

Lieb-Thirring bounds for interacting Bose gases

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based on joint work with
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Outline of Talk

- ① Introduction to quantum gases
- ② Old and new Lieb-Thirring inequalities
- ③ Repulsion \Rightarrow local exclusion principle
- ④ Local uncertainty principle
- ⑤ General Lieb-Thirring type inequalities
- ⑥ Generalizations to fractional operators, HLT, interpolation

The interacting quantum gas

N -particle Hamiltonian with repulsive pair interaction $W(\mathbf{x}) \geq 0$:

$$\hat{H}_N = \hat{T} + \hat{V} + \hat{W} = \sum_{j=1}^N (-\Delta_j + V(\mathbf{x}_j)) + \sum_{1 \leq j < k \leq N} W(\mathbf{x}_j - \mathbf{x}_k),$$

acting on normalized wave functions $\Psi \in L^2((\mathbb{R}^d)^N)$. $\frac{\hbar^2}{2m} = 1$.

Bosons: $\Psi \in \bigotimes_{\text{sym}}^N L^2(\mathbb{R}^d)$

Fermions: $\Psi \in \bigwedge^N L^2(\mathbb{R}^d)$

← Pauli's exclusion principle: $\psi \wedge \psi = 0$, $\psi \in L^2(\mathbb{R}^d)$

Total energy in the state Ψ :

$$E[\Psi] = \langle \Psi, \hat{H}_N \Psi \rangle = T_\Psi + V_\Psi + W_\Psi$$

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Local particle density

The one-body density associated to Ψ :

$$\rho_{\Psi}(\mathbf{x}) := \sum_{j=1}^N \int_{\mathbb{R}^{d(N-1)}} |\Psi(\mathbf{x}_1, \dots, \mathbf{x}_{j-1}, \mathbf{x}, \mathbf{x}_{j+1}, \dots, \mathbf{x}_N)|^2 \prod_{k \neq j} d\mathbf{x}_k$$

Normalized $\int_{\mathbb{R}^d} \rho_{\Psi} = N$,

$\int_Q \rho_{\Psi}$ = expected number of particles on $Q \subseteq \mathbb{R}^d$.

Aim: Replace functionals of $\Psi \in L^2(\mathbb{R}^{dN})$ (where $N \rightarrow \infty$)
by functionals of $\rho_{\Psi} \in L^1(\mathbb{R}^d)$

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The non-interacting Bose gas

Know: $\Psi_0 = \otimes^N \psi_0$,

ψ_0 normalized ground state of $\hat{H}_1 = -\Delta_{\mathbb{R}^d} + V(\mathbf{x})$

$$E[\Psi_0] = N \langle \psi_0, \hat{H}_1 \psi_0 \rangle = N \int_{\mathbb{R}^d} (|\nabla \psi_0|^2 + V |\psi_0|^2) d\mathbf{x},$$

$$\rho_{\Psi_0}(\mathbf{x}) = N |\psi_0(\mathbf{x})|^2$$

The dilute interacting Bose gas (3D)

Dilute limit $a\bar{\rho}^{1/3} \rightarrow 0$ while $N \rightarrow \infty$. Expect: $\Psi_0 \sim \psi^{\otimes N}$

Gross-Pitaevskii limit: $Na/L \sim \text{const.} \Rightarrow$

$$E[\Psi_0] \rightarrow \mathcal{E}_{\text{GP}}[\phi_0], \quad \rho_{\Psi_0}(\mathbf{x}) \rightarrow |\phi_0(\mathbf{x})|^2,$$

$$\mathcal{E}_{\text{GP}}[\phi] := \int_{\mathbb{R}^3} (|\nabla\phi|^2 + V|\phi|^2 + 4\pi a|\phi|^4) d\mathbf{x}, \quad \int_{\mathbb{R}^3} |\phi|^2 = N$$

'Thomas-Fermi' limit: $Na/L \rightarrow \infty \Rightarrow$

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Rigorous treatments first by Dyson 1957 (hard-sphere & $V = 0$),
more recently and generally by Lieb, Yngvason, Seiringer, ...

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The non-interacting Fermi gas (3D)

Know: $\Psi_0 = \bigwedge_{k=0}^{N-1} \psi_k$, ψ_k lowest states of $\hat{H}_1 = -\Delta_{\mathbb{R}^d} + V(\mathbf{x})$

The free Fermi gas in a box $Q \subset \mathbb{R}^3$:

$$E_0 = \sum_{k=0}^{N-1} \lambda_k \sim C_{\text{TF}} \underbrace{(N/|Q|)^{5/3}}_{\bar{\rho}} |Q|, \quad C_{\text{TF}} = \frac{3}{5} (6\pi^2)^{2/3}$$

\Rightarrow Thomas-Fermi approximation: (Thomas, Fermi, 1927)

$$T_{\Psi_0} + V_{\Psi_0} \approx \int_{\mathbb{R}^3} \left(C_{\text{TF}} \rho_{\Psi_0}(\mathbf{x})^{5/3} + V(\mathbf{x}) \rho_{\Psi_0}(\mathbf{x}) \right) d\mathbf{x}$$

(Precursor to modern density functional theory, DFT)

Pauli repulsion and Lieb-Thirring inequalities

Pauli exclusion: say $q \in \mathbb{N}$ particles allowed in each one-particle state of $\hat{H}_1 = -\Delta_{\mathbb{R}^d} + V(\mathbf{x})$

\Rightarrow Lieb-Thirring inequality: (Lieb, Thirring, 1975)

$$\begin{aligned}\hat{H}_{N,\text{Pauli}} = \hat{T} + \hat{V} &= \sum_{j=1}^N (-\Delta_j + V(\mathbf{x}_j)) \\ &\geq -q \sum_{k=0}^{\infty} |\lambda_k| \geq -q C_d \int_{\mathbb{R}^d} |V_-(\mathbf{x})|^{1+\frac{d}{2}} d\mathbf{x}\end{aligned}$$

\Leftrightarrow kinetic energy inequality: (cp. Thomas-Fermi. New approach due to Rumin, 2011)

$$T_{\Psi} = \int_{\mathbb{R}^{dN}} \sum_{j=1}^N |\nabla_j \Psi|^2 dx \geq \frac{C'_d}{q^{2/d}} \int_{\mathbb{R}^d} \rho_{\Psi}(\mathbf{x})^{1+\frac{2}{d}} dx$$

Bosons: $q = N \rightarrow \infty \Rightarrow$ trivial bounds

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The uncertainty principle and LT

For fermions, $\Psi \in \bigwedge^N L^2(\mathbb{R}^d)$, $\|\Psi\| = 1$:

$$T_\Psi = \int_{\mathbb{R}^{dN}} \sum_{j=1}^N |\nabla_j \Psi|^2 dx \geq \underbrace{C'_d}_{\leq C_{\text{TF}}} \int_{\mathbb{R}^d} \rho_\Psi(\mathbf{x})^{1+\frac{2}{d}} d\mathbf{x}$$

This can also be interpreted as a many-particle generalization of the Gagliardo-Nirenberg-Sobolev inequality

$$\int_{\mathbb{R}^d} |\nabla u|^2 dx \left(\int_{\mathbb{R}^d} |u|^2 dx \right)^{2/d} \geq C \int_{\mathbb{R}^d} |u|^{2(1+2/d)} dx,$$

which is a quantitative formulation of the uncertainty principle.

LT bounds for generalized particle statistics

DL, Solovej, 2011-2013

Abelian **anyons** in 2D, with interchange phase $e^{\alpha\pi i} \in U(1)$:

$$T_{\Psi}^{(\alpha)} := \int_{\mathbb{R}^{2N}} \sum_{j=1}^N \left| (-i\nabla_j + \mathbf{A}_j^{(\alpha)}) \Psi \right|^2 dx \geq C C_{\alpha}^2 \int_{\mathbb{R}^2} \rho_{\Psi}^2 dx,$$

$$C_{\alpha} := \inf_{p,q \in \mathbb{Z}} |(2p+1)\alpha - 2q| = \begin{cases} 1/\nu & \text{if } \alpha = \mu/\nu \in \mathbb{Q}, \mu \text{ odd} \\ 0, & \text{otherwise} \end{cases}$$

Intermediate statistics particles in 1D, modeled as bosons with a pair interaction $W(x) = \eta\delta(x)$ or $\alpha(\alpha-1)/|x|^2$: (cp. Lieb-Liniger / Calogero-Sutherland)

$$T_{\Psi} + W_{\Psi} \geq C \int_{\mathbb{R}} e(c/\rho_{\Psi}(x)) \rho_{\Psi}(x)^3 dx$$

$e(c/\rho) \sim$ local bound for the two-particle energy.

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LT bounds for repulsive Bose gases

DL, Portmann, Solovej, 2014

More generally, replace Pauli repulsion by $W \geq 0$.

Examples of new energy inequalities:

For the hard-sphere gas, $W = W_a^{\text{hs}}$ with diameter $a > 0$, in 3D:

$$T_\Psi + W_\Psi \geq C \int_{\mathbb{R}^3} \min \left\{ a \rho_\Psi(\mathbf{x})^2, \rho_\Psi(\mathbf{x})^{5/3} \right\} d\mathbf{x}$$

cp. $E[\Psi_0]/\text{Vol} \rightarrow 4\pi a \rho^2$ as $a \rho^{1/3} \rightarrow 0$

For hard disks, $W = W_a^{\text{hd}}$, $a > 0$, in 2D:

$$T_\Psi + W_\Psi \geq C \int_{\mathbb{R}^2} \frac{\rho_\Psi(\mathbf{x})^2}{2 + \left(-\ln(a \rho_\Psi(\mathbf{x})^{1/2}/2) \right)_+} d\mathbf{x}$$

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cp. $E[\Psi_0]/\text{Vol} \rightarrow 4\pi \rho^2 / |\ln a^2 \rho|$ as $a \rho^{1/2} \rightarrow 0$

Main idea: Local exclusion principle

Consider a d -dimensional box Q , and the local energy $(T + W)_\Psi^Q :=$

$$\sum_{j=1}^N \int_{\mathbb{R}^{dN}} \chi_Q(\mathbf{x}_j) \left(|\nabla_j \Psi|^2 + \frac{1}{2} \sum_{k \neq j} W(\mathbf{x}_j - \mathbf{x}_k) |\psi|^2 \right) dx.$$

If $W \geq 0$ then

$$(T + W)_\Psi^Q \geq \sum_{n=0}^N E_n p_n(Q),$$

where $E_n(|Q|; W)$ is the g.s. energy for n particles on Q with Neumann b.c., and $p_n(Q)$ the n -particle probability distribution,

$$\sum_{n=0}^N p_n(Q) = 1, \quad \sum_{n=0}^N n p_n(Q) = \int_Q \rho_\Psi.$$

Local exclusion for fermions

cp. Dyson, Lenard, 1967

Let $\psi \in \bigwedge^n L^2(\mathbb{R}^d)$ be a wave function of n fermions and let Q be a d -cube. Then

$$\int_{Q^n} \sum_{j=1}^n |\nabla_j \psi|^2 dx \geq (n-1) \frac{\pi^2}{|Q|^{2/d}} \int_{Q^n} |\psi|^2 dx,$$

hence $E_n \geq (n-1)_+ \pi^2 / |Q|^{2/d}$.

It follows that

$$(T + 'W_{\text{Pauli}}')_{\Psi}^Q \geq \frac{\pi^2}{|Q|^{2/d}} \left(\int_Q \rho_{\Psi}(x) dx - 1 \right)_+.$$

Similarly for $W(x) \sim |x|^{-2}$: $W_{\Psi}^Q \geq \frac{C}{|Q|^{2/d}} \left(\left(\int_Q \rho_{\Psi} \right)^2 - \int_Q \rho_{\Psi} \right)_+.$

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Local uncertainty principle

We combine exclusion with uncertainty:

Lemma (Local uncertainty principle)

Let Ψ be an N -particle wave function on \mathbb{R}^d , and Q a d -cube with volume $|Q|$. Then

$$T_{\Psi}^Q \geq c_1 \frac{\int_Q \rho_{\Psi}^{1+2/d} d\mathbf{x}}{(\int_Q \rho_{\Psi} d\mathbf{x})^{2/d}} - c_2 \frac{\int_Q \rho_{\Psi} d\mathbf{x}}{|Q|^{2/d}},$$

where the constants $c_1, c_2 > 0$ only depend on d .

Idea of proof: $\int_{\mathbb{R}^d} |\nabla \sqrt{\rho_{\Psi}}|^2$ and Poincaré-Sobolev inequality on Q

General Lieb-Thirring type inequalities

General assumptions on W :

Assumption 1 (Local exclusion)

Given W , there exists a function $e(\gamma)$ with

$$\gamma(|Q|) := \tau|Q|^{(2-\alpha)/d}, \quad \alpha, \tau > 0,$$

where $e(\gamma)$ is monotone increasing and concave in γ with $e(0) = 0$, such that for any finite cube Q , any $N \geq 1$ and all normalized $\Psi \in H^1(\mathbb{R}^{dN})$ the local energy satisfies

$$(T + W)_{\Psi}^Q \geq \frac{1}{2} \frac{e(\gamma(|Q|))}{|Q|^{2/d}} \left(\int_Q \rho_{\Psi} - 1 \right)_+,$$

General Lieb-Thirring type inequalities

General assumptions on W :

Assumption 2 (Local uncertainty)

Given W , there exist $\alpha > 0$ and constants $S_1, S_2 > 0$ such that for any finite cube Q , any $N \geq 1$ and all normalized $\Psi \in H^1(\mathbb{R}^{dN})$ we have

$$(T + W)_\Psi^Q \geq \begin{cases} S_1 \frac{\int_Q \rho_\Psi^{1+2/d}}{(\int_Q \rho_\Psi)^{2/d}} - S_2 \frac{\int_Q \rho_\Psi}{|Q|^{2/d}}, & \text{for } 0 < \alpha \leq 2, \\ S_1 \frac{(\int_Q \rho_\Psi^{1+\alpha/d})^{2/\alpha}}{(\int_Q \rho_\Psi)^{2/\alpha+2/d-1}} - S_2 \frac{\int_Q \rho_\Psi}{|Q|^{2/d}}, & \text{for } \alpha > 2. \end{cases}$$

General Lieb-Thirring type inequalities

We also need a boundedness assumption on $e(\gamma)$,

$$\underline{e}_K(\gamma) := \min\{e(\gamma), K\}, \quad K > 0,$$

(arbitrarily strong exclusion cannot be matched by uncertainty)

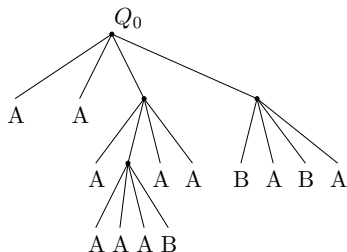
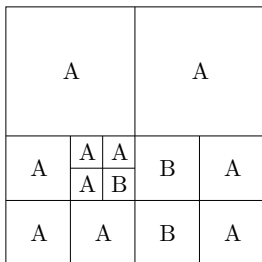
Theorem (Lieb-Thirring inequality)

Let W satisfy Assumption 1 & 2 with an $\alpha > 0$ and e replaced by \underline{e}_K . Then there exists an explicit constant $C_{d,\alpha,K} > 0$, such that for any $N \geq 1$ and all normalized $\Psi \in H^1(\mathbb{R}^{dN})$, the total energy satisfies the bound

$$T_\Psi + W_\Psi \geq C_{d,\alpha,K} \int_{\mathbb{R}^d} \underline{e}_K(\gamma(2/\rho_\Psi(\mathbf{x}))) \rho_\Psi(\mathbf{x})^{1+2/d} d\mathbf{x}.$$

Proof uses a splitting algorithm (Covering lemma)

DL, Solovej, 2011. Convenient reformulation in DL, Nam, Portmann, 2015



Split a cube $Q_0 \subset \mathbb{R}^d$ recursively until each sub-cube contains ≈ 2 particles (B) or < 2 particles (A). Apply local uncertainty on every cube with non-constant density. Apply local exclusion on B-cubes, which also cover for A-cubes with \sim constant density.

Generalizations to fractional operators

DL, Nam, Portmann, 2015

Fractional kin. en. & homogeneous interaction, $d \geq 1$, $s > 0$:

$$\left\langle \Psi, \left(\sum_{j=1}^N (-\Delta_j)^s + \sum_{j < k} \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|^{2s}} \right) \Psi \right\rangle \geq C \int_{\mathbb{R}^d} \rho_{\Psi}^{1 + \frac{2s}{d}} d\mathbf{x}$$

Special case $d = 3$, $s = 1/2$: N equally charged relativistic particles with Coulomb interaction,

$$\left\langle \Psi, \left(\sum_{j=1}^N \sqrt{-\Delta_j} + \sum_{j < k} \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|} \right) \Psi \right\rangle \geq C \int_{\mathbb{R}^3} \rho_{\Psi}^{4/3} d\mathbf{x}$$

Generalizations to fractional operators

Recall Hardy's inequality: $(-\Delta)^s - \frac{C_{d,s}}{|\mathbf{x}|^{2s}} \geq 0$ on $L^2(\mathbb{R}^d)$,

$d \geq 1$, $0 < s < d/2$. Hardy-Lieb-Thirring inequality:

(cp. Ekholm, Frank, Lieb, Seiringer)

$$\left\langle \Psi, \left(\sum_{j=1}^N \left((-\Delta_j)^s - \frac{C_{d,s}}{|\mathbf{x}_j|^{2s}} \right) + \sum_{j < k} \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|^{2s}} \right) \Psi \right\rangle \geq C \int_{\mathbb{R}^d} \rho_{\Psi}^{1 + \frac{2s}{d}} d\mathbf{x}$$

Special case $d = 3$, $s = 1/2$: N equally charged relativistic particles with Coulomb interaction and a static 'nucleus' at $\mathbf{x} = 0$,

$$\hat{H}_N = \sum_{j=1}^N \left(\sqrt{-\Delta_j} - \frac{2/\pi}{|\mathbf{x}_j|} \right) + \sum_{j < k} \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|}$$

One-body interpolation inequalities

Taking $\Psi = u^{\otimes N}$ in our Hardy-Lieb-Thirring inequality \Rightarrow

$$\left\langle u, \left((-\Delta)^s - \frac{C_{d,s}}{|x|^{2s}} \right) u \right\rangle^{1 - \frac{2s}{d}} \left(\iint_{\mathbb{R}^d \times \mathbb{R}^d} \frac{|u(x)|^2 |u(y)|^2}{|x - y|^{2s}} dx dy \right)^{\frac{2s}{d}} \\ \geq C \int_{\mathbb{R}^d} |u(x)|^{2(1+2s/d)} dx,$$

for $0 < s < d/2$. Such an inequality, *without the Hardy term*, was recently proved by Bellazzini, Frank, Ozawa, Visciglia.

Theorem

For $0 < s < d/2$ and $s \leq 1$ this inequality is **equivalent** to HLT.

Idea of proof: Use Hoffmann-Ostenhof and Lieb-Oxford inequalities

An isoperimetric inequality

Our approach to proving LT inequalities can also be applied to prove other interpolation inequalities, for example:

Theorem (Isoperimetric inequality with non-local term)

For any $d \geq 2$ and $1/2 \leq s < d/2$ there exists a constant $C > 0$ depending only on d and s , such that for all functions $u \in W^{1,2s}(\mathbb{R}^d)$ we have

$$\left(\int_{\mathbb{R}^d} |\nabla u|^{2s} dx \right)^{1 - \frac{2s}{d}} \left(\iint_{\mathbb{R}^d \times \mathbb{R}^d} \frac{|u(x)|^{2s} |u(y)|^{2s}}{|x - y|^{2s}} dx dy \right)^{\frac{2s}{d}} \geq C \int_{\mathbb{R}^d} |u|^{2s(1+2s/d)} dx.$$

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