Lieb-Thirring Inequalities: What we know and what we want to know

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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

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

- For $N = 1$ this is a well-known Sobolev-type inequality,

$$\int_{\mathbb{R}^d} |\nabla\psi|^2\,dx \geq \mathcal{K}_d^{(1)} \int_{\mathbb{R}^d} |\psi(x)|^{2(1+2/d)}dx\,, \qquad \|\psi\|_2 = 1$$

- 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.)
  Orthonormality allows to beat the triangle inequality.

- Relevant for quantum physics and quantum chemistry (stability of matter, density functional theory), as well as in PDEs (nonlinear evolution equations) and as a general principle in harmonic analysis.

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* $L^2(\mathbb{R}^d)$,

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

Equivalent formulation of the inequality:

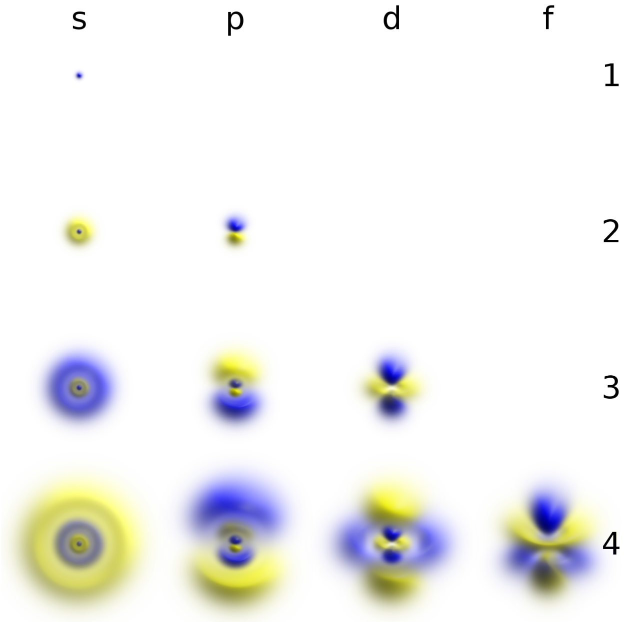
For norm., antisymmetric $\Psi \in L^2(\mathbb{R}^{dN})$ (i.e., $\Psi(\ldots,x_n,\ldots,x_m,\ldots) = -\Psi(\ldots,x_m,\ldots,x_n,\ldots)$, $n \neq m$)

$$\int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d} \sum_{n=1}^N |\nabla_n \Psi(x_1,\ldots,x_N)|^2 \, dx_1 \cdots dx_N \geq \mathcal{K}_d \int_{\mathbb{R}^d} \rho_\Psi(x)^{1+2/d} dx$$

with $\rho_\Psi(x) = \sum_{n=1}^N \int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d} |\Psi(x_1,\ldots,x_{n-1},x,x_n,\ldots,x_N)|^2 \, dx_1 \cdots dx_{n-1} \, dx_{n+1} \cdots dx_N \, .$

- LS: kinetic energy of a quantum mechanical state of N (spinless) fermions in $\mathbb{R}^d$, RS: (const times) Thomas–Fermi approximation involving the one-particle density
- Uncertainty principle: Since the power on the right side $1 + 2/d > 1$, the inequality restricts the possible concentration of the particle density ($\rightarrow$ Sobolev inequalities)
- Pauli exclusion principle: Since the constant $\mathcal{K}_d$ is independent of N, the $|\psi_n|^2$ 'go out of each other's way' ($\rightarrow$ atomic orbitals)

Atomic orbitals



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 as follows

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

The Lieb–Thirring conjecture in 3D, 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 $d \geq 3$. This is not understood at all and presents an intriguing problem.

Two recent results

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

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

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

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

$$\mathcal{K}_d \geq (0.4719)^{1/d} \, \mathcal{K}_d^{\mathrm{TF}} \qquad \textit{for all } d \geq 1$$

$(0.4719)^{1/3} \approx 0.7785$; compare with LT's 0.1850 (and other results since then).

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

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

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

$$\max\{L^{(1)}_{\gamma,d}, L^{\mathrm{cl}}_{\gamma,d}\}\,,$$

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

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

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

Denote by $L_{\gamma,d}^{(N)}$ the optimal constant in

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

so

$$L_{\gamma,d}^{(N)} \leq L_{\gamma,d}^{(N+1)} \quad \text{for all } N \qquad \text{and} \qquad \lim_{N\to\infty} L_{\gamma,d}^{(N)} = L_{\gamma,d}$$

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, the LT conjecture fails for

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

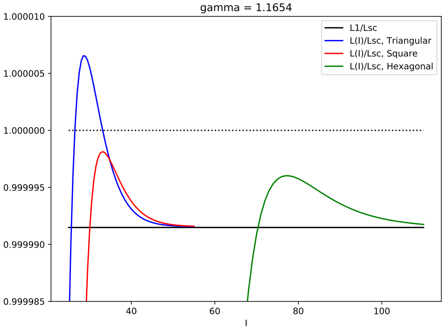
  At the same time, the result gives credence to its validity for $\gamma = 1$ if $d = 3$.
- Proof based on an exponentially small attraction between two distant pieces of V

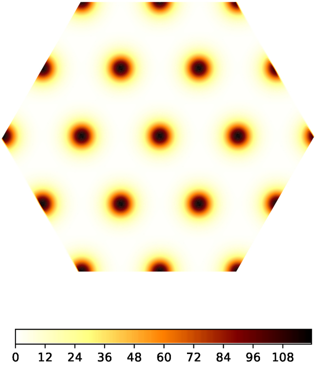
A new scenario for the optimal constant?

The result suggest a new scenario for the optimal constant $L_{\gamma,d}$, namely a

periodic, nonconstant V

- We have verified this analytically for $\gamma = 3/2$ in 1D.
- We have numerical evidence to support this in 2D for $\gamma \approx \gamma_{c,2}$, where we have found periodic potentials that beat both $L^{(1)}_{\gamma,2}$ and $L^{\mathrm{cl}}_{\gamma,2}$.





This corresponds to a 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 $T : \mathcal{H} \to L^q(X)$ for some $q > 2$,

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

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

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

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 several inequalities from harmonic analysis

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

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

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

Applications to dynamics of large fermionic systems by Lewin–Sabin

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

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

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

Application to bounds on eigenvalues of Schrödinger operators with complex potentials
Also, implies that Hausdorff dimension of a Kakeya set is $\geq \frac{d+1}{2}$ (Cuenin)

- There are some common features in the proofs, but there is no general method.
- There is a regime of q's for the Strichartz inequality which is not understood.
- Optimal constants have not been investigated.

Summary

- We have discussed the Lieb–Thirring inequality as a mathematical quantification of the uncertainty and Pauli exclusion principles in quantum mechanics, 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!