Interior-Boundary Conditions for Schrödinger Equations

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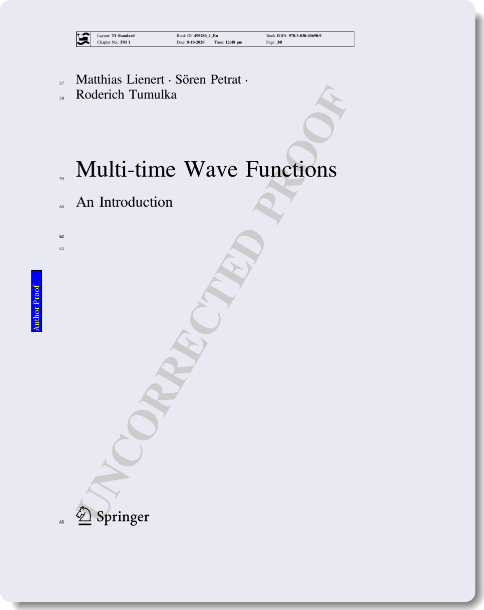
Upcoming book



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Multi-time Wave Functions

An Introduction

Author Proof

Springer

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Schrödinger equation of non-relativistic QM

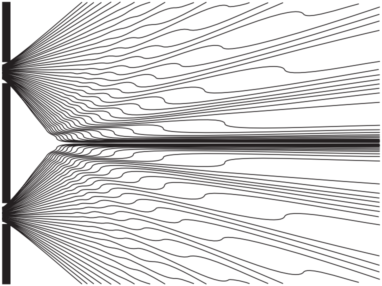
configuration space $\mathcal{Q} = \mathbb{R}^{3N}$, $\psi : \mathcal{Q} \times \mathbb{R}_t \to \mathbb{C}$

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

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

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

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

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

- built into the domain $\mathscr{D}$ of the Hamiltonian H: $H = -\frac{\hbar^2}{2m}\nabla^2$,

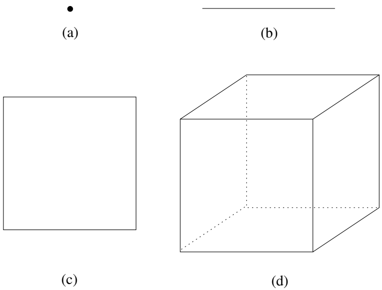
  $\mathscr{D} = \{\psi \in L^2([0,1]) : \nabla^2\psi \in L^2([0,1]), \psi \text{ satisfies (1)}\}$
- (1) are reflecting boundary conditions: make $(H, \mathscr{D})$ self-adjoint $\Rightarrow$ $U_t = e^{-iHt/\hbar}$ unitary $\Rightarrow$ no loss of probability
- Likewise for Robin BC ($\alpha, \beta \neq (0,0)$ 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

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. $\mathscr{H} = \mathscr{F}_y^+$
- 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

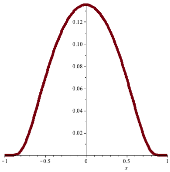
UV cut-off $\varphi \in L^2(\mathbb{R}^3)$:

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

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

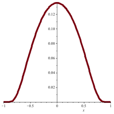
$$+ \; \frac{g}{\sqrt{n}}\sum_{i=1}^{m}\sum_{j=1}^{n}\varphi(\boldsymbol{y}_j)\,\psi(\boldsymbol{y}_1 \ldots \widehat{\boldsymbol{y}_j} \ldots \boldsymbol{y}_n)$$

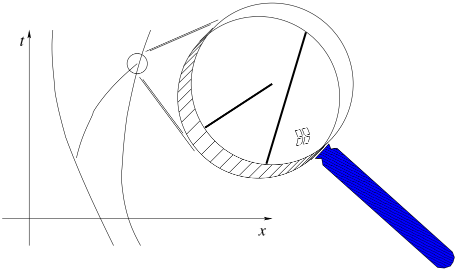
"smearing out" the x-particle
with "charge distribution" $\varphi(\cdot)$



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.

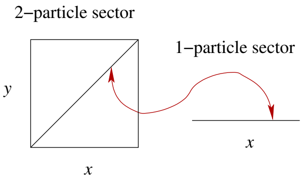
This UV problem can be solved!

[Teufel and Tumulka arxiv.org/abs/1505.04847, arxiv.org/abs/1506.00497]

Stefan Teufel

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

A derivation of an IBC in 1d

Stefan Keppeler

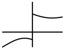
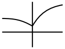
due to [Keppeler and Sieber arxiv.org/abs/1511.03071]

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

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

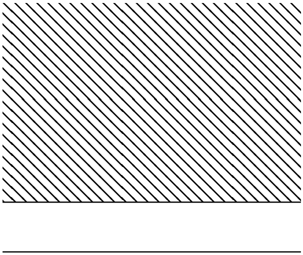
$\phi'(y) = \delta(y) \Rightarrow$ jump , likewise $\phi''(y) = \delta(y) \Rightarrow$ kink 

so $D = \Big\{(\psi^{(0)}, \psi^{(1)}) : \psi^{(1)\prime}(0+) - \psi^{(1)\prime}(0-) = 2mg\psi^{(0)}$ 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

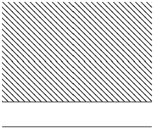
Consider quantum mechanics on a space $\mathcal{Q}$ with a boundary $\partial\mathcal{Q}$.



- 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: $\quad \psi^{(2)}(x,0) = -\frac{2mg}{\hbar^2}\, \psi^{(1)}(x)$
- 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, Tumulka 2015]

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:

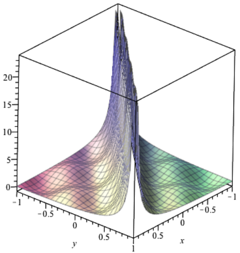
$$\partial_t|\psi^{(2)}|^2 = -\partial_x j_x^{(2)} - \partial_y j_y^{(2)},$$

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

IBC for particle creation model

Consider again

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



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 arxiv.org/abs/1703.04476]

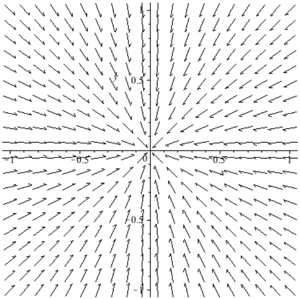
On a suitable dense domain $\mathscr{D}_{IBC}$ of ψs in $\mathscr{H}$ satisfying the IBC (2), H_{IBC} is well defined, self-adjoint, and positive.
No UV divergence!

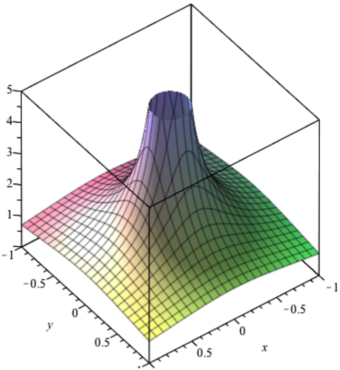
Jonas Lampart

Julian Schmidt

Why it works: flux of probability into a point

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

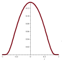


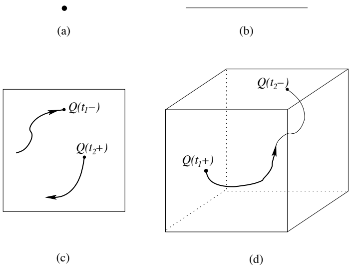


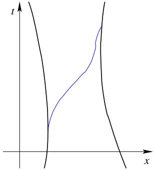
Bohmian picture

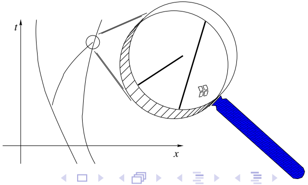
- $t \mapsto Q(t) \in \mathcal{Q}$ piecewise continuous, jumps between $\mathcal{Q}^{(n)}$ and $\mathcal{Q}^{(n+1)}$
- within $\mathcal{Q}^{(n)}$, Bohm's law of motion

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

- with IBC:
- when $Q(t) \in \mathcal{Q}^{(n)}$ reaches $\boldsymbol{y}_j = \boldsymbol{0}$, 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 )







H_{IBC} is not a perturbation of H_{free}

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

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

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

Ground state

Theorem [Lampart et al. 2017]

For $E_0 > 0$, H_{IBC} possesses a non-degenerate ground state ψ_0, which is

$$\psi_0(\boldsymbol{y}_1, \ldots, \boldsymbol{y}_n) = \mathcal{N} \frac{(-g)^n}{(4\pi)^n \sqrt{n}} \prod_{j=1}^{n} \frac{e^{-\sqrt{2mE_0}|\boldsymbol{y}_j|/\hbar}}{|\boldsymbol{y}_j|}$$

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 $\boldsymbol{x}_1 = (0,0,0)$ and $\boldsymbol{x}_2 = (R,0,0)$, $\mathscr{H} = \mathscr{F}_y^+$
- 2 IBCs, one at $\boldsymbol{x}_1$ and one at $\boldsymbol{x}_2$
- 2 creation and annihilation terms in H_{IBC}
- The ground state is

$$\psi_0 = c_n \prod_{j=1}^{n} \sum_{i=1}^{2} \frac{e^{-\sqrt{2mE_0}|\boldsymbol{y}_j - \boldsymbol{x}_i|/\hbar}}{|\boldsymbol{y}_j - \boldsymbol{x}_i|}$$

  with eigenvalue

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

- That is, x-particles effectively interact through an attractive Yukawa potential.

Comparison to renormalization procedure

- Consider again the scenario with 1 x-particle fixed at the origin, $\mathscr{H} = \mathscr{F}_y^+$.
- Consider $H_{\mathrm{cutoff}} = H_\varphi$ with $\varphi =$ , limit $\varphi \to \delta^3$.
- Then there exist constants $E_\varphi \to \infty$ and a self-adjoint operator H_∞ such that

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

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

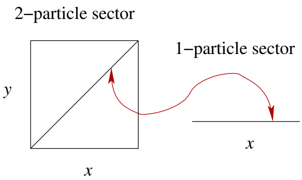
Theorem [Lampart et al. 2017]

$$H_\infty = H_{IBC} + const$$

Moving sources

- Now: x-particles can move, config. space $\mathcal{Q} = \bigcup_{m,n=0}^{\infty} (\mathbb{R}^3_x)^m \times (\mathbb{R}^3_y)^n$
- $\mathscr{H} = \mathscr{F}_x^- \otimes \mathscr{F}_y^+, \quad \psi : \mathcal{Q} \to \mathbb{C}, \quad \psi = \psi(x^m, y^n)$
- The original Hamiltonian is UV divergent.
- IBC $$\lim_{(\boldsymbol{x}_i,\boldsymbol{y}_j)\to(\boldsymbol{x},\boldsymbol{x})} |\boldsymbol{x}_i - \boldsymbol{y}_j|\, \psi(x^m, y^n) = \alpha_{n-1}\, \psi(\boldsymbol{x}_i = \boldsymbol{x}, \widehat{\boldsymbol{y}_j}) \qquad (4)$$

with $\alpha_{n-1} = \dfrac{g}{2\pi\hbar^2\sqrt{n}} \dfrac{m_x m_y}{m_x + m_y}$.
Here, "boundary" = diagonal;
boundary config: where $\boldsymbol{x}_i = \boldsymbol{y}_j$;
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 Dirac operators instead of $-\nabla^2$

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

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

or

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

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

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:

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

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 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 $x \leftrightarrows x + x$.
- Dirac eq in 1d: spin space $\mathbb{C}^2$, $\gamma^0 = \sigma_1$, $\gamma^1 = \sigma_1\sigma_3$.
- (truncated) Fock space $\mathscr{H} = \bigoplus_{n=0}^{N} S_- \, L^2(\mathbb{R}^1, \mathbb{C}^2)^{\otimes n}$

M. Lienert

Lukas Nickel

- For simplicity, let $N = 2$, $m = 0$, ignore the $n = 0$ sector, so $\mathscr{H} = \mathscr{H}^{(1)} \oplus \mathscr{H}^{(2)}$.
- $(H\psi)^{(1)}(x) = -i\alpha^1 \partial_x \psi^{(1)}(x) + N(x)^\dagger \, \psi^{(2)}(x, x)$
  $(H\psi)^{(2)}(x_1, x_2) = (-i\alpha^1_1 \partial_1 - i\alpha^1_2 \partial_2)\psi^{(2)}(x_1, x_2)$
  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, 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:

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, 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
$H^\circ(\psi^{(0)} = 0, \psi^{(1)}) = (0, (-i\boldsymbol{\alpha} \cdot \nabla + m\beta)\psi^{(1)})$
defined on $\mathscr{D}(H^\circ) = \{0\} \oplus C_c^\infty(\mathbb{R}^3 \setminus \{\mathbf{0}\}, \mathbb{C}^4)$
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, Tumulka arxiv.org/abs/2006.16755]

Let $H^\circ = -i\boldsymbol{\alpha}\cdot\nabla + m\beta + q/|\boldsymbol{x}|$ with $\sqrt{3}/2 < |q| < 1$ be defined on $\mathscr{D}^\circ = \{0\} \oplus C_c^\infty(\mathbb{R}^3 \setminus \{\boldsymbol{0}\}, \mathbb{C}^4)$. Set $B := \sqrt{1-q^2} \in (0, \frac{1}{2})$, let $0 \neq g \in \mathbb{R}$. There is a self-adjoint extension $(H, \mathscr{D})$ 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 $\psi^{(1)}(\boldsymbol{x}) =$
$$c_{-1}\, f_{-1}\big(\tfrac{\boldsymbol{x}}{|\boldsymbol{x}|}\big)\, |\boldsymbol{x}|^{-1-B} + \left(\sum_{k=0}^{3} c_k\, f_k\big(\tfrac{\boldsymbol{x}}{|\boldsymbol{x}|}\big)\right) |\boldsymbol{x}|^{-1+B} + o\big(|\boldsymbol{x}|^{-1/2}\big)$$
as $\boldsymbol{x} \to \boldsymbol{0}$ with $c_{-1} \dots c_3 \in \mathbb{C}$ and particular fcts $f_{-1} \dots f_3 : \mathbb{S}^2 \to \mathbb{C}^4$.
3. Every $\psi \in \mathscr{D}$ obeys IBC $\quad c_{-1} = g\, \psi^{(0)} \quad (g \in \mathbb{R})$
4. For $\psi \in \mathscr{D}$, $\quad (H\psi)^{(0)} = g\, c_0$
$$(H\psi)^{(1)}(\boldsymbol{x}) = \big(-i\boldsymbol{\alpha}\cdot\nabla + m\beta + \tfrac{q}{|\boldsymbol{x}|}\big)\psi^{(1)} \quad (\boldsymbol{x} \neq \boldsymbol{0}).$$

In short, IBCs at $\boldsymbol{0}$ 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