Interior-Boundary Conditions and Their Physical Meaning

Roderich Tumulka

EBERHARD KARLS UNIVERSITÄT TÜBINGEN

Mathematical physics colloquium
Tübingen, 2 December 2024

Schrödinger equation of non-relativistic QM

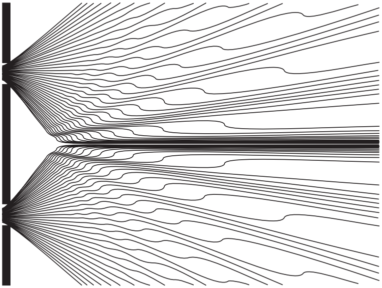
configuration space $\mathcal{Q} = \mathbb{R}^{3N}$, $\psi : \mathcal{Q} \times \mathbb{R}_t \to \mathbb{C}$

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

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

Born's rule

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

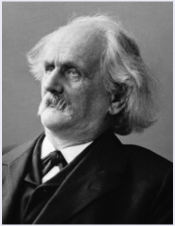


$\psi_t \in \mathscr{H} = L^2(\mathcal{Q}, \mathbb{C})$
$U_t : \mathscr{H} \to \mathscr{H}$ is unitary
$\Leftarrow H$ is self-adjoint
prob. current $\boldsymbol{j} = \frac{\hbar}{m}\mathrm{Im}[\psi^* \nabla \psi]$
$\frac{\partial \rho}{\partial t} + \nabla \cdot \boldsymbol{j} = 0$ continuity equation

Boundary conditions for the Schrödinger equation

- $\mathcal{Q} = [0,1]$
- for time evolution, PDE is not enough: also need boundary conditions (BCs) such as

$$\psi(0,t) = 0 \;\forall t \text{ (Dirichlet)},$$
$$\frac{\partial\psi}{\partial x}(1,t) = 0 \;\forall t \text{ (Neumann)} \qquad (1)$$



Carl Neumann

- built into the domain $\mathscr{D}$ of the Hamiltonian: $H = -\frac{\hbar^2}{2m}\nabla^2$,
  $\mathscr{D} = \left\{\psi \in L^2([0,1]) : \nabla^2\psi \in L^2([0,1]), \psi \text{ satisfies (1)}\right\}$
- (1) are reflecting boundary conditions: they make $(H, \mathscr{D})$ 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):

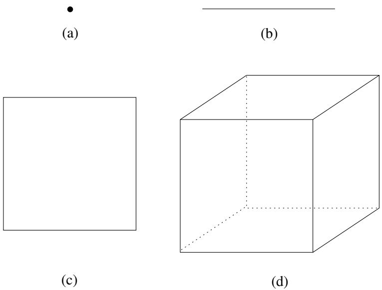
$$\alpha \frac{\partial\psi}{\partial x} + \beta\,\psi(x) = 0$$

Particle-position representation of a Fock space vector

Configuration space of a variable number of particles:

$$\mathcal{Q} = \bigcup_{n=0}^{\infty} \mathbb{R}^{3n}$$

$$= \bigcup_{n=0}^{\infty} \mathcal{Q}^{(n)}$$



here $d = 1$,
$n = 0, 1, 2, 3$

Fock space:

- $\mathscr{F}^{\pm} = \bigoplus_{n=0}^{\infty} S_{\pm} \mathscr{H}_1^{\otimes n}$
  with S_+ = symmetrizer, S_- = anti-symmetrizer, $\mathscr{H}_1$ = 1-particle Hilbert space = $L^2(\mathbb{R}^3, \mathbb{C}^k)$
- $\psi \in \mathscr{F} \Rightarrow \psi = \big(\psi^{(0)}, \psi^{(1)}, \psi^{(2)}, \ldots\big)$
- $\psi : \mathcal{Q} \to S$ with S = value space = $\cup_{n=0}^{\infty} (\mathbb{C}^k)^{\otimes n}$
- ψ is an (anti-)symmetric function

UV divergence problem

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

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

Original Hamiltonian in the particle-position representation:

$$
\begin{aligned}
(H_{\mathrm{orig}}\psi)^{(n)}(\boldsymbol{y}_1 \ldots \boldsymbol{y}_n) = &-\frac{\hbar^2}{2m_y} \sum_{j=1}^{n} \nabla^2_{\boldsymbol{y}_j} \psi^{(n)}(\boldsymbol{y}_1 \ldots \boldsymbol{y}_n) + nE_0 \psi^{(n)} \\
&+ g\sqrt{n+1}\, \psi^{(n+1)}(\boldsymbol{y}_1 \ldots \boldsymbol{y}_n, \boldsymbol{0}) \\
&+ \frac{g}{\sqrt{n}} \sum_{j=1}^{n} \delta^3(\boldsymbol{y}_j)\, \psi^{(n-1)}(\boldsymbol{y}_1 \ldots \widehat{\boldsymbol{y}}_j \ldots \boldsymbol{y}_n),
\end{aligned}
$$

is UV divergent. ($\widehat{\ }$ = omit, $E_0 \geq 0$ energy needed for creating y)

Well-defined, "regularized" version of H

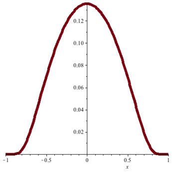
UV cut-off $\varphi \in L^2(\mathbb{R}^3)$:

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

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

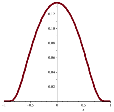
$$+ \; \frac{g}{\sqrt{n}}\sum_{i=1}^{m}\sum_{j=1}^{n}\varphi(\boldsymbol{y}_j)\,\psi\big(\boldsymbol{y}_1 \dots \widehat{\boldsymbol{y}}_j \dots \boldsymbol{y}_n\big)$$

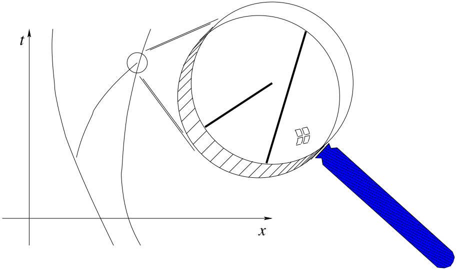
"smearing out" the x-particle with "charge distribution" $\varphi(\cdot)$



But then . . .

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

$\varphi =$ )



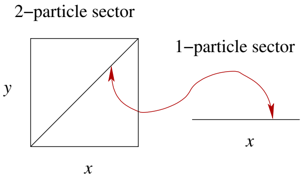
- There is no empirical evidence that an electron has positive radius.
- Positive radius leads to difficulties with Lorentz invariance.

This UV problem can be solved!

[Teufel and Tumulka 1505.04847, 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 $\mathbf{0}$,

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

with $y^n = (\boldsymbol{y}_1, \dots, \boldsymbol{y}_n)$.

A derivation of an IBC in 1d

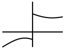
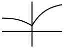
due to [Keppeler and Sieber 1511.03071]

for simplicity in a truncated Fock space

$$\mathscr{H} = \bigoplus_{n=0}^{1} S_+ \mathscr{H}_1^{\otimes n} = \mathbb{C} \oplus \mathscr{H}_1 = \mathbb{C} \oplus L^2(\mathbb{R}).$$

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

$$\partial_y^2 \psi^{(1)}(y) = 2mg\,\delta(y)\,\psi^{(0)} + f(y) \text{ with } f \in L^2$$

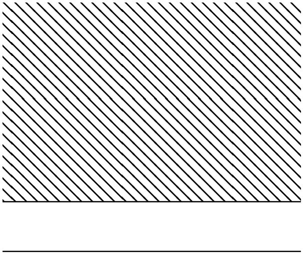
$\partial_y \phi(y) = \delta(y) \Rightarrow$ jump , likewise $\partial_y^2 \phi(y) = \delta(y) \Rightarrow$ kink 

so $\mathscr{D} = \Big\{ (\psi^{(0)}, \psi^{(1)}) : \partial_y \psi^{(1)}(0+) - \partial_y \psi^{(1)}(0-) = 2mg\psi^{(0)}$ and away from 0, $\nabla^2 \psi^{(1)} \in L^2 \Big\}$

and $H(\psi^{(0)}, \psi^{(1)}) = (g\psi^{(1)}(0), -\frac{1}{2m}\nabla^2 \psi^{(1)}$ away from 0$)$

The basic idea of IBCs: a toy example

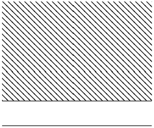
Consider quantum mechanics on a space $\mathcal{Q}$ with a boundary $\partial\mathcal{Q}$.



- E.g.,
  $\mathcal{Q} = \mathcal{Q}^{(1)} \cup \mathcal{Q}^{(2)} = \mathbb{R} \cup \big(\mathbb{R} \times [0,\infty)\big)$
  $\partial\mathcal{Q} = \partial\mathcal{Q}^{(2)} = \mathbb{R} \times \{0\}$
- Consider probability current vector field j on $\mathcal{Q}$.
- Suppose j has nonzero flux into $\partial\mathcal{Q}$, $0 \neq \int_{\partial\mathcal{Q}} dx\, j \cdot n$ ($n =$ normal to $\partial\mathcal{Q}$)
- We want the prob that disappears at $q \in \partial\mathcal{Q}$ to reappear at $f(q) \in \mathcal{Q}$.

- E.g., what disappears at $(x,0) \in \partial\mathcal{Q}^{(2)}$ reappears at $f(x,0) = x$, so $f : \partial\mathcal{Q}^{(2)} \to \mathcal{Q}^{(1)}$. In general, $f : \partial\mathcal{Q} \to \mathcal{Q}$.
- This is achieved through
  - $\to$ an extra term in H for $\mathcal{Q}^{(1)}$
  - $\to$ an interior-boundary condition $\psi(q) = (\text{const.})\, \psi(f(q))$

IBC in the toy example



- $\psi_t : \mathcal{Q} \to \mathbb{C}, \quad \psi = (\psi^{(1)}, \psi^{(2)})$
- $g \in \mathbb{R}$ coupling constant
- IBC: $\psi^{(2)}(x,0) = -\frac{2mg}{\hbar^2}\, \psi^{(1)}(x)$
- Hamiltonian:

$$(H\psi)^{(1)}(x) = -\frac{\hbar^2}{2m}\partial_x^2\psi^{(1)}(x) + g\,\partial_y\psi^{(2)}(x,0)$$

$$(H\psi)^{(2)}(x,y) = -\frac{\hbar^2}{2m}\Big(\partial_x^2 + \partial_y^2\Big)\psi^{(2)}(x,y) \quad \text{for } y > 0\,.$$

Theorem [Teufel and Tumulka 1506.00497]

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

$$\mathscr{D} = \Big\{(\psi^{(1)}, \psi^{(2)}) : \psi^{(n)} \in H^2(\mathcal{Q}^{(n)})\ \forall n, \quad \psi^{(2)}\Big|_{\mathbb{R}\times\{0\}} = -\frac{2mg}{\hbar^2}\psi^{(1)}\Big\}.$$

Probability balance equations:

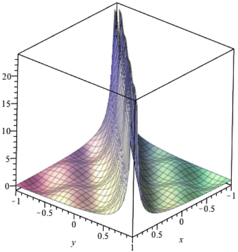
$$\partial_t|\psi^{(2)}|^2 = -\partial_x j_x^{(2)} - \partial_y j_y^{(2)},$$

$$\partial_t|\psi^{(1)}|^2 = -\partial_x j_x^{(1)} + \underbrace{\frac{2g}{\hbar}\,\mathrm{Im}\Big[\psi^{(1)}(x)^*\,\partial_y\psi^{(2)}(x,0)\Big]}_{= -j_y^{(2)}(x,0) \text{ by the IBC}}$$

IBC for particle creation model

Consider again

- x-particle at **0** emits and absorbs y-particles, $\mathscr{H} = \mathscr{F}_y^+$
- IBC $\quad \lim_{r\to 0+} r\psi(y^n, r\boldsymbol{\omega}) = \frac{gm}{2\pi\hbar^2\sqrt{n+1}}\,\psi(y^n)$ for all $\boldsymbol{\omega}\in\mathbb{S}^2$ (2)
- $$(H_{IBC}\psi)(y^n) = -\frac{\hbar^2}{2m}\nabla^2\psi + \frac{g\sqrt{n+1}}{4\pi}\int_{\mathbb{S}^2} d^2\boldsymbol{\omega}\,\lim_{r\to 0+}\partial_r\Big(r\psi(y^n, r\boldsymbol{\omega})\Big) + nE_0\psi + \frac{g}{\sqrt{n}}\sum_{j=1}^{n}\delta^3(\boldsymbol{y}_j)\,\psi(y^n\setminus\boldsymbol{y}_j) \quad (3)$$



IBC (2) $\Rightarrow$ ψ typically diverges like $1/r = 1/|\boldsymbol{y}_j|$ as $\boldsymbol{y}_j\to\mathbf{0}$. In fact,

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

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

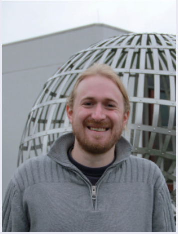
(3) $\Leftrightarrow$ $(H\psi)(y^n) = -\frac{\hbar^2}{2m}\nabla^2\psi + g\sqrt{n+1}\,c_0(y^n) + nE_0\psi + \frac{g}{\sqrt{n}}\sum\delta^3(\boldsymbol{y}_j)\,\psi(y^n\setminus\boldsymbol{y}_j)$

Rigorous absence of UV divergence in this model

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

Theorem [Lampart, Schmidt, Teufel, Tumulka 1703.04476]

On a suitable dense domain $\mathscr{D}_{IBC}$ of ψs in $\mathscr{H}$ satisfying the IBC (2), H_{IBC} is well defined, self-adjoint, and positive.
No UV divergence!

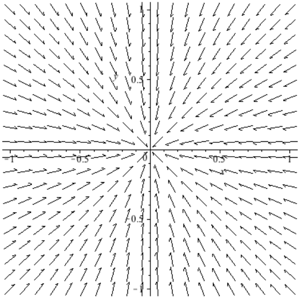


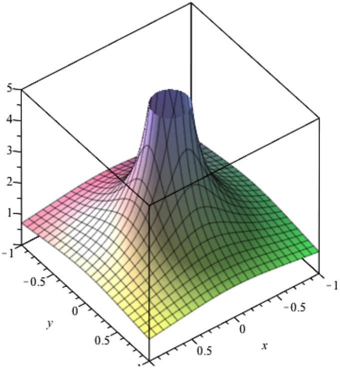
Jonas Lampart

Julian Schmidt

Why it works: flux of probability into a point

- probability current $\boldsymbol{j}_{\boldsymbol{y}_j}(y^n) = \frac{\hbar}{m} \mathrm{Im}\, \psi^* \nabla_{\boldsymbol{y}_j} \psi$
- $$\frac{\partial |\psi(y^n)|^2}{\partial t} = -\sum_{j=1}^{n} \nabla_{\boldsymbol{y}_j} \cdot \boldsymbol{j}_{\boldsymbol{y}_j} + (n+1) \lim_{r \to 0+} \underbrace{r^2 \int_{\mathbb{S}^2} d^2\boldsymbol{\omega}\, \boldsymbol{\omega} \cdot \boldsymbol{j}_{\boldsymbol{y}_{n+1}}(y^n, r\boldsymbol{\omega})}_{\text{flux into } \mathbf{0} \text{ on } (n+1)\text{-sector}}$$
- motion towards $\mathbf{0}$ $\Rightarrow$ $\rho \sim 1/r^2$ as $r \to 0$



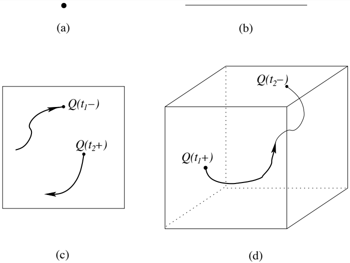


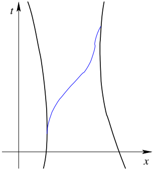
Bohmian picture

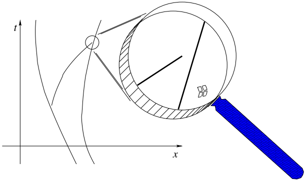
- $t \mapsto Q(t) \in \mathcal{Q}$ piecewise continuous, jumps between $\mathcal{Q}^{(n)}$ and $\mathcal{Q}^{(n+1)}$
- within $\mathcal{Q}^{(n)}$, Bohm's law of motion

$$\frac{dQ}{dt} = \frac{\hbar}{m_B} \mathrm{Im} \frac{\nabla\psi^{(n)}}{\psi^{(n)}}(Q(t))$$

- with IBC:
- when $Q(t) \in \mathcal{Q}^{(n)}$ reaches $\boldsymbol{y}_j = \mathbf{0}$, it jumps to $(y^n \setminus \boldsymbol{y}_j) \in \mathcal{Q}^{(n-1)}$
- emission of new y-particle at $\mathbf{0}$ at random time with random direction
- with UV cut-off:
- emission and absorption occurs anywhere in a ball around $\mathbf{0}$ (= in the support of φ )







Now Dirac operators instead of $-\nabla^2$

- Now suppose that y-particles are relativistic and have spin $\frac{1}{2}$.
- A free y-particle is described by the Dirac equation

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

or

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

- $\mathscr{H}_1 = L^2(\mathbb{R}^3, \mathbb{C}^4)$ for 1 particle
- Henceforth, $\hbar = 1 = c$.

Example of a reflecting boundary condition for the Dirac equation

- $\mathcal{Q} = \mathbb{R}^3_> = \{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_3 \geq 0\}$ 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 $i\partial_t\psi = (-i\boldsymbol{\alpha}\cdot\nabla + \beta m)\psi$
- α, β, γ 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 $L^2(\mathbb{R}^3_>, \mathbb{C}^4)$, $\mathscr{D} = \{\psi \in H^1(\mathbb{R}^3_>, \mathbb{C}^4) : (\gamma^3 - i)\psi\big|_{\partial\mathcal{Q}} = 0\}$.

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

$$j^3(x_1, x_2, 0) = \psi^\dagger\alpha^3\psi = \tfrac{1}{2}\psi^\dagger(\alpha^3\psi) + \tfrac{1}{2}(\alpha^3\psi)^\dagger\psi$$

$$\overset{(BC)}{=} \tfrac{1}{2}\psi^\dagger(i\beta\psi) + \tfrac{1}{2}(i\beta\psi)^\dagger\psi = \tfrac{i}{2}\psi^\dagger\beta\psi - \tfrac{i}{2}\psi^\dagger\beta\psi = 0$$

BC specifies half of the components

- (BC) $(\gamma^3 - i)\psi = 0$ on $\partial\mathcal{Q}$
- γ^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 ψ to 0 and leaves two components arbitrary.
- For comparison, the reflecting boundary conditions for the Laplacian,

$$\psi(x_1, x_2, 0) = 0 \text{ (Dirichlet)}$$
$$\partial_3\psi(x_1, x_2, 0) = 0 \text{ (Neumann)}$$
$$(\alpha + \beta\partial_3)\psi(x_1, x_2, 0) = 0 \text{ (Robin)}$$

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

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

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

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

Theorem [Schmidt, Teufel, Tumulka 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 and Nickel 1808.04192]

- particles move in $\mathbb{R}^1$, split or coalesce according to $x \leftrightarrows x + x$.
- Dirac eq in 1d: spin space $\mathbb{C}^2$, $\gamma^0 = \sigma_1$, $\gamma^1 = \sigma_1 \sigma_3$.
- (truncated) Fock space $\mathscr{H} = \bigoplus_{n=0}^{n_{\max}} S_- \, L^2(\mathbb{R}^1, \mathbb{C}^2)^{\otimes n}$

M. Lienert

Lukas Nickel

- For simplicity, let $n_{\max} = 2$, $m = 0$, ignore the $n = 0$ sector, so $\mathscr{H} = \mathscr{H}^{(1)} \oplus \mathscr{H}^{(2)}$.
- $(H\psi)^{(1)}(x) = -i\alpha^1 \partial_x \psi^{(1)}(x) + N(x)^\dagger \, \psi^{(2)}(x,x)$
  $(H\psi)^{(2)}(x_1,x_2) = (-i\alpha_1^1 \partial_1 - i\alpha_2^1 \partial_2)\psi^{(2)}(x_1,x_2)$
  with $N(x)$ a certain 4×2-matrix.
- IBC $\quad \psi^{(2)}_{-+}(x,x) - e^{i\theta} \psi^{(2)}_{+-}(x,x) = B \, \psi^{(1)}(x)$
  with B a certain 1×2-matrix.

Model with IBC for Dirac eq in 1d

Theorem [Lienert and Nickel 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:

Theorem [known]

There exist several self-adjoint extensions of
$(H^\circ, \mathscr{D}(H^\circ)) = (-\nabla^2, C_c^\infty(\mathbb{R}^3 \setminus \{\mathbf{0}\}, \mathbb{C}))$.

Not so for the Dirac Hamiltonian:

Theorem [Svendsen 1981]

There is only one self-adjoint extension of
$(H^\circ, \mathscr{D}(H^\circ)) = (-i\boldsymbol{\alpha} \cdot \nabla + m\beta, C_c^\infty(\mathbb{R}^3 \setminus \{\mathbf{0}\}, \mathbb{C}^4))$,
the free Dirac Hamiltonian.

This has consequences for IBCs:

Fact

The non-relativistic H_{IBC} in $\mathbb{C} \oplus L^2(\mathbb{R}^3)$ with source at $\mathbf{0}$ 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 $\mathscr{D}(H^\circ) = \{0\} \oplus C_c^\infty(\mathbb{R}^3 \setminus \{\mathbf{0}\}, \mathbb{C})$.

whereas

Theorem [Henheik and Tumulka 2006.16755]

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

Joscha Henheik

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

...we add a Coulomb potential...

Theorem [Henheik and Tumulka 2006.16755]

Let $H^\circ = -i\boldsymbol{\alpha}\cdot\nabla + m\beta + q/|\boldsymbol{y}|$ with $\sqrt{3}/2 < |q| < 1$ be defined on $\mathscr{D}^\circ = \{0\} \oplus C_c^\infty(\mathbb{R}^3 \setminus \{\mathbf{0}\}, \mathbb{C}^4)$. Set $B := \sqrt{1-q^2}$; note that $0 < B < \frac{1}{2}$. There is a self-adjoint extension $(H, \mathscr{D})$ of $(H^\circ, \mathscr{D}^\circ)$ 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 $\psi \in \mathscr{D}$, the upper sector is of the form

$$\psi^{(1)}(\boldsymbol{y}) = c_{-B}\, f_-\Big(\tfrac{\boldsymbol{y}}{|\boldsymbol{y}|}\Big)\, |\boldsymbol{y}|^{-B} + c_B\, f_+\Big(\tfrac{\boldsymbol{y}}{|\boldsymbol{y}|}\Big)\, |\boldsymbol{y}|^{B} + o(|\boldsymbol{y}|^{1/2}) \qquad (5)$$

   as $\boldsymbol{y} \to \mathbf{0}$ with $c_{-B}, c_B \in \mathbb{C}$ and fixed functions $f_\pm : \mathbb{S}^2 \to \mathbb{C}^4$.
3. Every $\psi \in \mathscr{D}$ obeys IBC $\quad c_{-B} = g\,\psi^{(0)}$
4. For $\psi \in \mathscr{D}$, $\quad (H\psi)^{(0)} = \tilde{g}\, c_B$

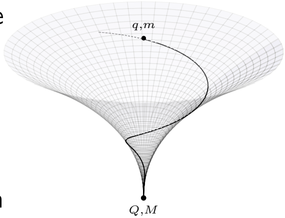
$$(H\psi)^{(1)}(\boldsymbol{y}) = \Big(-i\boldsymbol{\alpha}\cdot\nabla + m\beta + \tfrac{q}{|\boldsymbol{y}|}\Big)\psi^{(1)}(\boldsymbol{y}) \qquad (\boldsymbol{y} \neq \mathbf{0})$$

   with constants $g, \tilde{g} = 4B(1+q)g^*$.

...or have a space-time singularity

[Tumulka 0708.0070]

According to general relativity, the curved space-time created by a point with mass $M > 0$ and charge $Q > M$ is the Reissner-Nordström geometry



$$ds^2 = \lambda(r)\,dt^2 - \frac{1}{\lambda(r)}\,dr^2 - r^2\,d\vartheta^2 - r^2\sin^2\vartheta\,d\varphi^2$$

with $\lambda(r) = 1 - \frac{2M}{r} + \frac{Q^2}{r^2}$. Its metric is static in coordinates $(t, r, \vartheta, \varphi)$ and has singularity at $r = 0$.

- Dirac spin spaces form a vector bundle S with fibers $S_x \cong \mathbb{C}^4$.
- The metric defines a covariant derivative on S.
- $\mathscr{H}_1 = L^2$ sections of S over $\Sigma = \{t = \text{const.}\}$.
- Let H_1 be the free Dirac operator (depends on the curved metric).

IBC works with a space-time singularity

Theorem [Henheik, Poudyal, Tumulka 2409.00677]

Let $H^\circ = 0 \oplus H_1$ on $\mathscr{D}^\circ = \{0\} \oplus C_c^\infty(\Sigma \setminus \{\mathbf{0}\}, S)$. There is a self-adjoint extension $(H, \mathscr{D})$ of $(H^\circ, \mathscr{D}^\circ)$ with

1. The sectors $\mathbb{C} \oplus L^2(\Sigma, S)$ do not decouple (i.e., creation occurs).
2. For every $\psi \in \mathscr{D}$, the upper sector is of the form
$$\psi^{(1)}(r,\vartheta,\varphi) = c(\vartheta,\varphi)\, r^{-1/2} + \mathcal{O}(r^{1/2}) \quad \text{as } r \to 0.$$
3. Every $\psi \in \mathscr{D}$ obeys IBC
$$\tfrac{1}{2}(I - \beta)\, c(\vartheta,\varphi) = f_-(\vartheta,\varphi)\, \psi^{(0)}$$
with fixed functions $f_\pm : \mathbb{S}^2 \to \mathbb{C}^4$.
4. For $\psi \in \mathscr{D}$,
$$(H\psi)^{(0)} = \langle f_+, c\rangle_{L^2(\mathbb{S}^2,\mathbb{C}^4)}$$
$$(H\psi)^{(1)} = H_1\psi^{(1)} \quad \text{for } r > 0$$

Bipul Poudyal

Summary: 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