Probability of Particle Creation and Interior-Boundary Conditions for Fock Space

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- Hamiltonians *H* on Fock space with particle creation and annihilation usually are UV divergent.
- To obtain a well-defined H you can introduce a UV cut-off by
 - discretizing space or
 - smearing out the creation/annihilation terms
- The novel approach of interior-boundary conditions (IBCs) can provide a well-defined *H* without need for a UV cut-off.
- I will present
 - rigorous results for the non-relativistic case
 - Bohmian trajectories

Particle-position representation of a Fock space vector

Configuration space of a variable number of particles:



Example: a non-relativistic QFT

- There are two species of particles, x-particles and y-particles.
- x-particles can emit and absorb y-particles.
- configuration space $\mathcal{Q} = \bigcup_{m,n=0}^{\infty} (\mathbb{R}^3_x)^m imes (\mathbb{R}^3_y)^n$
- Hilbert space $\mathscr{H} = \mathscr{F}_x^- \otimes \mathscr{F}_y^+$
- $\psi : \mathcal{Q} \to \mathbb{C}, \ \psi = \psi(x^m, y^n)$, where x^m is any x-configuration with m particles
- As always, $i\partial_t \psi = H\psi$ Schrödinger eq

Naive original Hamiltonian (UV divergent)

$$H_{\mathrm{orig}} = H_x^{\mathrm{free}} + H_y^{\mathrm{free}} + g \int_{\mathbb{R}^3} d^3 x \; a_x^{\dagger}(x) \left(a_y(x) + a_y^{\dagger}(x) \right) a_x(x)$$

 $g = \mathsf{coupling constant} \in \mathbb{R}$

$H_{\rm orig}$ in the particle-position representation

Naive original Hamiltonian (UV divergent)

$$\begin{aligned} (\mathcal{H}_{\mathrm{orig}}\psi)(x^m,y^n) &= -\frac{\hbar^2}{2m_x}\sum_{i=1}^m \nabla^2_{\mathbf{x}_i}\psi(x^m,y^n) - \frac{\hbar^2}{2m_y}\sum_{j=1}^n \nabla^2_{\mathbf{y}_j}\psi(x^m,y^n) + \\ &+ nE_0\psi(x^m,y^n) + \\ &+ g\sqrt{n+1}\sum_{i=1}^m\psi(x^m,(y^n,\mathbf{x}_i)) + \\ &+ \frac{g}{\sqrt{n}}\sum_{i=1}^m\sum_{j=1}^n \delta^3(\mathbf{x}_i-\mathbf{y}_j)\psi(x^m,y^n\setminus\mathbf{y}_j) \,, \end{aligned}$$

with E_0 = rest energy, $y^n \setminus y_j$ = leave out y_j .

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

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

$$(\mathcal{H}_{\text{cutoff}}\psi)(\mathbf{x}^{m},\mathbf{y}^{n}) = -\frac{\hbar^{2}}{2m_{\mathbf{x}}}\sum_{i=1}^{m}\nabla_{\mathbf{x}_{i}}^{2}\psi(\mathbf{x}^{m},\mathbf{y}^{n}) - \frac{\hbar^{2}}{2m_{\mathbf{y}}}\sum_{j=1}^{n}\nabla_{\mathbf{y}_{j}}^{2}\psi(\mathbf{x}^{m},\mathbf{y}^{n}) + \\ + nE_{0}\psi(\mathbf{x}^{m},\mathbf{y}^{n}) + \\ + g\sqrt{n+1}\sum_{i=1}^{m}\int_{\mathbb{R}^{3}}d^{3}\mathbf{y}\,\varphi^{*}(\mathbf{x}_{i}-\mathbf{y})\,\psi(\mathbf{x}^{m},(\mathbf{y}^{n},\mathbf{y})) + \\ + \frac{g}{\sqrt{n}}\sum_{i=1}^{m}\sum_{j=1}^{n}\varphi(\mathbf{x}_{i}-\mathbf{y}_{j})\,\psi(\mathbf{x}^{m},\mathbf{y}^{n}\setminus\mathbf{y}_{j})$$

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



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Novel idea: Interior-boundary condition

Interior-boundary condition (IBC) basic form

For q on the boundary of Q,

 $\psi(\boldsymbol{q}) = \alpha \, \psi(\boldsymbol{q}') \,,$

where q' is an interior point of Q and $\alpha = \alpha(q) \in \mathbb{R}$ independent of ψ .

Here, "boundary" = diagonal; boundary config: where $\mathbf{x}_i = \mathbf{y}_j$; interior config q': one y-particle removed Ex: $q = (\mathbf{x}, \mathbf{x}), q' = \mathbf{x}$



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Toy example of a configuration space with boundary

- Consider configuration space $Q = Q^{(1)} \cup Q^{(2)}$ with $Q^{(1)} = \mathbb{R}$ and $Q^{(2)} = \{(x, y) \in \mathbb{R}^2 : y > 0\}.$
- Correspondingly, $\mathscr{H} = \mathscr{H}^{(1)} \oplus \mathscr{H}^{(2)}$ with $\mathscr{H}^{(n)} = L^2(\mathcal{Q}^{(n)}).$



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- boundary $\partial \mathcal{Q} = \left\{ (x, y) \in \mathbb{R}^2 : y = 0 \right\}$
- IBC: For every $x \in \mathbb{R}$, $\psi^{(2)}(x,0) = \frac{2mg}{\hbar^2} \psi^{(1)}(x)$ (1)
- Hamiltonian:

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

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

Theorem (TT 2015 arXiv:1506.00497)

On a domain $\mathscr{D} \subseteq \mathscr{H}$ of functions satisfying the IBC (1), H is rigorously defined and self-adjoint.

Probability balance

$$\begin{aligned} \text{IBC:} \quad \psi^{(2)}(x,0) &= \frac{2mg}{\hbar^2} \psi^{(1)}(x) \qquad (1) \\ (H\psi)^{(1)}(x) &= -\frac{\hbar^2}{2} \partial_x^2 \psi^{(1)}(x) - g \, \partial_y \psi^{(2)}(x,0) \\ (H\psi)^{(2)}(x,y) &= -\frac{\hbar^2}{2} \left(\partial_x^2 + \partial_y^2 \right) \psi^{(2)}(x,y) \end{aligned}$$



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• Loss of probability in $\mathcal{Q}^{(2)}$ at (x,0): $-j_y^{(2)}(x,0)$

 \bullet is compensated by gain in $\mathcal{Q}^{(1)}$:

$$\frac{\partial |\psi^{(1)}|^2}{\partial t}(x) = -\partial_x j^{(1)} - \frac{2}{\hbar} \operatorname{Im} \left[\psi^{(1)}(x)^* g \, \partial_y \psi^{(2)}(x,0) \right]$$
$$\stackrel{(1)}{=} -\partial_x j^{(1)} - j_y^{(2)}(x,0) \, .$$

Bohmian trajectories

• Bohm's equation of motion:

$$egin{aligned} rac{dQ}{dt} &= rac{j^\psi(Q)}{
ho^\psi(Q)} \ &= rac{\hbar}{m} \mathrm{Im} rac{\psi^*
abla \psi}{\psi^* \psi} \end{aligned}$$

- in every sector $\mathcal{Q}^{(1)}, \mathcal{Q}^{(2)}$.
- When the trajectory hits the boundary at (x, 0), it jumps to x.
- When $Q(t) = x \in Q^{(1)}$, it jumps to $(x, 0) \in Q^{(2)}$ with rate

$$\sigma_t(x \to (x, 0)) = \frac{j_y^{(2)}(x, 0)^+}{\rho^{(1)}(x)}$$

$$= \frac{\hbar}{m} \frac{\mathrm{Im}^{+} \big[\psi^{(2)}(x,0)^{*} \partial_{y} \psi^{(2)}(x,0) \big]}{|\psi^{(1)}(x)|^{2}}$$





- Markov process
- time reversal invariant
- $Q_t \sim |\psi_t|^2$ at all t

Simplified QFT model ("Lee model")

- There is only 1 x-particle, and it is fixed at the origin. $\mathscr{H} = \mathscr{F}_{v}^{+}$
- configuration space $Q = \bigcup_{n=0}^{\infty} \mathbb{R}^{3n}$
- boundary configurations: any particle at the origin (r = 0 in spherical coordinates)
- IBC $\lim_{r \searrow 0} r\psi(y^n, r\omega) = \frac{g m_y}{2\pi\hbar^2 \sqrt{n+1}} \psi(y^n)$ for all $\omega \in \mathbb{S}^2$ (2)

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

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

Theorem (LSTT 2017 arXiv:1703.04476)

On a suitable dense domain \mathscr{D}_{IBC} of ψ s in \mathscr{F}_{y}^{+} satisfying the IBC (2), H_{IBC} is well defined, self-adjoint, and positive.

Comparison H_{orig}, H_{IBC}

$$\begin{split} H_{\rm orig} \psi &= H_{\rm free} \psi + g \sqrt{n+1} \, \psi \big(y^n, \mathbf{0} \big) + \\ &+ \frac{g}{\sqrt{n}} \sum_{j=1}^n \delta^3(\mathbf{y}_j) \, \psi \big(y^n \setminus \mathbf{y}_j \big) \,, \end{split}$$

$$\begin{aligned} H_{IBC}\psi &= H_{\text{free}}\psi + \\ &+ \frac{g\sqrt{n+1}}{4\pi} \int_{\mathbb{S}^2} d^2 \omega \underbrace{\lim_{r \searrow 0} \frac{\partial}{\partial r} \left[r\psi(y^n, r\omega) \right]}_{b} \\ &+ \frac{g}{\sqrt{n}} \sum_{j=1}^n \delta^3(\boldsymbol{y}_j) \,\psi(y^n \setminus \boldsymbol{y}_j) \end{aligned}$$

$$\begin{split} \psi^{(1)}(r\omega) &= a r^{-1} + b + o(1); & \text{IBC: } a = \alpha_n \psi^{(0)} \\ \ln \mathbb{R}^d \text{ instead of } \mathbb{R}^3 \text{, replace } r^{-1} \to r^{-(d-1)/2} \text{ for } d \geq 3, \\ \log r \text{ for } d = 2, \ r^0 \text{ for } d = 1. \end{split}$$

Why it works: flux of probability into a point

• probability current
$$\mathbf{j}_{\mathbf{y}_{j}}(\mathbf{y}^{n}) = \frac{\hbar}{m_{\mathbf{y}}} \operatorname{Im} \psi^{*} \nabla_{\mathbf{y}_{j}} \psi$$

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

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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

$$rac{dQ}{dt} = rac{\hbar}{m} \mathrm{Im} rac{
abla \psi^{(n)}}{\psi^{(n)}} ig(Q(t)ig)$$

- with IBC:
- when $Q(t) \in \mathcal{Q}^{(n)}$ reaches $\mathbf{y}_j = \mathbf{0}$, it jumps to $(y^n \setminus \mathbf{y}_j) \in \mathcal{Q}^{(n-1)}$
- 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 ${\bf 0}~(=$ in

the support of φ^{f}



Trajectories starting at r = 0

- It turns out that for functions in the domain of H_{IBC} , $\psi^{(1)}(r\omega) = ar^{-1} + b + o(1)$ with a and b independent of ω .
- As a consequence, the last velocity of the *y*-particle before absorption at **0** is purely radial.
- Hence, the *y*-trajectory reaches **0** in a definite direction and has an endpoint in spherical coordinates (r, ω) at $(0, \omega_{\text{final}})$.
- Different trajectories in $\mathcal{Q}^{(1)}$ reaching **0** at the same time have different ω_{final} .
- Time reverse: for every t and $\omega_{initial}$ there is a unique trajectory beginning at **0** at time t in the direction $\omega_{initial}$ whenever $\lim_{r \to 0} j_r^{(1)}(r\omega_{initial}, t) > 0.$
- Thus, whenever Q_t jumps from $Q^{(0)}$ to $\mathbf{0} \in Q^{(1)}$, there starts a trajectory at $\mathbf{0}$ for each direction.
- The process chosses the direction randomly.
- This is key for showing that the IBC process Q_t is well defined.

Comparison to renormalization procedure

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

$$H_{\varphi} - E_{\varphi} o H_{\infty}$$
.

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

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Theorem (LSTT 2017 arXiv:1703.04476)

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

Previously, it was unknown what the domain of H_∞ looks like and how H_∞ acts on it.

Shown non-rigorously:

The Bohmian process Q_t^{φ} for H_{φ} converges in distribution, as $\varphi \to \delta^3$, to the IBC process Q_t^{IBC} .

Moving x-particles

$$\begin{array}{l} \text{Hilbert space } \mathcal{H} = \mathscr{F}_x^- \otimes \mathscr{F}_y^+ \\ \mathcal{H}_{\text{orig}} = \mathcal{H}_x^{\text{free}} + \mathcal{H}_y^{\text{free}} + g \int_{\mathbb{R}^3} d^3 x \ a_x^{\dagger}(x) \left(a_y(x) + a_y^{\dagger}(x) \right) a_x(x) \end{array}$$

There is a natural formulation of the IBC and H_{IBC} in this setting.

Theorem (Lampart and Schmidt 2017 forthcoming)

Let the space dimension be $d \in (1, 2, 3)$. On a suitable dense domain \mathcal{D}_{IBC} of ψ s in \mathcal{H} satisfying the IBC, H_{IBC} is well defined, self-adjoint, and positive.

With moving x-particles in 3d, the growth of ψ near the boundary is no longer $ar^{-1} + b + o(1)$ but instead

$$\psi^{(1)}(r\omega) = a r^{-1} + b \log r + c + o(1)$$

where $b = \tilde{\alpha} a$ with certain constant $\tilde{\alpha} \in \mathbb{R}$ independent of ψ .

 H_{IBC} and the IBC process Q_t respect the symmetries of H_{orig} including (if appropriate)

- Galilean boosts, rotations, space and time translations, time reversal
- gauge invariance

Thank you for your attention

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