}$ and d_-, d_+ for those of $\phi^{(1)}$, then condition (88) is equivalent to

$$\langle \eta, \psi \rangle_{\widehat{\mathcal{H}}} = \langle \phi^{(0)}, (\widehat{H}\psi)^{(0)} \rangle_{\mathbb{C}} + \langle \phi^{(1)}, h^* \psi^{(1)} \rangle_{L^2((0,\infty), \mathcal{H})} \tag{89}$$

$$\stackrel{(41),(83)}{=} \phi^{(0)*} g^* (a_3 c_- + a_4 c_+) + \langle h^* \phi^{(1)}, \psi^{(1)} \rangle_{L^2((0,\infty), \mathcal{H})} - (d_-^* c_+ - d_+^* c_-) 4B(1+q) \tag{90}$$

$$\stackrel{(42)}{=} [g\phi^{(0)}]^* (a_3 c_- + a_4 c_+) + \langle h^* \phi^{(1)}, \psi^{(1)} \rangle_{L^2((0,\infty), \mathcal{H})} - \begin{vmatrix} d_-^* & d_+^* \\ c_- & c_+ \end{vmatrix} \begin{vmatrix} a_1 & a_3 \\ a_2 & a_4 \end{vmatrix} \tag{91}$$

$$= [g\phi^{(0)}]^* (a_3 c_- + a_4 c_+) + \langle h^* \phi^{(1)}, \psi^{(1)} \rangle_{L^2((0,\infty), \mathcal{H})} - \begin{vmatrix} d_-^* a_1 + d_+^* a_2 & d_-^* a_3 + d_+^* a_4 \\ c_- a_1 + c_+ a_2 & c_- a_3 + c_+ a_4 \end{vmatrix} \tag{92}$$

$$= [-(a_1 d_- + a_2 d_+) + g\phi^{(0)}]^* (a_3 c_- + a_4 c_+) + \langle h^* \phi^{(1)}, \psi^{(1)} \rangle_{L^2((0,\infty), \mathcal{H})} + (a_3 d_-^* + a_4 d_+^*) (a_1 c_- + a_2 c_+) \tag{93}$$

$$= [-(a_1 d_- + a_2 d_+) + g\phi^{(0)}]^* (a_3 c_- + a_4 c_+) + \langle h^* \phi^{(1)}, \psi^{(1)} \rangle_{L^2((0,\infty), \mathcal{H})} + \langle g^* (a_3 d_- + a_4 d_+), \psi^{(0)} \rangle_{\mathbb{C}}. \tag{94}$$

The only way this can be true for all $\psi \in \widehat{D}$ is that

$$\eta^{(0)} = g^* (a_3 d_- + a_4 d_+), \tag{95a}$$

$$\eta^{(1)} = h^* \phi^{(1)}, \tag{95b}$$

and the product in the first line of (94) vanishes. For one thing, we obtain from this an expression for $\widehat{H}^* \phi = \eta$. Moreover, since the product in the first line of (94) consists of one factor depending on ϕ and one depending on ψ , and since the product needs to vanish for every $\psi \in \widehat{D}$ but the second factor will not, the first factor has to vanish for every $\phi \in D(\widehat{H}^*)$. As a consequence, ϕ also needs to satisfy the IBC (40), i.e.,

$$a_1 d_- + a_2 d_+ = g\phi^{(0)}, \tag{96}$$

so that we arrive at

$$\widehat{D} = D(\widehat{H}^*) \quad (97)$$

and \widehat{H} (and, thus, H) is self-adjoint. This completes the proof of Theorem 6. \square

Remark 7. Here is an alternative argument for the part after (86), after it has been shown that H is symmetric. While this alternative argument does not show that H is self-adjoint, it shows that H possesses a self-adjoint extension, which suffices for proving Theorem 6. The argument is based on the von Neumann theorem about conjugations (Ref. 45, Theorem X.3), which asserts the following: let \mathcal{H} be a Hilbert space. An antilinear map $C : \mathcal{H} \rightarrow \mathcal{H}$ [i.e., such that $C(\alpha\phi + \beta\psi) = \alpha^*C\phi + \beta^*C\psi$] is called a conjugation if it is norm-preserving and $C^2 = I$. Let $[A, D(A)]$ be a densely defined symmetric operator, and suppose that there exists a conjugation C with $C(D(A)) \subseteq D(A)$ and $AC = CA$. Then, A has equal deficiency indices and, therefore, has self-adjoint extensions.

In our case, we use that the differential expression (64) for h has only real entries. We assume for the argument that the coupling constant g is real; if this is not the case, it can be arranged through a unitary transformation of \mathcal{H} that merely changes the phase of $\psi^{(0)}$ by the phase of g . So, we take $C : \mathcal{H} \rightarrow \mathcal{H}$ to be complex conjugation of $\psi^{(0)}$ and of the coefficients of $\psi^{(1)} \in L^2((0, \infty)) \otimes \mathcal{H}$ relative to $\Phi_{\vec{m}, \vec{k}}^\pm$. Since the coefficients a_1, \dots, a_4 are real, H commutes with C , and the von Neumann theorem applies.

Remark 8. In Ref. 39, the authors established short-distance asymptotics of wave functions for the case of general Coulomb-type potentials (27), very similarly to Lemmas 3 and 4. Having their analog at hand, constructing a similar IBC Hamiltonian for certain parameter ranges of $\nu, \mu, \lambda \in \mathbb{R}$ from (27) is reasonably straightforward.

Proof of Lemma 1. Suppose ψ was a nonzero vector in $L^2(\mathbb{R}^3, \mathbb{C}^4)$ invariant under the representation of the covering group of $SO(3)$. A rotation (about any axis) through 360° is a particular element g of the covering group that acts on vectors \mathbf{x} in \mathbb{R}^3 as the identity and on spinors as $-I$ with I the identity. Thus, g maps ψ to $-\psi$, and if ψ is invariant, it must vanish. \square

Proof of Theorem 7. If H were a self-adjoint extension of H° that involves particle creation, then the initial Fock vector $\psi_0 = (\psi_0^{(0)}, \psi_0^{(1)}) = (1, 0)$ (i.e., the Fock vacuum) would evolve by some time $t > 0$ to a non-vacuum state, i.e., one with nonzero $\psi_t^{(1)}$, that would be invariant under rotations. Since rotations do not mix particle number sectors, also $\psi_t^{(1)}$ by itself would be invariant under rotations. However, by Lemma 1 no such state exists. \square

Note added in proof. After the completion of this work, Binz and Lampart posted a preprint⁴⁶ in which they described a general abstract framework for the construction of IBC Hamiltonians. The one given in Theorem 6 can also be cast in this form.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Joscha Henheik: Formal analysis (equal); Investigation (equal); Writing – original draft (equal); Writing – review & editing (equal). **Roderich Tumulka:** Formal analysis (equal); Investigation (equal); Writing – original draft (equal); Writing – review & editing (equal).

DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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