

Recent Results on Lieb-Thirring Inequalities

Rupert L. Frank

Caltech / LMU Munich

8 ECM, Portoroz, June 22, 2021

The Lieb–Thirring inequality

Theorem (Lieb–Thirring (1975))

There is a constant $\mathcal{K}_d > 0$ such that for all $(\psi_n)_{n=1}^N$ that are orthonormal in $L^2(\mathbb{R}^d)$,

$$\sum_{n=1}^N \int_{\mathbb{R}^d} |\nabla \psi_n(x)|^2 dx \geq \mathcal{K}_d \int_{\mathbb{R}^d} \left(\sum_{n=1}^N |\psi_n(x)|^2 \right)^{1+2/d} dx.$$

- **Orthonormality** in $L^2(\mathbb{R}^d)$ means that

$$\int_{\mathbb{R}^d} \overline{\psi_n(x)} \psi_m(x) dx = \delta_{n,m} \quad \text{for all } 1 \leq n, m \leq N.$$

- The key feature is that the constant \mathcal{K}_d is **independent of N** . Without orthonormality, the constant would be $\sim N^{-2/d}$. (Take all ψ_n equal.)
- The left side is the **kinetic energy** of a quantum mechanical state of N (spinless) fermionic particles in \mathbb{R}^d described by the **Slater determinant**

$$\det(\psi_n(x_k))_{n,k=1}^N \quad (x_1, \dots, x_N) \in \mathbb{R}^{dN}.$$

The right side involves the **one-particle density**

$$\sum_{n=1}^N |\psi_n(x)|^2.$$

- The inequality remains valid for general antisymmetric functions.

The Lieb–Thirring inequality, cont'd

Theorem (Lieb–Thirring (1975))

There is a constant $\mathcal{K}_d > 0$ such that for all $(\psi_n)_{n=1}^N$ that are orthonormal in $L^2(\mathbb{R}^d)$,

$$\sum_{n=1}^N \int_{\mathbb{R}^d} |\nabla \psi_n(x)|^2 dx \geq \mathcal{K}_d \int_{\mathbb{R}^d} \left(\sum_{n=1}^N |\psi_n(x)|^2 \right)^{1+2/d} dx.$$

- This is a mathematical quantification of the **uncertainty** and **exclusion principles**, more precisely:
- Since the power on the right side $1 + 2/d > 1$, the inequality restricts the possible concentration of the particle density (\rightarrow **Sobolev inequalities**)
- Since the constant \mathcal{K}_d is independent of N , the $|\psi_n|^2$ 'go out of each other's way' (\rightarrow **atomic orbitals**)
- Important **locality property**: integral is bounded by an integral
- Relevant for stability of matter, density functional theory, nonlinear evolution equations and as a general principle in harmonic analysis.

Atomic orbitals

s

p

d

f



1



2



3



4

Source:

https://en.wikipedia.org/wiki/Atomic_orbital

The Lieb–Thirring conjecture

Theorem (Lieb–Thirring (1975))

There is a constant $\mathcal{K}_d > 0$ such that for all $(\psi_n)_{n=1}^N$ that are orthonormal in $L^2(\mathbb{R}^d)$,

$$\sum_{n=1}^N \int_{\mathbb{R}^d} |\nabla \psi_n(x)|^2 dx \geq \mathcal{K}_d \int_{\mathbb{R}^d} \left(\sum_{n=1}^N |\psi_n(x)|^2 \right)^{1+2/d} dx.$$

What is the optimal value of the constant \mathcal{K}_d ?

Lieb–Thirring (1976) conjectured that the optimal constant is given by

- if $d = 1, 2$ by the constant for $N = 1$
- if $d \geq 3$ by a constant corresponding to $N = \infty$ (free Fermi gas, $(2\pi)^{-d/2} e^{ip \cdot x}$)

The Lieb–Thirring conjecture, if correct, would mean that the Thomas–Fermi approximation is a rigorous lower bound to quantum mechanics, which would be a fundamental result in density functional theory.

The Lieb–Thirring conjecture predicts a fundamental difference between dimensions $d = 1, 2$ and $d \geq 3$, which is not understood at all and presents an intriguing problem.

Two recent results

The **Thomas–Fermi** (or **semiclassical**) constant is, with $\omega_d = \text{vol of unit ball in } \mathbb{R}^d$,

$$\mathcal{K}_d^{\text{TF}} = \frac{d}{d+2} \frac{(2\pi)^2}{\omega_d^{2/d}}$$

The **LT conjecture** is that, if $d \geq 3$, $\mathcal{K}_d = \mathcal{K}_d^{\text{TF}}$.

Theorem (F.–Hundertmark–Jex–Nam (2021))

$$\mathcal{K}_d \geq (0.4719)^{1/d} \mathcal{K}_d^{\text{TF}} \quad \text{for all } d \geq 1$$

$(0.4719)^{1/3} \approx 0.7785$; compare with **LT's** 0.1850 and **Dolbeault–Laptev–Loss's** 0.7400.

Denote by $\mathcal{K}_d^{(N)}$ the optimal constant with $\leq N$ functions, so

$$\mathcal{K}_d^{(N)} \geq \mathcal{K}_d^{(N+1)} \quad \text{for all } N \quad \text{and} \quad \lim_{N \rightarrow \infty} \mathcal{K}_d^{(N)} = \mathcal{K}_d$$

Theorem (F.–Gontier–Lewin (2021))

Let $d \geq 3$. There is a sequence (N_j) , diverging to infinity, such that for all j

$$\mathcal{K}_d^{(N_j+1)} < \mathcal{K}_d^{(N_j)}$$

We see a **dimensional dependence**, but we still don't know what \mathcal{K}_d is.

A more general family of Lieb–Thirring inequalities

The Lieb–Thirring inequality mentioned before is equivalent to the special case $\gamma = 1$ of

Theorem (Lieb–Thirring, Cwikel, Lieb, Rozenblum, Weidl)

Let $\gamma \geq 1/2$ if $d = 1$, $\gamma > 0$ if $d = 2$ and $\gamma \geq 0$ if $d \geq 3$. The negative eigenvalues (E_j) of the Schrödinger operator $-\Delta + V$ in $L^2(\mathbb{R}^d)$ satisfy

$$\sum_j |E_j|^\gamma \leq L_{\gamma,d} \int_{\mathbb{R}^d} V(x)_-^{\gamma+d/2} dx.$$

What is the optimal value of the constant $L_{\gamma,d}$?

Lieb–Thirring (1976) conjectured that the optimal constant is given by

$$\max\{L_{\gamma,d}^{(1)}, L_{\gamma,d}^{\text{cl}}\},$$

where $L_{\gamma,d}^{(1)}$, or more generally $L_{\gamma,d}^{(N)}$, is the best constant with the sum on the left side restricted to $j \leq N$, and $L_{\gamma,d}^{\text{cl}}$ is the constant appearing in Weyl asymptotics (with $V \mapsto \lambda V$ and $\lambda \gg 1$)

$$\sum_j |E_j(\lambda)|^\gamma = \text{Tr}(-\Delta + \lambda V)_-^\gamma \sim \iint_{\mathbb{R}^d \times \mathbb{R}^d} (|\xi|^2 + \lambda V(x))_-^\gamma \frac{dx d\xi}{(2\pi)^d} = L_{\gamma,d}^{\text{cl}} \int_{\mathbb{R}^d} (\lambda V)_-^{\gamma+d/2} dx$$

This conjecture is known to hold sometimes (Gardner–Greene–Kruskal–Miura, LT, Aizenman–Lieb, Hundertmark–Lieb–Thomas, Laptev–Weidl) and to fail sometimes (Glaser–Grosse–Martin, Helffer–Robert). Many cases, including $\gamma = 1$, are still open.

The Lieb–Thirring inequality for eigenvalues of Schrödinger operators

$$\sum_{j=1}^N |E_j|^\gamma \leq L_{\gamma,d}^{(N)} \int_{\mathbb{R}^d} V(x)_-^{\gamma+d/2} dx.$$

Theorem (F.–Gontier–Lewin (2021))

Let $d \geq 1$ and $\gamma > \max\{0, 2-d/2\}$. There is a sequence (N_j) , diverging to infinity, such that for all j

$$L_{\gamma,d}^{(N_j+1)} > L_{\gamma,d}^{(N_j)}$$

- In particular, for $N = 1$ we have the strict inequality $L_{\gamma,d}^{(2)} > L_{\gamma,d}^{(1)}$.
- Together with known results, we see that the LT conjecture **fails** if

$$\begin{cases} 1 < \gamma \leq \gamma_{c,2} & \text{if } d = 2, \\ 1/2 < \gamma < 1 & \text{if } d = 3, \\ 0 < \gamma < 1 & \text{if } 4 \leq d \leq 6, \\ 0 \leq \gamma < 1 & \text{if } d \geq 7. \end{cases}$$

It is still believed to **hold**, however, in $d = 1$, as well as for $1 \leq \gamma < 3/2$ in $d \geq 3$.

- Proof based on an **exponentially small attraction** between two distant pieces of V
- Interesting questions about the behavior of optimizing V for $L_{\gamma,d}^{(N)}$ as $N \rightarrow \infty$ / **phase transition** with respect to the parameter γ

Where are we, and where do we go from here?

Summary so far: We have seen that a classical inequality in analysis (namely a certain type the Sobolev inequality) has a generalization to the setting of **orthonormal functions** with an improved dependence (wrt triangle inequality) on the number of functions.

Is this a general principle, valid for a larger class of inequalities?

Is such a principle, if it exists, useful in applications?

More formally: Let \mathcal{H} be a Hilbert space, X a measure space and assume there is a bounded linear operator $T : \mathcal{H} \rightarrow L^q(X)$ for some $q > 2$,

$$\|T\psi\|_{L^q(X)} \lesssim \|\psi\|_{\mathcal{H}}.$$

Question: Is it true that, for some $\sigma < \frac{q}{2}$,

$$\int_X \left(\sum_{n=1}^N |T\psi_n|^2 \right)^{\frac{q}{2}} dx \lesssim N^\sigma \quad \text{if } (\psi_n, \psi_m)_{\mathcal{H}} = \delta_{n,m} \quad ?$$

The bound with $\sigma = \frac{q}{2}$ holds in general, even without orthogonality
A bound with $\sigma < \frac{q}{2}$, if true, relies on the particular operator T in question

Example. Lieb (1983) **Fractional integration:** If $0 < \alpha < d/2$, then

$$\int_{\mathbb{R}^d} \left(\sum_{n=1}^N \left| |x|^{-d+\alpha} * \psi_n \right|^2 \right)^{\frac{d}{d-2\alpha}} dx \lesssim N$$

Equivalent to bound on number of negative eigenvalues of $(-\Delta)^s + V$ through $\int V_-^{\frac{d}{2s}} dx$

Some results of this type

Recently, this principle was investigated in inequalities from harmonic analysis

Theorem (Strichartz ineq – F.–Lewin–Lieb–Seiringer (2014), F.–Sabin (2018))

For $1 \leq q < 1 + 2/(d-1)$, $2/p + d/q = d$, then for orthonormal $(\psi_n) \subset L^2(\mathbb{R}^d)$,

$$\int_{\mathbb{R}} \left(\int_{\mathbb{R}^d} \left(\sum_n |e^{it\Delta} \psi_n|^2 \right)^q dx \right)^{\frac{p}{q}} dt \lesssim N^{\frac{p(q+1)}{2q}}$$

Applications to dynamics of fermions at positive density by [Lewin–Sabin](#)

Theorem (Stein–Tomas inequality – F.–Sabin (2018))

For orthonormal $(\psi_n) \subset L^2(\mathbb{S}^{d-1})$,

$$\int_{\mathbb{R}^d} \left(\sum_n \left| \int_{\mathbb{S}^{d-1}} e^{ix \cdot \omega} \psi_n(\omega) d\omega \right|^2 \right)^{\frac{d+1}{d-1}} dx \lesssim N^{\frac{d}{d-1}}$$

Application to bounds on eigenvalues of Schrödinger operators with [complex potentials](#)

- There are some common features in the proofs, but there is no general method.
- The N dependence in these bounds is [best possible](#).
- There is a regime of q 's for the Strichartz inequality which is not understood.
- **Optimal constants** have not been investigated.

- We have discussed the [Lieb–Thirring inequality](#) as a mathematical quantification of the uncertainty and exclusion principles in physics, with many applications in mathematical physics, analysis and PDE.
- We have seen some recent progress in the quest for the [optimal constant](#) and the structure of optimal configurations.
- We have shown that a mathematical idea behind the Lieb–Thirring inequality extends to other inequalities in harmonic analysis, namely the [Strichartz](#) and the [Stein–Thomas](#) inequalities, and we have established versions of these with an optimal dependence on the number of functions.

THANK YOU FOR YOUR ATTENTION!