Lieb–Thirring bounds and other inequalities for orthonormal functions

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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

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

- 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

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

  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

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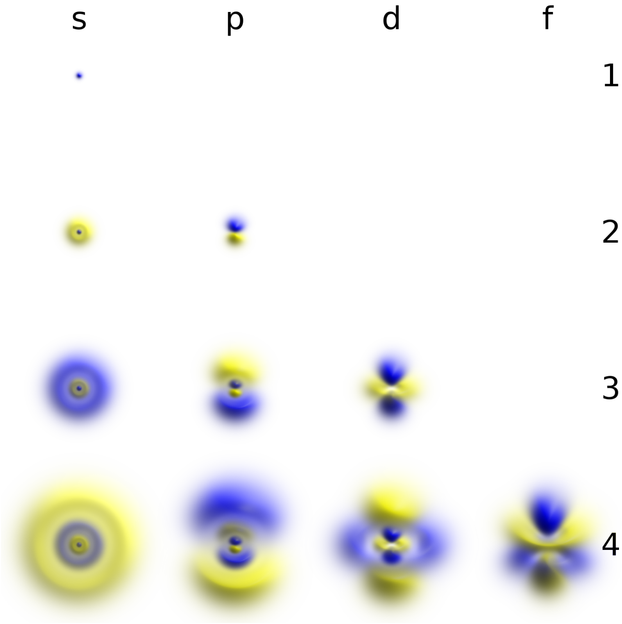
$$\sum_{n=1}^{N} \int_{\mathbb{R}^d} |\nabla \psi_n(x)|^2 \, dx \geq \mathcal{K}_d \int_{\mathbb{R}^d} \left(\sum_{n=1}^{N} |\psi_n(x)|^2 \right)^{1+2/d} dx \, .$$

- 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 (→ Sobolev inequalities)
- Since the constant $\mathcal{K}_d$ is independent of N, the $|\psi_n|^2$ 'go out of each other's way' (→ 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



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 at all understood and presents an intriguing problem.

Two recent results

The Thomas–Fermi (or semiclassical) constant is, with $\omega_d =$ 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 (2018))

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

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

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

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

Theorem (F.–Gontier–Lewin (2020))

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

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

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 $L_{\gamma,d}^{\mathrm{cl}}$ is the constant appearing in Weyl asymptotics (with $V \mapsto \lambda V$ and $\lambda \gg 1$)

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

This conjecture is known to hold sometimes (LT, Aizenman–Lieb, Laptev–Weidl, Hundertmark–Lieb–Thomas) 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

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

Theorem (F.–Gontier–Lewin (2020 & 2021))

Let $d \ge 1$ 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

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

  It is still believed to hold, however, in $d = 1$, as well as for $1 \le \gamma < 3/2$ in $d \ge 3$.
- 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 $N \to \infty$ / 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 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 $\sigma < \frac{q}{2}$,

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

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

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

Applications to dynamics of 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.

The Strichartz inequality for orthonormal functions

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

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

The proof of the inequality uses techniques from harmonic analysis.

Why is $\iint \left(\sum_{n=1}^N \left| \left(e^{it\Delta} \psi_n \right)(x) \right|^2 \right)^{(2+d)/d} dx\, dt \leq C_d\ N^{(d+1)/d}$ best possible?

Heuristics: At $t = 0$ consider N electrons in a box of size L with const density $\rho = L^{-d} N$. For $|t| \geq T$ the electrons have (approximately) disjoint supports and therefore

$$\iint_{|t| \geq T} \left(\sum_{n=1}^N \left| \left(e^{it\Delta} \psi_n \right)(x) \right|^2 \right)^{(2+d)/d} dx\, dt \approx N \ll N^{(d+1)/d}.$$

We think of T as the typical time it takes an electron to move a distance comparable with the size of the system. By Thomas–Fermi theory the expected momentum per particle is $\approx \rho^{1/d}$ and therefore, if the electrons move ballistically $T \approx L \rho^{-1/d}$. Thus,

$$\iint_{|t| \leq T} \left(\sum_{n=1}^N \left| \left(e^{it\Delta} \psi_n \right)(x) \right|^2 \right)^{(2+d)/d} dx\, dt \approx T L^d \rho^{(2+d)/d} \approx N^{(d+1)/d}.$$

Summary

- 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!