Mathematical methods for uncertainty and exclusion in quantum mechanics

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Quantum Mechanics

Classical mechanics in symbiosis with math: Newton, Lagrange, ...

Quantum mechanics resolves several issues, in particular **stability**.

Built around **two fundamental principles:**

- The **uncertainty** principle (Heisenberg 1927; Hardy, Sobolev)
- The **exclusion** principle (Pauli 1925)

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Interests as a **mathematical physicist**:

- new mathematics to make these precise and robust
- allow generalizations according to modern developments in physics (new interactions, geometries/dimensionalities, ...).

Methods from

- **analysis**: functional inequalities and variational methods
- **geomety and topology**: ex. deformations and index theory
- **algebra and representation theory**: ex. braid groups, Clifford algebras

Outline

1. The uncertainty principle in quantum mechanics
2. Quantum statistics and the exclusion principle
3. The Lieb–Thirring inequality
4. Quantum statistics in 2D (anyons)

The uncertainty principle: Heisenberg

"Heisenberg's uncertainty principle": $(\hbar = 1)$ [Kennard, Weyl]

$$\boxed{\Delta x \Delta p \geq \tfrac{1}{2}}$$

In QM we replace classical **observables** x and p with operators $\hat{x} = x$ (multiplication) resp. $\hat{p} = -i\frac{d}{dx}$, acting on **wave functions** $\psi \in L^2(\mathbb{R})$, with $|\psi(x)|^2$ its probability density at $x \in \mathbb{R}$.
$\Rightarrow$ non-commutativity:

$$(i\hat{p})\hat{x} - \hat{x}(i\hat{p}) = \mathbb{1}$$

Application of Cauchy-Schwarz, for ψ smooth and normalized:

$$\begin{aligned}\sqrt{\langle \hat{x}^2 \rangle_\psi}\sqrt{\langle \hat{p}^2 \rangle_\psi} &= \left(\int_{\mathbb{R}} x^2 |\psi(x)|^2 \, dx\right)^{\frac{1}{2}} \left(\int_{\mathbb{R}} \xi^2 |\hat{\psi}(\xi)|^2 \, d\xi\right)^{\frac{1}{2}} \\ &\geq \int_{\mathbb{R}} |\hat{x}\psi||i\hat{p}\psi| \, dx \geq \frac{1}{2}\int_{\mathbb{R}} |\psi|^2 \, dx\end{aligned}$$

The uncertainty principle: Hardy

The Hardy inequality: For $\psi \in H^1(\mathbb{R}^d)$, $d \geq 3$,

$$\int_{\mathbb{R}^d} |\nabla \psi(\mathbf{x})|^2 \, d\mathbf{x} \geq \frac{(d-2)^2}{4} \int_{\mathbb{R}^d} \frac{1}{|\mathbf{x}|^2} |\psi(\mathbf{x})|^2 d\mathbf{x}$$

Application: the **stability** of an atom ($d = 3$)

$$\hat{H}_{\text{electron}} = \frac{1}{2m}\hat{\mathbf{p}}^2 - \frac{1}{|\hat{\mathbf{x}}|} = \frac{1}{2m}(-\Delta_{\mathbb{R}^3}) - \frac{1}{|\mathbf{x}|}$$

$\Rightarrow$

$$\inf \operatorname{spec} \hat{H}_{\text{electron}} \geq \inf_{\mathbf{x} \in \mathbb{R}^3} \left(\frac{1}{8m} \frac{1}{|\mathbf{x}|^2} - \frac{1}{|\mathbf{x}|} \right) = -2m > -\infty.$$

The uncertainty principle: Sobolev and GNS

Other examples:

Sobolev (ex. $d = 3$, and for f vanishing at ∞):

$$\int_{\mathbb{R}^3} |\nabla f|^2 \, d\mathbf{x} \geq C \left(\int_{\mathbb{R}^3} |f(\mathbf{x})|^6 \, d\mathbf{x} \right)^{\frac{1}{3}}$$

Gagliardo-Nirenberg-Sobolev $(d \geq 1)$:

$$\int_{\mathbb{R}^d} |\nabla f|^2 \, d\mathbf{x} \geq C_d \left(\int_{\mathbb{R}^d} |f(\mathbf{x})|^2 \, d\mathbf{x} \right)^{-\frac{2}{d}} \int_{\mathbb{R}^d} |f(\mathbf{x})|^{2(1+2/d)} \, d\mathbf{x}$$

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$$\int_{\mathbb{R}^d} |\xi|^{2s} |\hat{f}(\xi)|^2 \, d\xi \geq C_d \left(\int_{\mathbb{R}^d} |f(\mathbf{x})|^2 \, d\mathbf{x} \right)^{-\frac{2s}{d}} \int_{\mathbb{R}^d} |f(\mathbf{x})|^{2(1+2s/d)} \, d\mathbf{x}$$

Many-body Quantum Mechanics

Typical operator for N particles in $\mathbb{R}^d$:

$$\hat{H}_N = \sum_{j=1}^{N} \big(-\Delta_{\mathbf{x}_j} + V(\mathbf{x}_j)\big) + \sum_{1 \le j < k \le N} W(\mathbf{x}_j - \mathbf{x}_k)$$

acts on $\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_N)$ in $L^2(\mathbb{R}^{dN})$, normalized $\int |\Psi|^2 = 1$.

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As $N \to \infty$, we look for a **Density Functional Theory** (DFT)

$$\inf \operatorname{spec} \hat{H}_N \approx \inf_{\varrho \ge 0,\, \int \varrho = N} \int_{\mathbb{R}^d} \big(e_W(\varrho(\mathbf{x})) + V \varrho(\mathbf{x})\big) d\mathbf{x}$$

From Ψ we have a one-body density on $\mathbb{R}^d$: ($\Rightarrow V$ is ok)

$$\varrho_\Psi(\mathbf{x}) := \sum_{j=1}^{N} \int_{\mathbb{R}^{d(N-1)}} |\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_{j-1}, \mathbf{x}, \mathbf{x}_{j+1}, \ldots, \mathbf{x}_N)|^2 \prod_{i \ne j} d\mathbf{x}_i$$

The exclusion principle

Fundamental principle: **indistinguishability** (identical particles)

$$|\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_k, \ldots, \mathbf{x}_N)|^2 = |\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_k, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_N)|^2$$

Possibilities:

symmetry of phase ⇒ **bosons**

$$\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_k, \ldots, \mathbf{x}_N) = +\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_k, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_N)$$

antisymmetry of phase ⇒ **fermions**

$$\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_k, \ldots, \mathbf{x}_N) = -\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_k, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_N)$$

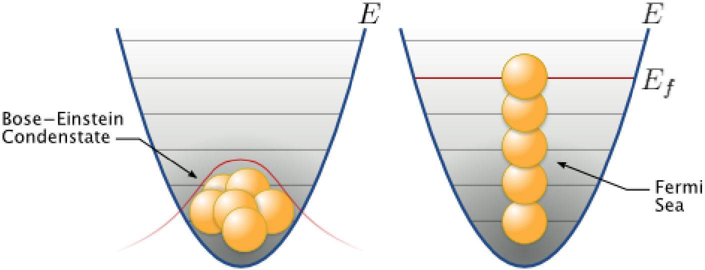
satisfy **Pauli's exclusion principle:**

$$\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_j, \ldots, \mathbf{x}_k, \ldots, \mathbf{x}_N) = 0 \quad \text{if } \mathbf{x}_j = \mathbf{x}_k,\ j \neq k,$$

or, generally, $\Psi \in \bigwedge^N L^2(\mathbb{R}^d)$, spanned by **"Slater determinants"**

$$(\psi_1 \wedge \ldots \wedge \psi_N)(\mathbf{x}_1, \ldots, \mathbf{x}_N) := \frac{1}{\sqrt{N!}} \det \Big[\psi_j(\mathbf{x}_k)\Big]_{j,k}.$$

Quantum statistics (in 3D)



Cold **bosons**   Cold **fermions**

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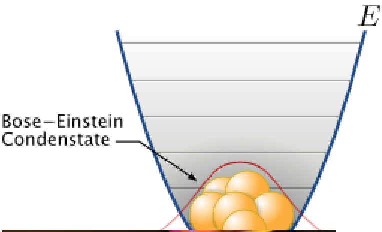
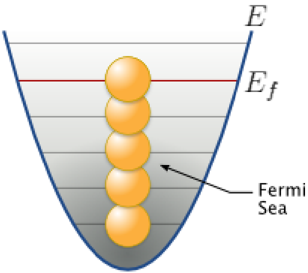


force carriers (fluffy)



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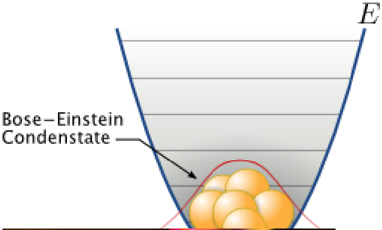

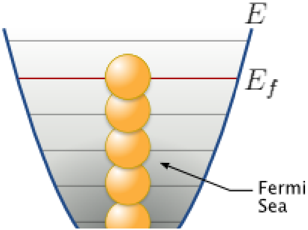

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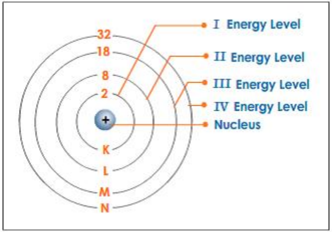


matter (stable)

The Lieb–Thirring inequality

Unifies uncertainty and exclusion & leads to **stability** as $N \to \infty$.

Theorem: For any $s > 0$ there exists a constant $K > 0$ such that

$$\left\langle \sum_{j=1}^{N} (-\Delta_{\mathbf{x}_j})^s \right\rangle_{\Psi} \geq K \int_{\mathbb{R}^d} \varrho_\Psi(\mathbf{x})^{1+2s/d} d\mathbf{x}$$

for all $N \geq 1$ and $\Psi \in H^s(\mathbb{R}^{dN})$, $\int_{\mathbb{R}^{dN}} |\Psi|^2 = 1$, satisfying
Pauli's exclusion principle (fermions):

$$\Psi(\mathbf{x}_1, ..., \mathbf{x}_i, ..., \mathbf{x}_j, ..., \mathbf{x}_N) = -\Psi(\mathbf{x}_1, ..., \mathbf{x}_j, ..., \mathbf{x}_i, ..., \mathbf{x}_N) \quad \forall i \neq j.$$

Note: without this (ex. bosons) $K \to K/N^{2s/d}$ (and **no** stability).

[Dyson, Lenard, 1967; Lieb, Thirring, 1975 ($s = 1$); Daubechies, 1983 ($s > 0$)..]

A Lieb–Thirring inequality for bosons

Theorem: For any $s > 0$, $\beta \geq 0$ there exists a constant K_β s.t.

$$\left\langle \sum_{j=1}^{N} (-\Delta_{\mathbf{x}_j})^s + \beta \sum_{1 \leq j < k \leq N} |\mathbf{x}_j - \mathbf{x}_k|^{-2s} \right\rangle_\Psi \geq K_\beta \int_{\mathbb{R}^d} \varrho_\Psi(\mathbf{x})^{1+2s/d} d\mathbf{x}$$

for all $N \geq 1$ and $\Psi \in H^s(\mathbb{R}^{dN})$, $\int_{\mathbb{R}^{dN}} |\Psi|^2 = 1$, where

- if $\beta > 0$ then $K_\beta > 0$,
- if $\beta \to 0$ and $2s < d$ then $K_\beta \sim \beta^{2s/d} \to 0$,
- if $\beta = 0$ and $\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_N) = 0$ whenever $\mathbf{x}_j = \mathbf{x}_k$, $j \neq k$, then $K_{\beta=0} > 0$ if $2s > d$ and $K_{\beta=0} = 0$ if $2s \leq d$.

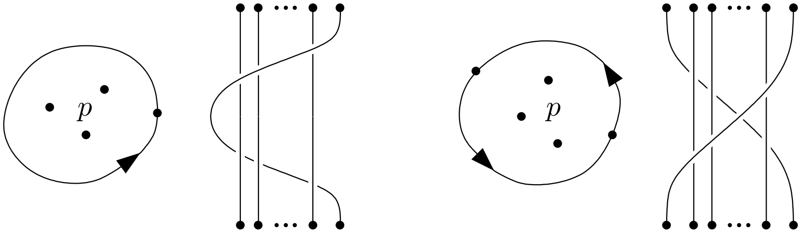
Also $\Rightarrow$ **stability** for such **repulsive bosons**.

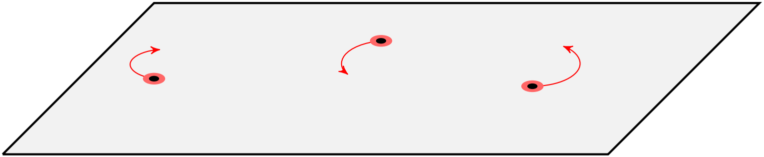
[L., Portmann, Solovej, 2015; L., Nam, Portmann, 2016; Larson, L., Nam, 2019]

Quantum statistics in 2D

More possibilities in 2D!

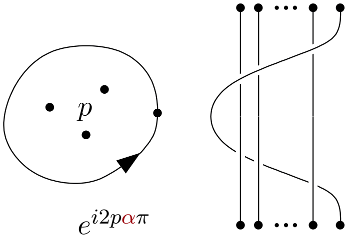
Quantum statistics in 2D — braided exchange

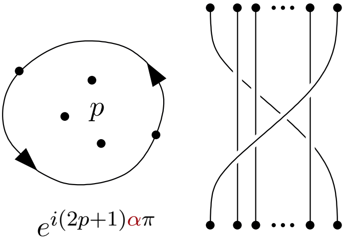


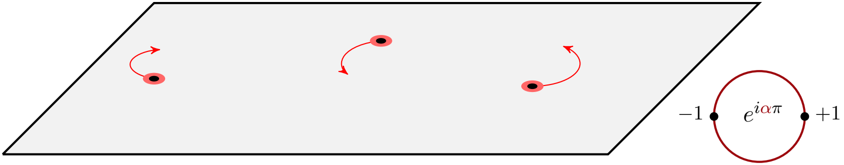


Exchange symmetry $B_N \to \mathrm{U}(1)$

Quantum statistics in 2D — braided exchange







Exchange symmetry $B_N \to \mathrm{U}(1)$ any phase $\Rightarrow$ “**anyons**”

Main results for the many-anyon gas

Instead of studying the spectrum of the Laplacian on $\Omega^N \subseteq \mathbb{R}^{2N}$,

$$\hat{H}_N = \sum_{j=1}^{N} (-\Delta_{\mathbf{x}_j}),$$

we study the magnetically interacting operator (act. on bosons)

$$\hat{H}_N^\alpha = \sum_{j=1}^{N} \left(-i\nabla_{\mathbf{x}_j} + \alpha \sum_{k \neq j} \frac{(\mathbf{x}_j - \mathbf{x}_k)^\perp}{|\mathbf{x}_j - \mathbf{x}_k|^2} \right)^2,$$

with $\alpha \in [0,1]$ and $\mathbf{x}^\perp = (x,y)^\perp = (-y,x)$.

1. Proof of extensivity of the ideal anyon gas g.s.e. (upper/lower bounds) via uncertainty–exclusion (Hardy, Lieb–Thirring).
2. An effective (mean-field) theory for almost-bosonic anyons.
3. A new route to prove its emergence from bosons/fermions.

Main results for the many-anyon gas

Many-body Hardy inequality:

Theorem: For any $\alpha \in [0,1]$, $N \geq 2$ and Ψ in the q.f. domain

$$\langle \hat{H}_N^\alpha \rangle_\Psi \geq \frac{1}{N} \int_{\mathbb{R}^{2N}} \sum_{1 \leq j < k \leq N} \left(\big|\partial_{r_{jk}} |\Psi|\big|^2 + \alpha_N^2 \frac{|\Psi|^2}{r_{jk}^2} \right) d\mathrm{x},$$

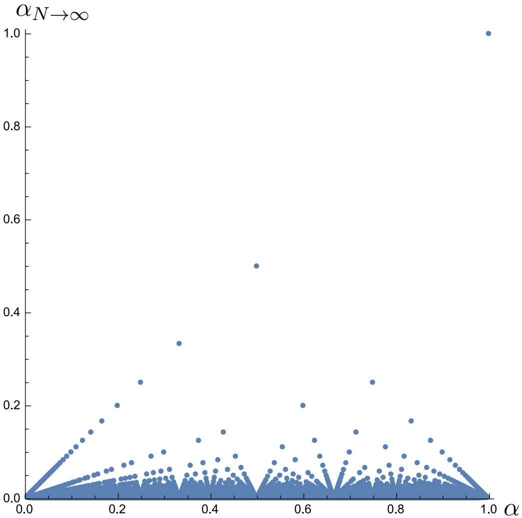
where $r_{jk} = |\mathbf{x}_j - \mathbf{x}_k|/2$ and

$$\alpha_N = \min_{\substack{p \in \{0,1,\ldots,N-2\} \\ q \in \mathbb{Z}}} |(2p+1)\alpha - 2q|$$

$$\geq \frac{1}{n} \quad \text{if } \alpha = \frac{m}{n} \in \mathbb{Q} \text{ reduced, } m \text{ odd.}$$

[L., Solovej, 2013; Larson, L., 2018]

Main results for the many-anyon gas



odd-numerator popcorn / Thomae function

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for all $\alpha \in [0,1]$, $N \geq 1$ and Ψ in q.f. domain, $\int_{\mathbb{R}^{2N}} |\Psi|^2 = 1$.

[L., Solovej, 2013; Larson, L., 2018; L., Seiringer, 2018]

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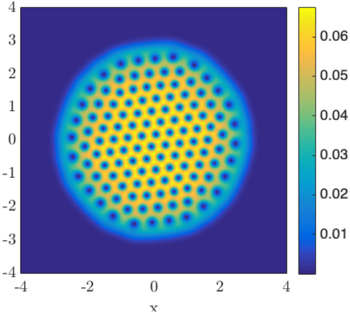

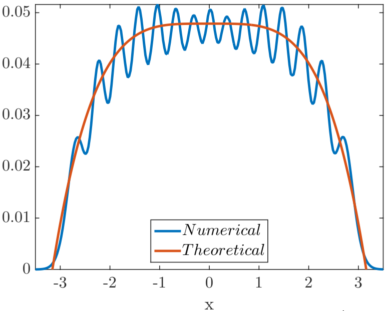

An effective description for **almost-bosonic anyons** $\alpha = \beta/N \to 0$

$$\mathcal{E}^{\mathrm{af}}[\psi] = \int_{\mathbb{R}^2} \left(\left| (-i\nabla + \beta \mathbf{A}[|\psi|^2])\psi \right|^2 + V|\psi|^2 \right)$$

$$\mathcal{E}^{\mathrm{TF}}[\varrho] = \int_{\mathbb{R}^2} \left(2\pi e(1,1)\beta \varrho^2 + V\rho \right)$$

[L., Rougerie, 2015; Correggi, L., Rougerie, 2017; +Duboscq 2019]