The approach to Lieb-Thirring inequalities for Schrödinger operators

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Agenda

We overview Lieb-Thirring inequalities, which estimate the moments of negative eigenvalues of Schrödinger operators in terms of potentials. In particular, we are interested in the optimal constant in the inequalities. Some recent results will be reviewed with the sketch of proof, and numerical approach will also be introduced.

- Lieb-Thirring inequalities
    - Analytical approach
    - Numerical approach

http://www.cc.matsuyama-u.ac.jp/~dan/stability/

Schrödinger operators

Definition (Schrödinger operators)

Let

$$H = -\triangle + V(x) \quad \text{on } L^2(\mathbb{R}^d),$$

where $\triangle = \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2}$ denotes the Laplace operator in $\mathbb{R}^d$ and $V : \mathbb{R}^d \to \mathbb{R}$ is a potential term.

Example (Hydrogenic atom)

$$H = -\triangle - \frac{Z}{|x|} \quad \text{on } L^2(\mathbb{R}^d),$$

Stability of Matter

Quantum systems for N electrons and M nuclei is described by

$$H_{N,M} = \sum_{j=1}^{N} \left(-i\nabla_j + \sqrt{\alpha}A(x_j)\right)^2 + \alpha V(X,R),$$

where $\alpha = e^2/\hbar c \approx 1/137 > 0$ is Sommerfeld's fine structure constant, A is an arbitrary magnetic vector potential in $L^2_{\mathrm{loc}}(\mathbb{R}^3;\mathbb{R}^3)$. The Coulomb potential is written by

$$V(X,R) = \sum_{j=1}^{N}\sum_{k=j+1}^{N} \frac{1}{|x_j - x_k|} - \sum_{j=1}^{N}\sum_{k=1}^{M} \frac{Z_k}{|x_j - R_k|} + \sum_{j=1}^{M}\sum_{k=j+1}^{M} \frac{Z_j Z_k}{|R_j - R_k|},$$

where R_j is the fixed position of j^{th} nucleus.

Stability of Matter

Why is our world stable?

Lieb and Thirring (1976) have improved the result by Dyson and Lenard for the stability of non-relativistic matter.

Theorem (Stability of matter of the second kind)

For all normalized, antisymmetric wavefunction ψ with q spin states, there is a constant $C_{LT} > 0$ such that

$$(\psi, H_{N,M}\psi) \geq -C_{LT}\alpha^2 q^{2/3} (N + M) .$$

It should be remarked that the ground state energy is bounded by the linear dependence on the total number of particles.

Riesz mean

Energy eigenvalues for Schrödinger operators

$E_0, E_1, E_2, \ldots$ denote all non-positive eigenvalues of H.

The moment of order $\gamma \geq 0$ of non-positive eigenvalues for H

$$\mathrm{Tr}\ H_-^\gamma = \sum_j |E_j|^\gamma$$

should be estimated in terms of V. In particular,

$$\sum_j |E_j|^\gamma = \begin{cases} \text{the number of eigenvalues} & \text{for } \gamma = 0 \\ \text{the sum of possible energies} & \text{for } \gamma = 1. \end{cases}$$

Lieb-Thirring inequalities

Theorem (Lieb and Thirring, 1976)

Let $\gamma \geq 0$. Assume $V_- \in L^{\gamma+d/2}(\mathbb{R}^d)$. Then, there is a constant $L_{\gamma,d} > 0$ independent of V such that

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

holds when

$$\begin{cases} \gamma \geq 1/2 & \text{for } d = 1, \\ \gamma > 0 & \text{for } d = 2, \\ \gamma \geq 0 & \text{for } d \geq 3. \end{cases}$$

Otherwise, there is V that violates the above inequalities.

- $V_-(x) = \max\{-V(x), 0\}$, the negative part of V.

Remarks on Lieb-Thirring inequalities

Almost all cases in Lieb-Thirring inequalities was proved by Lieb and Thirring (1976), moreover

- The critical case $\gamma = 0$ for $d \geq 3$, known as CLR bound, Cwikel (1977), Lieb (1980) and Rozenbljum (1972, 1976), independently.
- The remaining case $\gamma = 1/2$ for $d = 1$, Weidl (1996)

The bound cannot hold for

- $\gamma < 1/2$ when $d = 1$ by scaling argument or approximate δ-functions,
- $\gamma = 0$ when $d = 2$, because any arbitrarily small potential in two dimension creates at least one bound state. See also Landau-Lifshitz (1968) or Simon (1976) etc.

Semi-classical approximation

One can prove the semi-classical approximation using Weyl asymptotics

$$L^{\mathrm{cl}}_{\gamma,d} = \lim_{\lambda\to\infty} \frac{\mathrm{Tr}\,(-\triangle + \lambda V(x))^{\gamma}_{-}}{\int (\lambda V(x))^{\gamma+d/2}\, dx}$$

The coefficients $L_{\gamma,d}$ should be compared to classical ones obtained also by

$$L^{\mathrm{cl}}_{\gamma,d} = (2\pi)^d \int_{|p|\le 1} (1-|p|^2)^{\gamma}\ dp = \frac{\Gamma(\gamma+1)}{(4\pi)^{d/2}\Gamma(\gamma+d/2+1)}$$

where Γ is the Gamma function.

Comparison of $L_{\gamma,d}$ with $L^{\mathrm{cl}}_{\gamma,d}$

Some well-known facts about $R_{\gamma,d} = L_{\gamma,d}/L^{\mathrm{cl}}_{\gamma,d}$

- $R_{\gamma,d} \geq 1$ for all possible γ and d, and $R_{\gamma,d}$ is non-increasing on γ. (Aizenman and Lieb, 1978)
- $R_{\gamma,d} > 1$ for $\gamma < 1$. (Helffer and Robert, 1990)
- $R_{1/2,1} = 2$. (Hundertmark, Lieb and Thomas, 1998)
- $R_{\gamma,1} = 1$ for $\gamma \geq 3/2$. (Hundertmark, Laptev and Weidl, 2000)
- $R_{\gamma,d} = 1$ if $\gamma \geq 3/2$ for all d. (Laptev and Weidl, 2000)

Proposition

There exist $\gamma_{C,d} \in [1, 3/2] \subset \mathbb{R}$ such that

$$\begin{cases} R_{\gamma,d} > 1 & \textit{if } \gamma < \gamma_{C,d} \\ R_{\gamma,d} = 1 & \textit{if } \gamma \geq \gamma_{C,d}. \end{cases}$$

Open Question

Computational approach suggests the value of $\gamma_{C,d}$ with restriction of only one eigenvalue.

$\gamma_{C,1} = 3/2$	analytical (solved)
$\gamma_{C,2} \approx 1.165$	computational (unsolved)
$\gamma_{C,3} \approx 0.863$	computational (unsolved)

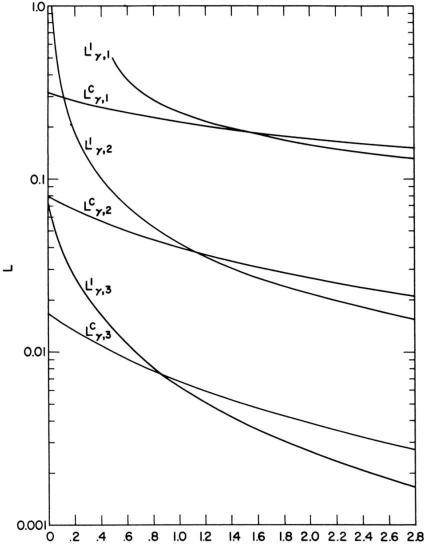
Conjecture (Lieb and Thirring, 1976)

There exist $\gamma_{C,d} > 0$ such that

$$L_{\gamma,d} = \begin{cases} L^C_{\gamma,d} & \gamma \geq \gamma_{C,d} \\ L^1_{\gamma,d} & \gamma \leq \gamma_{C,d}, \end{cases}$$

where $L^1_{\gamma,d}$ denotes the LT constant for only one eigenvalue.

Numerical Studies by Barnes in Lieb-Thirring 1976



Recent results: Case I

Dolbeault, Laptev and Loss (2008) have improved the coefficient which is also known as best possible at the present time.

Dolbeault, Laptev and Loss, 2008

$$R_{1,d} = L_{1,d}/L^{\mathrm{cl}}_{1,d} \leq \pi/\sqrt{3} = 1.81\ldots \quad \text{for all } d.$$

$$L^{\mathrm{cl}}_{1,1} = \frac{\Gamma(1+1)}{(4\pi)^{1/2}\Gamma(1+1/2+1)} = \frac{2}{3\pi}$$

- J. Dolbeault, A. Laptev and M. Loss; J. Eur. Math. Soc., Vol. 10, pp. 1121-1126. (2008)

Lemma I - 1

Lemma

Assume that $\{\phi_n\}_{n=1}^N$ *is orthonormal in* $H^1(\mathbb{R};\mathbb{C}^M)$*. Then,*

$$\int_{\mathbb{R}} Tr\left[U(x,x)^3\right]\ dx \leq \sum_{n=1}^{N} \int_{\mathbb{R}} |\nabla\phi_n(x)|^2\ dx,$$

where $U = \{u_{jk}\}_{j,k=1}^M$ *with*

$$u_{jk}(x,y) = \sum_{n=1}^{N} \phi_n(x,j)\overline{\phi_n(y,k)}$$

for $j,k = 1,\ldots,M$.

Sketch of Proof for the Case I

Let ϕ_n be an eigenfunction corresponding to the eigenvalue E_n,

$$\sum_{n=1}^{N} E_n = \sum_{n=1}^{N} \sum_{j=1}^{M} \int_{\mathbb{R}} |\phi_n'(x,j)|^2 \, dx - \int_{\mathbb{R}} \mathrm{Tr}\left[V(x)U(x,x)\right] \, dx.$$

The Hölder inequality implies

$$\begin{aligned} &\int_{\mathbb{R}} \mathrm{Tr}\left[V(x)U(x,x)\right] \, dx \\ &\quad \leq \left(\int_{\mathbb{R}} \mathrm{Tr}\left[V(x)^{3/2}\right] \, dx \right)^{2/3} \left(\int_{\mathbb{R}} \mathrm{Tr}\left[U(x,x)^{3}\right] \, dx \right)^{1/3}. \end{aligned}$$

Using Lemma and $X = \int_{\mathbb{R}} \mathrm{Tr}\left[U(x,x)^3\right] \, dx$,

$$\begin{aligned} \sum_{n=1}^{N} E_n &\geq X - \left(\int_{\mathbb{R}} \mathrm{Tr}\left[V(x)^{3/2}\right] \, dx \right)^{2/3} X^{1/3} \\ &\geq -\frac{2}{3\sqrt{3}} \int_{\mathbb{R}} \mathrm{Tr}\left[V(x)^{3/2}\right] \, dx. \end{aligned}$$

Recent results: Case II

Rumin and Solovej has proposed a new approach of proving that

Rumin and Solovej, 2011

$$R_{1,d} = L_{1,d}/L^{\mathrm{cl}}_{1,d} \le \left(\frac{d+4}{d}\right)^{d/2}.$$

- M. Rumin, Duke Math. J., **160**, no. 3, 567–597. (2011)
- J. P. Solovej, "The Lieb-Thirring inequality." (2011)

Energy cutoff method

For $\phi \in L^2(\mathbb{R}^d)$ we use

$$\phi^\varepsilon(x) = \mathcal{F}^{-1}\left[\chi_{[0,\varepsilon)}(|p|^2)\hat{\phi}(p)\right],$$

where $\mathcal{F}^{-1}$ is the Fourier inverse transform and χ denotes the characteristic function

$$\chi_{[0,\varepsilon)}(x) = \begin{cases} 1 & \text{if } 0 \le x < \varepsilon, \\ 0 & \text{otherwise.} \end{cases}$$

Lemma II - 1

Lemma

For every $\phi \in H^1$

$$\int_{\mathbb{R}^d} |\nabla \phi(x)|^2 \, dx = \int_{\mathbb{R}^d} \int_0^\infty |\phi(x) - \phi^\varepsilon(x)|^2 \, d\varepsilon dx.$$

$$\begin{aligned}
\int_{\mathbb{R}^d} |\nabla \phi(x)|^2 \, dx &= \int_{\mathbb{R}^d} |p|^2 |\hat{\phi}(p)|^2 dp \\
&= \int_{\mathbb{R}^d} \int_0^{|p|^2} |\hat{\phi}(p)|^2 \, d\varepsilon dp \\
&= \int_{\mathbb{R}^d} \int_0^\infty (1 - \chi_{[0,\varepsilon)}(|p|^2)) |\hat{\phi}(p)|^2 \, d\varepsilon dp.
\end{aligned}$$

Lemma II - 2

Lemma

For any sequence $\{\phi_j\}_j \subset L^2(\mathbb{R}^d)$

$$(\sum_j |\phi_j(x) - \phi_j^\varepsilon(x)|^2)^{1/2} \geq \left[(\sum_j |\phi_j(x)|^2)^{1/2} - (\sum_j |\phi_j^\varepsilon(x)|^2)^{1/2} \right]_+ ,$$

where $[f]_+$ *denotes the positive part of* f.

$$(\sum_j |\phi_j(x)|^2)^{1/2} \leq (\sum_j |\phi_j(x) - \phi_j^\varepsilon(x)|^2)^{1/2} + (\sum_j |\phi_j^\varepsilon(x)|^2)^{1/2}$$

Lemma II - 3

Lemma

Let $\{\phi_j\}_j$ be an orthonormal system in $L^2(\mathbb{R}^d)$. Then

$$\sum_j |\phi_j^\varepsilon(x)|^2 \leq (2\pi)^{-d} d^{-1} |S^{d-1}| \varepsilon^{d/2},$$

where $|S^{d-1}|$ denotes the surface area of the unit ball in $\mathbb{R}^d$.

For any sequence $\{\phi_j\}_j \subset L^2(\mathbb{R}^d)$, we call $\{\phi_j\}_j$ is an orthonormal system in $L^2(\mathbb{R}^d)$ if $(\phi_j, \phi_k) = \delta_{jk}$ for any j and k, where

$$\delta_{jk} = \begin{cases} 1 & \text{if } j = k \\ 0 & \text{if } j \neq k \end{cases}.$$

We begin with

$$\phi_j^\varepsilon(x) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} e^{ix\cdot p} \hat{\phi}_j^\varepsilon(p)\ dp.$$

Since $\{\hat{\phi}_j\}_j$ is also an orthonormal system in momentum space by assumption, we obtain

$$\begin{aligned}
\sum_j |\phi_j^\varepsilon(x)|^2 &= (2\pi)^{-d} \sum_j \left| \int_{\mathbb{R}^d} e^{ix\cdot p} \hat{\phi}_j^\varepsilon(p)\ dp \right|^2 \\
&= (2\pi)^{-d} \sum_j \left| \int_{\mathbb{R}^d} e^{ix\cdot p} \chi_{[0,\varepsilon)}(|p|^2) \hat{\phi}_j(p)\ dp \right|^2 \\
&\leq (2\pi)^{-d} \int_{\mathbb{R}^d} \left| e^{ix\cdot p} \chi_{[0,\varepsilon)}(|p|^2) \right|^2\ dp
\end{aligned}$$

by Bessel's inequality.

At the last integral, we change variables $p = r\omega$ with $r \in [0, \infty)$ and $\omega \in S^{d-1} = \left\{\omega \in \mathbb{R}^d; |\omega| = 1\right\}$, then $dp = r^{d-1} dr d\omega$ and

$$\int_{\mathbb{R}^d} \left| e^{ix\cdot p} \chi_{[0,\varepsilon)}(|p|^2) \right|^2 \, dp = \int_{S^{d-1}} d\omega \int_0^\infty \left| \chi_{[0,\varepsilon)}(r^2) \right|^2 \, r^{d-1} \, dr.$$

By the definition of χ, we have

$$\int_0^\infty \left| \chi_{[0,\varepsilon)}(r^2) \right|^2 \, r^{d-1} dr = \int_0^{\varepsilon^{1/2}} \, r^{d-1} \, dr = d^{-1} \varepsilon^{d/2},$$

which completes the proof of Lemma.

Estimate for Kinetic Energy

We need to estimate the lower bound of kinetic energies for orthonormal systems in order to estimate the Riesz mean.

Proposition (Solovej, 2011)

Let $\{\phi_j\}_j$ be an orthonormal system in $L^2(\mathbb{R}^d)$. Then

$$\begin{aligned}&\sum_j \int_{\mathbb{R}^d} |\nabla \phi_j(x)|^2 \, dx \\ &\geq \frac{(2\pi)^2 d^{2+2/d} |S^{d-1}|^{-2/d}}{(d+2)(d+4)} \int_{\mathbb{R}^d} \Big(\sum_j |\phi_j(x)|^2\Big)^{1+2/d} \, dx.\end{aligned} \tag{1}$$

Solovej's approach

$$\int_{\mathbb{R}^d}\int_0^\infty \left[(\sum_j |\phi_j(x)|^2)^{1/2} - (\sum_j |\phi_j^\varepsilon(x)|^2)^{1/2}\right]_+^2 \, d\varepsilon dx$$
$$\geq \int_{\mathbb{R}^d}\int_0^\infty \left[A_0(x) - B\varepsilon^{d/4}\right]_+^2 \, d\varepsilon dx.$$

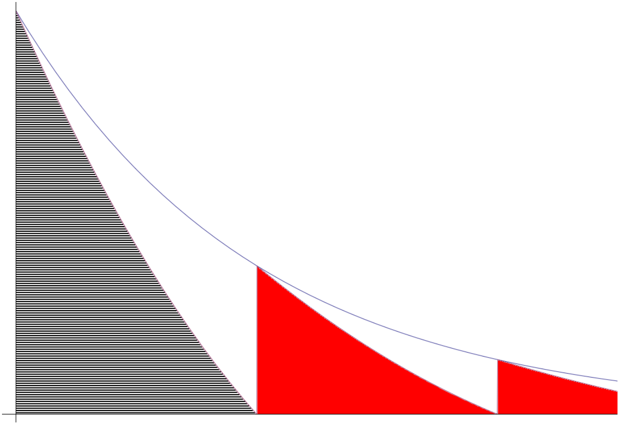
In the last inequality, we have used

$$A_0(x) = \left(\sum_j |\phi_j(x)|^2\right)^{1/2}$$

and

$$B = (2\pi)^{-d/2} d^{-1/2} |S^{d-1}|^{1/2}.$$

Figure



Applications

Lieb-Thirring inequalities can be applied

- to estimate the ground state energy of quantum systems, Lieb and Thrring (1976)
- to estimate dimensions of attractors in theory of the Navier-Stokes equations, Lieb (1984)
- to prove a geometrical problem for ovals in the plane, Benguria and Loss (2004)

Lieb-Thirring conjecture

It is conjectured by Lieb and Thirring (1976) that the optimal $L_{1,3}$ coincides with $L_{1,3}^{\mathrm{cl}}$.

Conjecture (Lieb and Thirring, 1976)

$$L_{1,3} = L_{1,3}^{cl}$$

Case I (Dolbeault, Laptev and Loss, 2008)

$$R_{1,d} = L_{1,d}/L_{1,d}^{\mathrm{cl}} \leq \pi/\sqrt{3} = 1.81\ldots \quad \text{for all } d.$$

Case II (Rumin and Solovej, 2011)

$$L_{1,d}/L_{1,d}^{\mathrm{cl}} \leq \left(\frac{d+4}{d}\right)^{d/2} = \left(\frac{3+4}{3}\right)^{3/2} \approx 3.56 \text{ when } d = 3.$$

Numerical Studies for Conjecture by Barnes, 1976

II. *The Exponential Potential*

To test the conjecture that $L_{1,3} = L^C_{1,3}$, the eigenvalues of the potential $V_\lambda = -\lambda \exp(-|x|)$ in three dimensions were evaluated for $\lambda = 5, 10, 20, 30, 40, 50$, and 100. These are listed in the table according to angular momentum and radial nodes. These numbers have been corroborated by H. Grosse, and they can be used to calculate $L_{\gamma,3}(V_\lambda)$ for any γ. The final column gives $L_{1,3}(V_\lambda)$, since $\int |V_\lambda|^{5/2} = \lambda^{5/2}(64\pi)/125$. It is to be noted that the classical value $L^C_{1,3} = 0.006755$, is approached from below, in agreement with the conjecture, but *not monotonically*.

$$V_\lambda = -\lambda e^{-r}$$

	ℓ	$\lvert e\rvert$	nodes	states	$\sum \lvert e\rvert$	$\dfrac{\sum \lvert e\rvert}{\lambda^{5/2}\frac{64\pi}{125}}$
$\lambda = 5$	0	0.55032	0	$\frac{1}{1}$	$\frac{0.55032}{0.55032}$	0.006120
$\lambda = 10$	0	0.06963	1			
		2.18241	0	2	2.2520	

Recent result through numerical approach

Conjecture (Levitt, 2014)

$$R_{\gamma,1} = 2\left(\frac{\gamma - 1/2}{\gamma + 1/2}\right)^{\gamma - 1/2} \quad \textit{for } \gamma \leq \frac{3}{2}$$

Conjecture (Levitt, 2014)

$$\gamma_{C,2} = \gamma^1_{C,2} \approx 1.16$$

Conjecture (Levitt, 2014)

$$\gamma_{C,3} = 1, \quad \textit{that is, } L_{1,3} = L^{cl}_{1,3}.$$

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Concluding remarks

- We reviewed the analytical and numerical approach to Lieb-Thirring inequalities for Schrödinger operators.
- We have struggled at the challenge to Lieb-Thirring conjecture $L_{1,3} = L_{1,3}^{\mathrm{cl}}$.
- Numerical studies agree with Lieb-Thirring conjecture within mainly radial potentials.

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