

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

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Joint work with Stefan Teufel, Julian Schmidt, and Jonas Lampart

Congratulations to Guenter Ahlers, Cristina Marchetti, and Shelly Goldstein!

- 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:

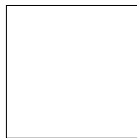
$$\begin{aligned} \mathcal{Q} &= \bigcup_{n=0}^{\infty} \mathbb{R}^{3n} \\ &= \bigcup_{n=0}^{\infty} \mathcal{Q}^{(n)} \end{aligned}$$



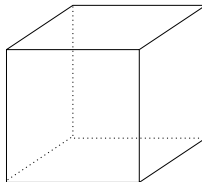
(a)



(b)



(c)



(d)

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

Fock space:

$$\bullet \quad \mathcal{F}^{\pm} = \bigoplus_{n=0}^{\infty} S_{\pm} \mathcal{H}_1^{\otimes n}$$

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

- $\psi \in \mathcal{F} \Rightarrow \psi = (\psi^{(0)}, \psi^{(1)}, \psi^{(2)}, \dots)$
- $\psi : \mathcal{Q} \rightarrow \mathbb{C}$ with S = value space = $\bigcup_{n=0}^{\infty} (\mathbb{C}^k)^{\otimes n}$
- ψ is an (anti-)symmetric function

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 $\mathcal{Q} = \bigcup_{m,n=0}^{\infty} (\mathbb{R}_x^3)^m \times (\mathbb{R}_y^3)^n$
- Hilbert space $\mathcal{H} = \mathcal{F}_x^- \otimes \mathcal{F}_y^+$
- $\psi : \mathcal{Q} \rightarrow \mathbb{C}$, $\psi = \psi(x^m, y^n)$, 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)

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

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

H_{orig} in the particle-position representation

Naive original Hamiltonian (UV divergent)

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

with $E_0 = \text{rest energy}$, $y^n \setminus \mathbf{y}_j = \text{leave out } \mathbf{y}_j$.

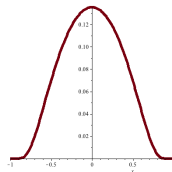
H_{orig} is ill-defined because the wave fct of the newly created y-particle, $\delta^3(\mathbf{x} - \mathbf{y})$, does not lie in $L^2(\mathbb{R}^3)$ (or, has infinite energy).

Well-defined, regularized version of H

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

$$\begin{aligned}(H_{\text{cutoff}}\psi)(x^m, y^n) = & -\frac{\hbar^2}{2m_x} \sum_{i=1}^m \nabla_{\mathbf{x}_i}^2 \psi(x^m, y^n) - \frac{\hbar^2}{2m_y} \sum_{j=1}^n \nabla_{\mathbf{y}_j}^2 \psi(x^m, y^n) + \\ & + nE_0 \psi(x^m, y^n) + \\ & + g\sqrt{n+1} \sum_{i=1}^m \int_{\mathbb{R}^3} d^3\mathbf{y} \varphi^*(\mathbf{x}_i - \mathbf{y}) \psi(x^m, (y^n, \mathbf{y})) + \\ & + \frac{g}{\sqrt{n}} \sum_{i=1}^m \sum_{j=1}^n \varphi(\mathbf{x}_i - \mathbf{y}_j) \psi(x^m, y^n \setminus \mathbf{y}_j)\end{aligned}$$

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



Novel idea: Interior–boundary condition

Interior–boundary condition (IBC) basic form

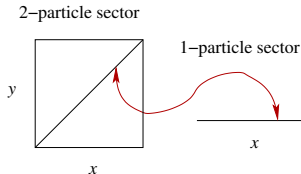
For q on the boundary of $\mathcal{Q}$,

$$\psi(q) = \alpha \psi(q'),$$

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

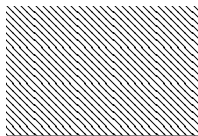
Here, “boundary” = diagonal;
boundary config: where $\mathbf{x}_i = \mathbf{y}_j$;
interior config q' : one y-particle removed

Ex: $q = (\mathbf{x}, \mathbf{x})$, $q' = \mathbf{x}$



Toy example of a configuration space with boundary

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



- Correspondingly, $\mathcal{H} = \mathcal{H}^{(1)} \oplus \mathcal{H}^{(2)}$
with $\mathcal{H}^{(n)} = L^2(\mathcal{Q}^{(n)})$.

- boundary $\partial\mathcal{Q} = \{(x, y) \in \mathbb{R}^2 : y = 0\}$

- IBC: For every $x \in \mathbb{R}$, $\psi^{(2)}(x, 0) = \frac{2mg}{\hbar^2} \psi^{(1)}(x)$ (1)

- Hamiltonian:

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

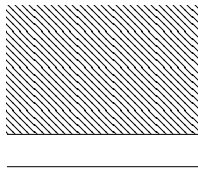
Theorem (TT 2015 arXiv:1506.00497)

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

$$\text{IBC: } \psi^{(2)}(x, 0) = \frac{2mg}{\hbar^2} \psi^{(1)}(x) \quad (1)$$

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

$$(H\psi)^{(2)}(x, y) = -\frac{\hbar^2}{2} (\partial_x^2 + \partial_y^2) \psi^{(2)}(x, y)$$



- Loss of probability in $\mathcal{Q}^{(2)}$ at $(x, 0)$: $-j_y^{(2)}(x, 0)$
- is compensated by gain in $\mathcal{Q}^{(1)}$:

$$\begin{aligned} \frac{\partial |\psi^{(1)}|^2}{\partial t}(x) &= -\partial_x j^{(1)} - \frac{2}{\hbar} \text{Im}[\psi^{(1)}(x)^* g \partial_y \psi^{(2)}(x, 0)] \\ &\stackrel{(1)}{=} -\partial_x j^{(1)} - j_y^{(2)}(x, 0). \end{aligned}$$

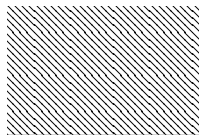
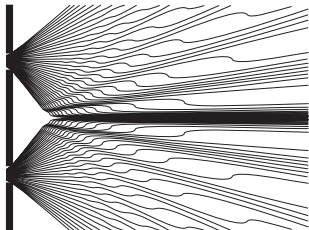
Bohmian trajectories

- Bohm's equation of motion:

$$\begin{aligned}\frac{dQ}{dt} &= \frac{j^\psi(Q)}{\rho^\psi(Q)} \\ &= \frac{\hbar}{m} \operatorname{Im} \frac{\psi^* \nabla \psi}{\psi^* \psi}\end{aligned}$$

- in every sector $Q^{(1)}, Q^{(2)}$.
- 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

$$\begin{aligned}\sigma_t(x \rightarrow (x, 0)) &= \frac{j_y^{(2)}(x, 0)^+}{\rho^{(1)}(x)} \\ &= \frac{\hbar}{m} \frac{\operatorname{Im}^+ [\psi^{(2)}(x, 0)^* \partial_y \psi^{(2)}(x, 0)]}{|\psi^{(1)}(x)|^2}\end{aligned}$$



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

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

- 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)

- $$H_{IBC}\psi = H_y^{\text{free}}\psi + \frac{g\sqrt{n+1}}{4\pi} \int_{\mathbb{S}^2} d^2\omega \lim_{r \searrow 0} \frac{\partial}{\partial r} [r\psi(y^n, r\omega)]$$
$$+ \frac{g}{\sqrt{n}} \sum_{j=1}^n \delta^3(\mathbf{y}_j) \psi(y^n \setminus \mathbf{y}_j)$$
 (3)

Theorem (LSTT 2017 arXiv:1703.04476)

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

Comparison $H_{\text{orig}}, H_{\text{IBC}}$

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

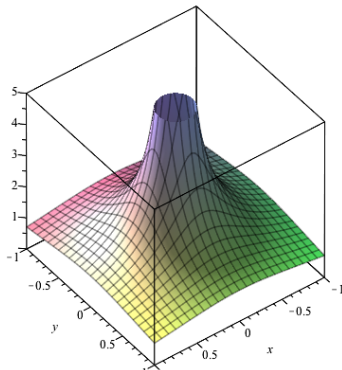
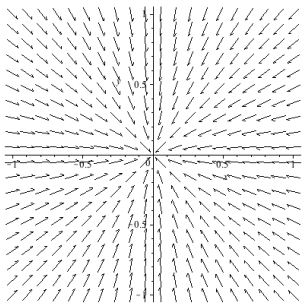
$$H_{\text{IBC}}\psi = H_{\text{free}}\psi + \\ + \frac{g\sqrt{n+1}}{4\pi} \int_{\mathbb{S}^2} d^2\omega \underbrace{\lim_{r \searrow 0} \frac{\partial}{\partial r} [r\psi(y^n, r\omega)]}_b \\ + \frac{g}{\sqrt{n}} \sum_{j=1}^n \delta^3(\mathbf{y}_j) \psi(y^n \setminus \mathbf{y}_j)$$

$\psi^{(1)}(r\omega) = ar^{-1} + b + o(1); \quad \text{IBC: } a = \alpha_n \psi^{(0)}$

In $\mathbb{R}^d$ instead of $\mathbb{R}^3$, replace $r^{-1} \rightarrow r^{-(d-1)/2}$ for $d \geq 3$,
 $\log r$ for $d = 2$, r^0 for $d = 1$.

Why it works: flux of probability into a point

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



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

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

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

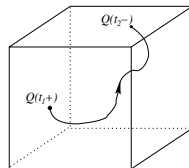
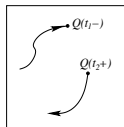
the support of φ )



(a)

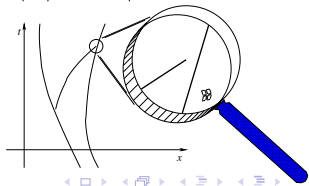
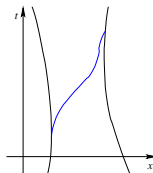


(b)



(c)

(d)



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 $\mathbf{0}$ is purely radial.
- Hence, the y -trajectory reaches $\mathbf{0}$ in a definite direction and has an endpoint in spherical coordinates (r, ω) at $(0, \omega_{\text{final}})$.
- Different trajectories in $Q^{(1)}$ reaching $\mathbf{0}$ at the same time have different ω_{final} .
- Time reverse: for every t and ω_{initial} there is a unique trajectory beginning at $\mathbf{0}$ at time t in the direction ω_{initial} whenever $\lim_{r \rightarrow 0} j_r^{(1)}(r\omega_{\text{initial}}, t) > 0$.
- 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 crosses 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 $\varphi = \text{[Gaussian plot]}$, limit $\varphi \rightarrow \delta^3$.
- Then there exist constants $E_\varphi \rightarrow \infty$ and a self-adjoint operator H_∞ such that

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

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

Theorem (LSTT 2017 arXiv:1703.04476)

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

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 $\varphi \rightarrow \delta^3$, to the IBC process Q_t^{IBC} .

Moving x-particles

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

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

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 $a r^{-1} + b + o(1)$ 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