Novel Type of Hamiltonians Without Ultraviolet Divergence for Quantum Field Theories

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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

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Hamiltonians Without Ultraviolet Divergence
Particle–position representation of a Fock space vector

Configuration space of a variable number of particles:

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

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

\[ \text{here } d = 1, \quad n = 0, 1, 2, 3 \]

Fock space:

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

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

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

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

\( \psi \) is an (anti-)symmetric function
There are issues with the particle–position representation in relativistic QFT...

- Some QFTs lead to $\infty$ number of particles [cf. Deckert, Merkl et al.] BUT perhaps one can get along with that
- Photons are believed not to have a good position representation BUT photon wave functions are believed to be mathematically equivalent to (complexified) classical Maxwell fields, and that may be good enough
- $Q = \bigcup_{n=0}^{\infty} \mathbb{R}^{3n}$ depends on a choice of hypersurface ("$\mathbb{R}^{3}$") in space-time $M$
  BUT multi-time wave function may be defined on (the spacelike subset of) $\bigcup_{n=0}^{\infty} M^n$ [Petrat & Tumulka Ann. Phys., J. Math. Phys. 2014]

...BUT they do not seem fatal.
There are two species of particles, \( x \)-particles and \( y \)-particles.

\( x \)-particles can emit and absorb \( y \)-particles.

Configuration space \( \mathcal{Q} = \bigcup_{m,n=0}^{\infty} (\mathbb{R}_x^3)^m \times (\mathbb{R}_y^3)^n \)

Hilbert space \( \mathcal{H} = \mathcal{F}_x^- \otimes \mathcal{F}_y^+ \)

\( \psi : \mathcal{Q} \to \mathbb{C}, \psi = \psi(x^m, y^n) \), where \( x^m \) is any \( x \)-configuration with \( m \) particles

As always, \( i\partial_t \psi = H\psi \) Schrödinger eq
The original Hamiltonian is UV divergent

**Naive original Hamiltonian:**

\[
(H_{\text{orig}} \psi)(x^m, y^n) = -\frac{\hbar^2}{2m_x} \sum_{i=1}^m \nabla^2_{x_i} \psi(x^m, y^n) - \frac{\hbar^2}{2m_y} \sum_{j=1}^n \nabla^2_{y_j} \psi(x^m, y^n) +
\]

\[
+ nE_0 \psi(x^m, y^n) +
\]

\[
+ g \sqrt{n + 1} \sum_{i=1}^m \psi(x^m, (y^n, x_i)) +
\]

\[
+ \frac{g}{\sqrt{n}} \sum_{i=1}^m \sum_{j=1}^n \delta^3(x_i - y_j) \psi(x^m, y^n \setminus y_j),
\]

with \( g = \) coupling constant, \( E_0 = \) rest energy, \( y^n \setminus y_j = \) leave out \( y_j \).

\( H_{\text{orig}} \) is ill-defined because the wave fct of the newly created \( y \)-particle, \( \delta^3(x - y) \), does not lie in \( L^2(\mathbb{R}^3) \) (or, has infinite energy).
Well-defined, regularized version of $H$

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

$$(H_{\text{cutoff}} \psi)(x^m, y^n) = -\frac{\hbar^2}{2m_x} \sum_{i=1}^{m} \nabla^2_{x_i} \psi(x^m, y^n) - \frac{\hbar^2}{2m_y} \sum_{j=1}^{n} \nabla^2_{y_j} \psi(x^m, y^n) +$$

$$ + nE_0 \psi(x^m, y^n) +$$

$$ + g \sqrt{n + 1} \sum_{i=1}^{m} \int_{\mathbb{R}^3} d^3y \, \varphi^*(x_i - y) \psi(x^m, (y^n, y)) +$$

$$ + \frac{g}{\sqrt{n}} \sum_{i=1}^{m} \sum_{j=1}^{n} \varphi(x_i - y_j) \psi(x^m, y^n \setminus y_j)$$

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

- There is only 1 x-particle, and it is fixed at the origin. $\mathcal{H} = \mathbb{F}_y^+$
- Configuration space $\mathcal{Q} = \bigcup_{n=0}^{\infty} \mathbb{R}^{3n}$
- $\psi = \psi(y^n)$

Original Hamiltonian:

$$(H_{\text{orig}}\psi)(y^n) = -\frac{\hbar^2}{2m_y} \sum_{j=1}^{n} \nabla^2_{y_j} \psi(y^n) + nE_0 \psi(y^n)$$

$$+ g\sqrt{n+1} \psi(y^n, 0)$$

$$+ \frac{g}{\sqrt{n}} \sum_{j=1}^{n} \delta^3(y_j) \psi(y^n \setminus y_j) ,$$

Still UV divergent.
Novel idea: Interior–boundary condition

Interior–boundary condition (IBC)

For every \( y^n \in (\mathbb{R}^3 \setminus \{0\})^n \) and every \( \omega \in S^2 \),

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

Here, “boundary” means: config with any particle at the origin, i.e.,

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

interior config: one \( y \)-particle removed
For every $y^n \in (\mathbb{R}^3 \setminus \{0\})^n$ and every $\omega \in S^2$, 

$$\lim_{r \searrow 0} r \psi(y^n, r \omega) = \frac{g m_y}{2\pi \hbar^2 \sqrt{n + 1}} \psi(y^n)$$

IBC (1) $\Rightarrow$ $\psi$ typically diverges like $1/r$ at the boundary

1-sector in 2D

2-sector in 1D
Interior–boundary condition and corresponding Hamiltonian

**IBC**

For every \( y^n \in (\mathbb{R}^3 \setminus \{0\})^n \) and every \( \omega \in S^2 \),

\[
\lim_{r \searrow 0} r \psi(y^n, r\omega) = \frac{g m_y}{2\pi \hbar^2 \sqrt{n+1}} \psi(y^n) \tag{1}
\]

**\( H = H_{IBC} \)**

\[
(H_{IBC}\psi)(y^n) = -\frac{\hbar^2}{2m_y} \sum_{j=1}^{n} \nabla^2_{y_j} \psi(y^n) + nE_0 \psi(y^n)
\]

\[
+ \frac{g \sqrt{n+1}}{4\pi} \int_{S^2} d^2\omega \lim_{r \searrow 0} \frac{\partial}{\partial r} \left( r \psi(y^n, r\omega) \right)
\]

\[
+ \frac{g}{\sqrt{n}} \sum_{j=1}^{n} \delta^3(y_j) \psi(y^n \setminus y_j) \tag{2}
\]
Comparison $H_{\text{orig}}, H_{IBC}$

$$
(H_{\text{orig}} \psi)(y^n) = H_{\text{free}} \psi(y^n) + g \sqrt{n+1} \sum_{i=1}^{m} \psi(y^n, 0) + \\
+ \frac{g}{\sqrt{n}} \sum_{j=1}^{n} \delta^3(y_j) \psi(y^n \setminus y_j),
$$

$$
(H_{IBC} \psi)(y^n) = H_{\text{free}} \psi(y^n) + \frac{g \sqrt{n+1}}{4\pi} \int d^2\omega \lim_{r \to 0} \frac{\partial}{\partial r} \left(r \psi(y^n, r\omega)\right) \\
+ \frac{g}{\sqrt{n}} \sum_{j=1}^{n} \delta^3(y_j) \psi(y^n \setminus y_j)
$$
Self-adjointness of $H_{IBC}$

- $\text{IBC } \lim_{r \downarrow 0} r \psi(y^n, r\omega) = \frac{g m_y}{2\pi \hbar^2 \sqrt{n+1}} \psi(y^n)$ for all $\omega \in \mathbb{S}^2$ (1)

- $H_{IBC}\psi = H_{y,\text{free}}\psi + \frac{g \sqrt{n+1}}{4\pi} \int_{\mathbb{S}^2} d^2\omega \lim_{r \downarrow 0} \frac{\partial}{\partial r} \left(r \psi(y^n, r\omega)\right)$

$$+ \frac{g}{\sqrt{n}} \sum_{j=1}^{n} \delta^3(y_j) \psi(y^n \setminus y_j)$$ (2)

**Theorem (LSTT 2014)**

On a suitable dense domain $\mathcal{D}_{IBC}$ of $\psi$s in $\mathcal{F}_y^+$ satisfying the IBC (1), $H_{IBC}$ is well defined, self-adjoint, and positive.
Why it works: flux of probability into a point

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

\[
\frac{\partial |\psi(y^n)|^2}{\partial t} = - \sum_{j=1}^{n} \nabla_{y_j} \cdot j_{y_j} + (n+1) \lim_{r \to 0} r^2 \int_{S^2} d^2\omega \cdot j_{y_{n+1}}(y^n, r\omega)
\]

- motion towards \( 0 \Rightarrow \rho \sim \frac{1}{r^2} \) 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

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

- 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 $Q^{(n)}$).
Back to the model with moving x-particles

- configuration space \( Q = \bigcup_{m,n=0}^{\infty} (\mathbb{R}_x^3)^m \times (\mathbb{R}_y^3)^n \)

- Hilbert space \( \mathcal{H} = \mathcal{H}_x^- \otimes \mathcal{H}_y^+ \)

**IBC**

For every \((x^m, y^n) \in Q\) with \(x^m \cap y^n = \emptyset\), every \(i \leq m\) and \(j \leq n\),

\[
\lim_{(x_i, y_j) \to (x, x)} |y_j - x_i| \psi(x^m, y^n) = \alpha_{n-1} \psi(x_i = x, \hat{y}_j)
\]

with \(\alpha_{n-1} = \frac{g}{2\pi \hbar^2 \sqrt{n}} \frac{m_x m_y}{m_x + m_y}\) and \(\hat{\cdots}\) = omission.

Here, “boundary" = diagonal; boundary config: where \(x_i = y_j\); interior config: one y-particle removed
Interior–boundary condition

**IBC**

For every \((x^m, y^n) \in Q\) with \(x^m \cap y^n = \emptyset\), every \(i \leq m\) and \(j \leq n\),

\[
\lim_{(x_i, y_j) \to (x, x)} |y_j - x_i| \psi(x^m, y^n) = \alpha_{n-1} \psi(x_i = x, \hat{y}_j)
\]

IBC (3) \(\Rightarrow\) \(\psi\) typically diverges like \(1/r = 1/|y_j - x_i|\) on the diagonal \(y_j = x_i\)
Interior–boundary condition and corresponding Hamiltonian

**IBC**

For every \((x^m, y^n) \in Q\) with \(x^m \cap y^n = \emptyset\), every \(i \leq m\) and \(j \leq n\),

\[
\lim_{(x_i, y_j) \rightarrow (x, x)} |y_j - x_i| \psi(x^m, y^n) = \alpha_{n-1} \psi(x_i = x, \hat{y}_j)
\]

(3)

**\(H = H_{IBC}\)**

\[
(H \psi)(x^m, y^n) = -\frac{\hbar^2}{2m_x} \sum_{i=1}^{m} \nabla^2_{x_i} \psi - \frac{\hbar^2}{2m_y} \sum_{j=1}^{n} \nabla^2_{y_j} \psi + nE_0 \psi
\]

\[
+ \frac{g \sqrt{n+1}}{4\pi} \sum_{i=1}^{m} \int d^2\omega \lim_{r \searrow 0} \frac{\partial}{\partial r} \left[ r \psi(x_i \rightarrow x_i - \mu_x r \omega, y_{n+1} \rightarrow x_i + \mu_y r \omega) \right]
\]

\[
+ \frac{g}{\sqrt{n}} \sum_{i=1}^{m} \sum_{j=1}^{n} \delta^3(x_i - y_j) \psi(x^m, y^n \setminus y_j)
\]

(4)

with \(\mu_x = m_y/(m_x + m_y)\), \(\mu_y = m_x/(m_x + m_y)\)

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Hamiltonians Without Ultraviolet Divergence
Comparison of IBC to a known boundary condition

Interior–boundary conditions have not been considered before, but other boundary conditions have. In particular, in order to define on $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C})$ a Schrödinger equation with $\delta$-potential,

$$H = -\frac{\hbar^2}{2m} \nabla^2 + \delta^3(x),$$

one employs the

**Bethe–Peierls boundary condition [1935]**

$$\lim_{r \searrow 0} \left( \frac{\partial}{\partial r} \psi(r\omega) - \alpha \psi(r\omega) \right) = 0 \quad \forall \omega \in S^2 \text{ with known constant } \alpha \in \mathbb{R}$$

which leads to 0 current into the origin. For comparison,

**IBC**

$$\lim_{r \searrow 0} r\psi(y^n, r\omega) = \alpha_n \psi(y^n) \quad \forall \omega \in S^2 \text{ with suitable constant } \alpha_n \in \mathbb{R}$$

which leads to nonzero current into $Q^{(n)} \times \{0\}$. 
Again, 1 x-particle fixed at the origin, $\mathcal{H} = \mathcal{F}_y^+$. 

**Theorem (LSTT 2014)**

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

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

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 $\mathbf{x}_1 = (0, 0, 0)$ and $\mathbf{x}_2 = (R, 0, 0)$, $\mathcal{H} = \mathcal{F}_y^+$
- 2 IBCs, one at $\mathbf{x}_1$ and one at $\mathbf{x}_2$
- 2 creation and annihilation terms in $H_{IBC}$
- Presumably, 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

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

That is, x-particles effectively interact through an attractive Yukawa potential
Consider again the scenario with 1 x-particle fixed at the origin, \( \mathcal{H} = \mathcal{F}_y^+ \). Let \( E_0 > 0 \).

Consider \( H_{\text{cutoff}} = H_\varphi \) with \( \varphi = \frac{\lambda}{\delta^3} \), 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 (LSTT 2014)**

\[
H_\infty = H_{IBC} + \text{const}
\]
Neumann vs. Dirichlet conditions

Usually, Neumann \( \frac{\partial u}{\partial n} \bigg|_{\partial Q} = 0 \), Dirichlet \( u \bigg|_{\partial Q} = 0 \), Robin \( (\alpha \frac{\partial u}{\partial n} + \beta u) \bigg|_{\partial Q} = 0 \).

In the previous example: Dirichlet-type IBC

\[
\lim_{r \downarrow 0} r \psi(y^n, r\omega) = \alpha_n \psi(y^n) \quad \text{(IBC)}
\]

\[
H_{IBC}\psi(y^n) = H_{\text{free}}\psi + \frac{g\sqrt{n+1}}{4\pi} \int_{S^2} d^2\omega \lim_{r \downarrow 0} \frac{\partial}{\partial r} \left( r \psi(y^n, r\omega) \right)
\]

One can also use instead: a Neumann-type IBC. Leads to a different \( H \).

\[
\lim_{r \downarrow 0} \frac{\partial}{\partial r} \left( r \psi(y^n, r\omega) \right) = \alpha_n \psi(y^n) \quad \text{(IBC)}
\]

\[
H_{IBC}\psi(y^n) = H_{\text{free}}\psi + \frac{g\sqrt{n+1}}{4\pi} \int_{S^2} d^2\omega \lim_{r \downarrow 0} r \psi(y^n, r\omega)
\]

Similarly, one can use Robin-type conditions.
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.
Again, 1 x-particle is fixed at the origin. Add Coulomb potential.
Let us restrict ourselves to $0 \leq n \leq 1$, i.e., $\mathcal{H} = \mathcal{H}^{(0)} \oplus \mathcal{H}^{(1)}$
with $\mathcal{H}^{(0)} = \mathbb{C}^4$ and $\mathcal{H}^{(1)} = L^2(\mathbb{R}^3, \mathbb{C}^4)$.

Theorem (LSTT 2014)
Suppose $|q_x q_y| > 1$. Then there is a self-adjoint operator $H_{IBC}$ on a
dense domain $D$ in $\mathcal{H} = \mathbb{C}^4 \oplus L^2(\mathbb{R}^4, \mathbb{C}^4)$ such that:
- For any $\psi = (0, \psi^{(1)})$ with $\psi^{(1)} \in H^1(\mathbb{R}^3, \mathbb{C}^4)$ (first Sobolev space)
  and $\psi^{(1)}(x) = 0$ on a neighborhood of the origin,

$$\psi \in D \text{ and } H\psi = \left(0, \left(-i\hbar \alpha \cdot \nabla + \beta m + \frac{q_x q_y}{|y|}\right)\psi^{(1)}\right).$$

- $H_{IBC}$ does not conserve particle number, i.e., $H_{IBC}$ is not of
  block-diagonal form w.r.t. $\mathcal{H}^{(0)} \oplus \mathcal{H}^{(1)}$. 
Formulate quantum electrodynamics in terms of IBCs, building on

Quantenelektrodynamik im Konfigurationsraum.
Von L. Landau und R. Peierls in Zürich.
(Eingegangen am 12. Februar 1930.)


(QED in the particle–position representation)
Thank you for your attention