Interior-Boundary Conditions for Schrödinger Equations

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Multi-time Wave Functions

An Introduction

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configuration space $Q = \mathbb{R}^{3N}$, $\psi : Q \times \mathbb{R}_t \rightarrow \mathbb{C}$

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi = -\frac{\hbar^2}{2m}\nabla^2 \psi + V\psi$$

$\psi_t = U_t \psi_0 = e^{-iHt/\hbar} \psi_0$

**Born’s rule**

$$\rho_t(x) = |\psi_t(x)|^2$$

$\psi_t \in \mathcal{H} = L^2(Q, \mathbb{C})$

$U_t : \mathcal{H} \rightarrow \mathcal{H}$ is unitary

$\Leftarrow H$ is self-adjoint

prob. current $j = \frac{\hbar}{m} \text{Im}[\psi^* \nabla \psi]$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot j = 0 \text{ continuity equation}$$
Boundary conditions for the Schrödinger equation

- $Q = [0, 1]$
- for time evolution, PDE is not enough: also need boundary conditions (BCs) such as
  
  \[ \psi(0, t) = 0 \ \forall t \ (\text{Dirichlet}), \quad \frac{\partial \psi}{\partial x}(1, t) = 0 \ \forall t \ (\text{Neumann}) \]  

  (1)

- built into the domain $\mathcal{D}$ of the Hamiltonian $H$: $H = -\frac{\hbar^2}{2m} \nabla^2$,
  
  $\mathcal{D} = \{ \psi \in L^2([0, 1]): \nabla^2 \psi \in L^2([0, 1]), \psi \text{ satisfies (1)} \} $

- (1) are reflecting boundary conditions: make $(H, \mathcal{D})$ self-adjoint $\Rightarrow$$U_t = e^{-iHt/\hbar}$ unitary $\Rightarrow$ no loss of probability

- Likewise for Robin BC ($\alpha, \beta \neq (0, 0)$ real constants):
  
  \[ \alpha \frac{\partial \psi}{\partial x} + \beta \psi(x) = 0 \]
Particle–position representation of a Fock space vector

Configuration space of a variable number of particles:

\[ Q = \bigcup_{n=0}^{\infty} \mathbb{R}^{3n} = \bigcup_{n=0}^{\infty} Q^{(n)} \]

Fock space:

\[ \mathcal{F}^{\pm} = \bigoplus_{n=0}^{\infty} S^{\pm} \mathcal{H}_1^\otimes n \]

with \( S_+ = \) symmetrizer, \( S_- = \) anti-symmetrizer, \( \mathcal{H}_1 = \) 1-particle Hilbert space = \( L^2(\mathbb{R}^3, \mathbb{C}^k) \)

\[ \psi \in \mathcal{F} \implies \psi = (\psi^{(0)}, \psi^{(1)}, \psi^{(2)}, \ldots) \]

\[ \psi : Q \to S \text{ with } S = \text{value space} = \bigcup_{n=0}^{\infty} (\mathbb{C}^k)^\otimes n \]

\( \psi \) is an (anti-)symmetric function

here \( d = 1, n = 0, 1, 2, 3 \)
An UV divergence problem

For example, consider a simplified model quantum field theory (QFT):

- x-particles can emit and absorb y-particles.
- There is only 1 x-particle, and it is fixed at the origin. \( \mathcal{H} = \mathcal{F}_y^+ \)
- configuration space \( \mathcal{Q} = \bigcup_{n=0}^{\infty} \mathbb{R}^{3n} \), coupling constant \( g \in \mathbb{R} \)

Original Hamiltonian in the particle-position representation:

\[
(H_{\text{orig}}\psi)^{(n)}(y_1 \cdots y_n) = -\frac{\hbar^2}{2m_y} \sum_{j=1}^{n} \nabla^2_{y_j} \psi^{(n)}(y_1 \cdots y_n) + nE_0 \psi^{(n)}
\]

\[
+ g \sqrt{n+1} \psi^{(n+1)}(y_1 \cdots y_n, 0)
\]

\[
+ \frac{g}{\sqrt{n}} \sum_{j=1}^{n} \delta^3(y_j) \psi^{(n-1)}(y_1 \cdots \hat{y}_j \cdots y_n),
\]

is UV divergent. (\( \hat{\ } = \) omit, \( E_0 \geq 0 \) energy needed for creating \( y \))
Well-defined, “regularized” version of $H$

UV cut-off $\varphi \in L^2(\mathbb{R}^3)$:

$$
(H_{\text{cutoff}} \psi)(\mathbf{y}_1 \ldots \mathbf{y}_n) = -\frac{\hbar^2}{2m} \sum_{j=1}^{n} \nabla^2_{\mathbf{y}_j} \psi(\mathbf{y}_1 \ldots \mathbf{y}_n) + nE_0 \psi^{(n)} + 
$$

$$
+ g \sqrt{n+1} \sum_{i=1}^{m} \int_{\mathbb{R}^3} d^3 \mathbf{y} \varphi^*(\mathbf{y}) \psi(\mathbf{y}_1 \ldots \mathbf{y}_n, \mathbf{y}) + 
$$

$$
+ \frac{g}{\sqrt{n}} \sum_{i=1}^{m} \sum_{j=1}^{n} \varphi(\mathbf{y}_j) \psi(\mathbf{y}_1 \ldots \hat{\mathbf{y}}_j \ldots \mathbf{y}_n)
$$

“smearing out” the $x$-particle with “charge distribution” $\varphi(\cdot)$
But then . . .

. . . emission and absorption occurs anywhere in a ball around the x-particle (= in the support of

\[ \varphi \]

There is no empirical evidence that an electron has positive radius.

Positive radius leads to difficulties with Lorentz invariance.

This UV problem can be solved!

[Teufel and Tumulka arxiv.org/abs/1505.04847, arxiv.org/abs/1506.00497]
Novel idea: Interior-boundary condition

Here: boundary config = where y-particle meets x-particle;
interior config = one y-particle removed

Interior–boundary condition (IBC)

\[ \psi^{(n+1)}(\text{bdy}) = (\text{const.}) \, \psi^{(n)} \]

links two configurations connected by the creation or annihilation of a particle.

For example, with an x-particle at 0,

\[ \psi^{(n+1)}(y^n, 0) = \frac{g \, m_y}{2\pi\hbar^2 \sqrt{n+1}} \, \psi^{(n)}(y^n) . \]

with \( y^n = (y_1, \ldots, y_n) \).
A derivation of an IBC in 1d

due to [Keppeler and Sieber arxiv.org/abs/1511.03071]

for simplicity in a truncated Fock space

\[ \mathcal{H} = \bigoplus_{n=0}^{\infty} S_+ \mathcal{H}_1^\otimes n = \mathbb{C} \oplus \mathcal{H}_1 = \mathbb{C} \oplus L^2(\mathbb{R}). \]

If \((H_{\text{orig}} \psi)^{(1)}(y) = -\frac{1}{2m} \frac{d^2}{dy^2} \psi^{(1)}(y) + g \delta(y) \psi^{(0)}\) lies in \(L^2(\mathbb{R})\), then

\[ \frac{d^2}{dy^2} \psi^{(1)}(y) = 2mg \delta(y) \psi^{(0)} + f(y) \text{ with } f \in L^2 \]

\(\phi'(y) = \delta(y) \Rightarrow \text{jump}\)

likewise \(\phi''(y) = \delta(y) \Rightarrow \text{kink}\)

so \(D = \left\{(\psi^{(0)}, \psi^{(1)}): \psi^{(1)'}(0+) - \psi^{(1)'}(0-) = 2mg\psi^{(0)} \right. \text{ and} \)

\(\left. \text{away from } 0, \nabla^2 \psi^{(1)} \in L^2 \right\}\)

and \(H(\psi^{(0)}, \psi^{(1)}) = (g \psi^{(1)}(0), -\frac{1}{2m} \nabla^2 \psi^{(1)} \text{ away from } 0)\)
The basic idea of IBCs: a toy example

Consider quantum mechanics on a space $Q$ with a boundary $\partial Q$.

- E.g.,
  
  $Q = Q^{(1)} \cup Q^{(2)} = \mathbb{R} \cup (\mathbb{R} \times [0, \infty))$
  
  $\partial Q = \partial Q^{(2)} = \mathbb{R} \times \{0\}$

- Consider probability current vector field $j$ on $Q$.

- Suppose $j$ has nonzero flux into $\partial Q$,
  
  $0 \neq \int_{\partial Q} dx \cdot j \cdot n$ ($n = $ normal to $\partial Q$)

- We want the prob that disappears at $q \in \partial Q$ to reappear at $f(q) \in Q$.

  - E.g., what disappears at $(x, 0) \in \partial Q^{(2)}$ reappears at $f(x, 0) = x$, so
    $f : \partial Q^{(2)} \rightarrow Q^{(1)}$. In general, $f : \partial Q \rightarrow Q$.

  - This is achieved through
    
    $\rightarrow$ an extra term in $H$ for $Q^{(1)}$
    
    $\rightarrow$ an interior-boundary condition $\psi(q) = (\text{const.}) \psi(f(q))$
IBC in the toy example

- \( \psi_t : Q \rightarrow \mathbb{C}, \quad \psi = (\psi^{(1)}, \psi^{(2)}) \)
- \( g \in \mathbb{R} \) coupling constant
- IBC: \( \psi^{(2)}(x, 0) = -\frac{2mg}{\hbar^2} \psi^{(1)}(x) \)
- Hamiltonian:
  \[
  (H\psi)^{(1)}(x) = -\frac{\hbar^2}{2m} \partial_x^2 \psi^{(1)}(x) + g \partial_y \psi^{(2)}(x, 0) \\
  (H\psi)^{(2)}(x, y) = -\frac{\hbar^2}{2m} \left( \partial_x^2 + \partial_y^2 \right) \psi^{(2)}(x, y) \quad \text{for} \ y > 0.
  \]

Theorem [Teufel, Tumulka 2015]

\( H \) is rigorously defined and self-adjoint on the dense-in-\( L^2(Q) \) domain

\[
D = \left\{(\psi^{(1)}, \psi^{(2)}): \psi^{(n)} \in H^2(Q^{(n)}) \ \forall n, \quad \psi^{(2)} \bigg|_{\mathbb{R} \times \{0\}} = -\frac{2mg}{\hbar^2} \psi^{(1)}\right\}.
\]

Probability balance equations:

\[
\begin{align*}
\partial_t |\psi^{(2)}|^2 &= -\partial_x j_x^{(2)} - \partial_y j_y^{(2)}, \\
\partial_t |\psi^{(1)}|^2 &= -\partial_x j_x^{(1)} + \frac{2g}{\hbar} \text{Im} \left[ \psi^{(1)}(x)^* \partial_y \psi^{(2)}(x, 0) \right] \\
&= -j_y^{(2)}(x, 0) \text{ by the IBC}
\end{align*}
\]
Consider again

- **x-particle at** 0 **emits and absorbs y-particles**, \( \mathcal{H} = \mathcal{F}_y^+ \)
- **IBC** \( \lim_{r \to 0} r \psi(y^n, r \omega) = \frac{g m}{2 \pi \hbar^2 \sqrt{n+1}} \psi(y^n) \) for all \( \omega \in S^2 \) (2)

\[
(H_{IBC} \psi)(y^n) = -\frac{\hbar^2}{2m} \nabla^2 \psi + \frac{g \sqrt{n+1}}{4\pi} \int_{S^2} d^2 \omega \lim_{r \to 0} \frac{\partial}{\partial r} \left( r \psi(y^n, r \omega) \right) \\
+ nE_0 \psi + \frac{g}{\sqrt{n}} \sum_{j=1}^{n} \delta^3(y_j) \psi(y^n \setminus y_j) \quad (3)
\]

IBC (2) ⇒ \( \psi \) typically diverges like \( 1/r = 1/|y_j| \) as \( y_j \to 0 \). In fact,

\[
\psi(y^n, r \omega) = c_{-1}(y^n) r^{-1} + c_0(y^n) r^0 + o(r^0)
\]

and (2) \( \Leftrightarrow \) \( c_{-1}(y^n) = \frac{g m}{2 \pi \hbar^2 \sqrt{n+1}} \psi(y^n) \)

(3) \( \Leftrightarrow \) \( (H \psi)(y^n) = -\frac{\hbar^2}{2m} \nabla^2 \psi + g \sqrt{n+1} c_0(y^n) \\
+ nE_0 \psi + \frac{g}{\sqrt{n}} \sum \delta^3(y_j) \psi(y^n \setminus y_j) \)
Rigorous absence of UV divergence in this model

- Note that $\nabla^2 \frac{1}{|y|} = -4\pi \delta^3(y)$ (cf. Poisson eq $\nabla^2 \phi = -4\pi \rho$).
- Thus, in $\nabla^2 \psi$ the $1/r$ divergent contribution to $\psi$ cancels the $\delta^3$!

**Theorem [Lampart, Schmidt, Teufel, Tumulka arxiv.org/abs/1703.04476]**

On a suitable dense domain $\mathcal{D}_{IBC}$ of $\psi$s in $\mathcal{H}$ satisfying the IBC (2), $H_{IBC}$ is well defined, self-adjoint, and positive. **No UV divergence!**
Why it works: flux of probability into a point

- probability current $j_y(y^n) = \frac{\hbar}{m} \text{Im} \psi^* \nabla_y \psi$

- $\frac{\partial |\psi(y^n)|^2}{\partial t} = - \sum_{j=1}^n \nabla_y \cdot j_y + (n+1) \lim_{r \downarrow 0} r^2 \int_{S^2} d^2 \omega \omega \cdot j_{y_{n+1}}(y^n, r\omega)$

- motion towards 0 $\Rightarrow$ 
  $\rho \sim 1/r^2$ as $r \to 0$
Bohmian picture

- $t \mapsto Q(t) \in Q$ piecewise continuous, jumps between $Q^{(n)}$ and $Q^{(n+1)}$
- within $Q^{(n)}$, Bohm's law of motion
  \[ \frac{dQ}{dt} = \frac{\hbar}{m_B} \text{Im} \frac{\nabla \psi^{(n)}}{\psi^{(n)}} (Q(t)) \]
  with IBC:
  - when $Q(t) \in Q^{(n)}$ reaches $y_j = 0$, it jumps to $(y^n \setminus y_j) \in Q^{(n-1)}$
  - emission of new $y$-particle at $0$ at random time with random direction
  - with UV cut-off:
    - emission and absorption occurs anywhere in a ball around $0$ (= in the support of $\varphi$)
Note that $H_{IBC}$ cannot be decomposed into a sum of two self-adjoint operators $H_{\text{free}} + H_{\text{interaction}}$.

That is because the domain $\mathcal{D}_{IBC}$ is different from the free domain $\mathcal{D}_{\text{free}}$.

The Laplacian is not self-adjoint on $\mathcal{D}_{IBC}$ (i.e., does not conserve probability) because it allows a nonzero flux of probability into the boundary

$$\partial Q^{(n+1)} = Q^{(n)} \times \{0\} \cup (\text{permutations thereof}) .$$

The additional terms in $H_{IBC}$ compensate that flux (by adding it to $Q^{(n)}$).
Ground state

Theorem [Lampart et al. 2017]

For $E_0 > 0$, $H_{IBC}$ possesses a non-degenerate ground state $\psi_0$, which is

$$\psi_0(y_1, \cdots, y_n) = \mathcal{N} \frac{(-g)^n}{(4\pi)^n \sqrt{n}} \prod_{j=1}^{n} \frac{e^{-\sqrt{2mE_0}|y_j|/\hbar}}{|y_j|}$$

with eigenvalue $E = g^2 m \sqrt{2mE_0}/\pi \hbar^3$.

That is, the $x$-particle is dressed with a cloud of $y$-particles.
Effective potential between x-particles

To compute effective interaction between x-particles by exchange of y-particles, consider

- 2 x-particles fixed at $x_1 = (0, 0, 0)$ and $x_2 = (R, 0, 0)$, $\mathcal{H} = \mathcal{F}_y^+$
- 2 IBCs, one at $x_1$ and one at $x_2$
- 2 creation and annihilation terms in $H_{IBC}$
- The ground state is

$$\psi_0 = c_n \prod_{j=1}^{n} \sum_{i=1}^{2} \frac{e^{-\sqrt{2mE_0}|y_j-x_i|/\hbar}}{|y_j-x_i|}$$

with eigenvalue

$$E = \frac{2g^2m}{\pi\hbar^2} \left( \frac{\sqrt{2mE_0}}{\hbar} - \frac{e^{-\sqrt{2mE_0}R/\hbar}}{R} \right)$$

- That is, x-particles effectively interact through an attractive Yukawa potential.
Consider again the scenario with 1 x-particle fixed at the origin, $\mathcal{H} = \mathcal{F}_y^+$. 

Consider $H_{\text{cutoff}} = H_\varphi$ with $\varphi = \delta^3$, limit $\varphi \to \delta^3$. Then there exist constants $E_\varphi \to \infty$ and a self-adjoint operator $H_\infty$ such that 

$$H_\varphi - E_\varphi \to H_\infty.$$ 

[van Hove 1952, Nelson 1964, see also Dereziński 2003]

**Theorem** [Lampart et al. 2017]

$$H_\infty = H_{IBC} + \text{const}$$
Moving sources

- Now: $x$-particles can move, config. space $Q = \bigcup_{m,n=0}^{\infty} (\mathbb{R}_x^3)^m \times (\mathbb{R}_y^3)^n$

- $\mathcal{H} = \mathcal{F}_x^- \otimes \mathcal{F}_y^+$, $\psi : Q \to \mathbb{C}$, $\psi = \psi(x^m, y^n)$

- The original Hamiltonian is UV divergent.

- IBC: $\lim_{(x_i, y_j) \to (x,x)} |x_i - y_j| \psi(x^m, y^n) = \alpha_{n-1} \psi(x_i = x, \hat{y}_j)$ (4)

with $\alpha_{n-1} = \frac{g}{2\pi\hbar^2 \sqrt{n} m_x + m_y}$. Here, “boundary” = diagonal; boundary config: where $x_i = y_j$; interior config: one $y$-particle removed

**Theorem** [Lampart and Schmidt arxiv.org/abs/1803.00872]

In 2d, $H_{IBC}$ is well defined and self-adjoint.

**Theorem** [Lampart arxiv.org/abs/1804.08295]

In 3d, $H_{IBC}$ is well defined and self-adjoint.
Now suppose that y-particles are relativistic and have spin $\frac{1}{2}$.

A free y-particle is governed by the Dirac equation

$$i\hbar \gamma^\mu \partial_\mu \psi = mc^2 \psi$$

or

$$i\hbar \frac{\partial \psi}{\partial t} = -i\hbar \mathbf{\alpha} \cdot \nabla \psi + mc^2 \beta \psi$$

$\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ for 1 particle
Example of a reflecting boundary condition for the Dirac equation

- \( Q = \mathbb{R}^3_+ = \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_3 \geq 0\} \) spatial domain with bdry
- \( \psi : \mathbb{R}_t \times \mathbb{R}^3_+ \to \mathbb{C}^4 \)
- current \( j^\mu = \overline{\psi} \gamma^\mu \psi \) or \( j^0 = |\psi|^2, \ j^i = \psi^\dagger \alpha^i \psi \)
- Dirac equation \( i \gamma^\mu \partial_\mu \psi = m \psi \) or \( i \partial_t \psi = (-i \alpha \cdot \nabla + \beta m) \psi \)
- \( \alpha, \beta, \gamma \) Dirac matrices; \( \alpha^i = \gamma^0 \gamma^i, \beta = \gamma^0 \) self-adjoint
- boundary condition (BC) \( (\gamma^3 - i)\psi(x_1, x_2, 0) = 0 \) or \( \alpha^3 \psi = i \beta \psi \)

Theorem [known]

The Dirac Hamiltonian is self-adjoint on a dense domain in \( L^2(\mathbb{R}^3_+, \mathbb{C}^4) \),
\( \mathcal{D} = \{ \psi \in H^1(\mathbb{R}^3_+, \mathbb{C}^4) : (\gamma^3 - i)\psi|_{\partial Q} = 0 \} \).

(BC) ensures there is no current into the boundary:

\[
j^3(x_1, x_2, 0) = \psi^\dagger \alpha^3 \psi = \frac{1}{2} \psi^\dagger (\alpha^3 \psi) + \frac{1}{2} (\alpha^3 \psi)^\dagger \psi
\]

\[
(BC) \quad = \frac{1}{2} \psi^\dagger (i \beta \psi) + \frac{1}{2} (i \beta \psi)^\dagger \psi = \frac{i}{2} \psi^\dagger \beta \psi - \frac{i}{2} \psi^\dagger \beta \psi = 0
\]
(BC) \((\gamma^3 - i)\psi = 0\) on \(\partial Q\)

\(\gamma^3\) is unitarily diagonalizable with eigenvalues \(\pm i\), each with multiplicity 2.

So, \(\gamma^3 - i\) is \(-2i\) times a 2d orthogonal projection.

So, \((\gamma^3 - i)\psi = 0\) sets two components of \(\psi\) to 0 and leaves two components arbitrary.

For comparison, the reflecting boundary conditions for the Laplacian,

\[
\begin{align*}
\psi(x_1, x_2, 0) &= 0 \quad \text{(Dirichlet)} \\
\partial_3 \psi(x_1, x_2, 0) &= 0 \quad \text{(Neumann)} \\
(\alpha + \beta \partial_3) \psi(x_1, x_2, 0) &= 0 \quad \text{(Robin)}
\end{align*}
\]

each set one component of the 2d pair \((\psi, \partial_3 \psi)\) to 0 and leave one component arbitrary.
Example of an interior-boundary condition for the Dirac equation

- configuration space $Q = Q^{(0)} \cup Q^{(1)} = \{\emptyset\} \cup \mathbb{R}^3$
- mini Fock space $\mathcal{H} = \mathcal{H}^{(0)} \oplus \mathcal{H}^{(1)} = \mathbb{C} \oplus L^2(\mathbb{R}_+^3, \mathbb{C}^4)$
- Hamiltonian

\[
(H\psi)^{(0)}(x) = \int_{\mathbb{R}^2} dx_1 \, dx_2 \, N(x_1, x_2)^\dagger \, \psi^{(1)}(x_1, x_2, 0)
\]

\[
(H\psi)^{(1)}(x) = -i\alpha \cdot \nabla \psi^{(1)}(x) + m\beta \psi^{(1)}(x), \quad x_3 > 0
\]

with $N(x_1, x_2) = e^{-x_1^2-x_2^2}(1, 0, 1, 0)$ in the Weyl representation

- $(\gamma^3 - i)\psi^{(1)}(x_1, x_2, 0) = (\gamma^3 - i)N(x_1, x_2)\psi^{(0)}$ (IBC)
- specifies two components of $\psi^{(1)}$ on $\partial Q$ and leaves two arbitrary
- $(\gamma^3 - i)\psi^{(1)}(x_1, x_2, 0) = 0$ reflecting BC to compare to.

Theorem [Schmidt, Teufel, Tumulka arxiv.org/abs/1811.02947]

$H$ is rigorously defined and self-adjoint on

\[
\{(\psi^{(0)}, \psi^{(1)}) \in \mathbb{C} \oplus H^1(\mathbb{R}_+^3, \mathbb{C}^4) : \text{(IBC)}\}\.
Model of creation of Dirac particles in 1d

[Lienert, Nickel
arxiv.org/abs/1808.04192]

- particles move in \( \mathbb{R}^1 \), split or coalesce according to \( x \rightleftharpoons x + x \).
- Dirac eq in 1d: spin space \( \mathbb{C}^2 \), \( \gamma^0 = \sigma_1 \), \( \gamma^1 = \sigma_1 \sigma_3 \).
- (truncated) Fock space
  \[ \mathcal{H} = \bigoplus_{n=0}^{N} S_- \mathcal{L}^2(\mathbb{R}^1, \mathbb{C}^2)^\otimes n \]
- For simplicity, let \( N = 2 \), \( m = 0 \), ignore the \( n = 0 \) sector, so \( \mathcal{H} = \mathcal{H}^{(1)} \oplus \mathcal{H}^{(2)} \).
- \((H\psi)^{(1)}(x) = -i\alpha^1 \partial_x \psi^{(1)}(x) + N(x)^{\dagger} \psi^{(2)}(x, x)\)
  \((H\psi)^{(2)}(x_1, x_2) = (-i\alpha^1_1 \partial_1 - i\alpha^1_2 \partial_2) \psi^{(2)}(x_1, x_2)\)
  with \( N(x) \) a certain \( 4 \times 2 \)-matrix.
- IBC \( \psi^{(2)}_{-+}(x, x) - e^{i\theta} \psi^{(2)}_{+-}(x, x) = B \psi^{(1)}(x)\)
  with \( B \) a certain \( 1 \times 2 \)-matrix.
Model with IBC for Dirac eq in 1d

Theorem [Lienert, Nickel arxiv.org/abs/1808.04192]

$$H_{IBC}$$ is well defined and self-adjoint.

They even gave a multi-time formulation and proved consistency of the multi-time equations.
Difficulty with Dirac operators in 3d

The Laplacian allows for BCs at a point:

\[ \text{Theorem [known]} \]
There exist several self-adjoint extensions of
\[ (H^\circ, \mathcal{D}(H^\circ)) = (-\nabla^2, C^\infty_\circ(\mathbb{R}^3 \setminus \{0\}, \mathbb{C})). \]

Not so for the Dirac Hamiltonian:

\[ \text{Theorem [Svendsen 1981]} \]
There is only one self-adjoint extension of
\[ (H^\circ, \mathcal{D}(H^\circ)) = (-i\mathbf{\alpha} \cdot \nabla + m\mathbf{\beta}, C^\infty_\circ(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4)), \]
the free Dirac Hamiltonian.

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This has consequences for IBCs:

**Fact**

The non-relativistic $H_{IBC}$ in $\mathbb{C} \oplus L^2(\mathbb{R}^3)$ with source at $0$ is a self-adjoint extension of the operator $H^\circ(\psi(0) = 0, \psi(1)) = (0, -\frac{\hbar^2}{2m} \nabla^2 \psi(1))$ defined on $\mathcal{D}(H^\circ) = \{0\} \oplus C^\infty_c(\mathbb{R}^3 \setminus \{0\}, \mathbb{C})$.

whereas

**Theorem**  [Henheik, Tumulka arxiv.org/abs/2006.16755]

All self-adjoint extensions in $\mathbb{C} \oplus L^2(\mathbb{R}^3, \mathbb{C}^4)$ of the operator $H^\circ(\psi(0) = 0, \psi(1)) = (0, (-i\alpha \cdot \nabla + m\beta)\psi(1))$ defined on $\mathcal{D}(H^\circ) = \{0\} \oplus C^\infty_c(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4)$ involve no particle creation and are the free Dirac operator on the upper sector.

In short, there is no IBC Hamiltonian for Dirac particles and a point source in 3d, unless...
...we add a Coulomb potential

Theorem [Henheik, Tumulka arxiv.org/abs/2006.16755]

Let $H^\circ = -i\alpha \cdot \nabla + m\beta + q/|x|$ with $\sqrt{3}/2 < |q| < 1$ be defined on $\mathcal{D}^\circ = \{0\} \oplus C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4)$. Set $B := \sqrt{1 - q^2} \in (0, \frac{1}{2})$, let $0 \neq g \in \mathbb{R}$. There is a self-adjoint extension $(H, \mathcal{D})$ of $(H^\circ, \mathcal{D}^\circ)$ with

1. The sectors $\mathbb{C} \oplus L^2(\mathbb{R}^3, \mathbb{C}^4)$ do not decouple (i.e., creation occurs).
2. For every $\psi \in \mathcal{D}$, the upper sector is of the form $\psi^{(1)}(x) =
   \begin{align*}
   c_{-1} f_{-1}(\frac{x}{|x|}) |x|^{-1-B} + \left( \sum_{k=0}^{3} c_k f_k(\frac{x}{|x|}) \right) |x|^{-1+B} + o(|x|^{-1/2})
   \end{align*}$

   as $x \to 0$ with $c_{-1} \ldots c_3 \in \mathbb{C}$ and particular fcts $f_{-1} \ldots f_3 : \mathbb{S}^2 \to \mathbb{C}^4$.
3. Every $\psi \in \mathcal{D}$ obeys IBC $c_{-1} = g \psi^{(0)}$ ($g \in \mathbb{R}$)
4. For $\psi \in \mathcal{D}$, $(H\psi)^{(0)} = g c_0$
   
   $(H\psi)^{(1)}(x) = (-i\alpha \cdot \nabla + m\beta + \frac{q}{|x|})\psi^{(1)}$ ($x \neq 0$).

In short, IBCs at $0$ for the 3d Dirac operator are possible with sufficiently strong Coulomb potential.
Further works

- Tumulka arxiv.org/abs/1808.06262: General form of IBCs
- Dürr, Goldstein, Teufel, Tumulka, and Zanghì arxiv.org/abs/1809.10235: Bohmian trajectories for IBCs
- Schmidt and Tumulka arxiv.org/abs/1810.02173: Time reversal of IBCs
- Schmidt arxiv.org/abs/1810.03313: IBCs for $\sqrt{m^2 - \nabla^2}$
- Schmidt, Teufel, and Tumulka arxiv.org/abs/1811.02947: General form of IBCs for the Dirac eq and codim-1 boundaries
- Henheik, Tumulka work in progress: Bohmian trajectories for $H_{IBC}$ for 3d Dirac eq with Coulomb potential
Features of the novel approach

Problem:
- Hamiltonian involving particle creation and annihilation is usually UV divergent, and thus ill defined

New approach:
- IBC = interior–boundary condition
- allows a new way of defining a Hamiltonian $H_{IBC}$
- provides rigorous definition of a self-adjoint $H_{IBC}$, at least for some scenarios (and we hope in many)
- no need for discretizing space, smearing out particles over positive radius, or other UV cut-off
- no need for renormalization, or taking limit of removing the UV cut-off
- makes use of particle–position representation
Thank you for your attention