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Spectral analysis of Schrödinger operators

Schrödinger operators

$$H = -\Delta + V(x)$$
 in $L^2(\mathbb{R}^d)$

where Δ denotes Laplacian in \mathbb{R}^d and V is a real-valued function of \mathbb{R}^d .

Non-positive eigenvalues

 $\{E_i\}$ = all non-positive eigenvalues of H

Lieb-Thirring inequalities (1976)

Let $\gamma \ge 0$. Assume that the negative part of the potential $V_-(x) = \max\{-V(x), 0\}$ satisfies the condition $V_- \in L^{\gamma+d/2}(\mathbb{R}^d)$. Then, there is a constant $L_{\gamma,d} > 0$ for suitable d defined below which is independent of V such that

$$\sum_{j} |E_{j}|^{\gamma} \leq L_{\gamma,d} \int_{\mathbb{R}^{d}} V_{-}(x)^{\gamma+d/2} dx. \tag{1}$$

This holds in the following cases:

$$\gamma \ge 1/2$$
 for $d = 1$,
 $\gamma > 0$ for $d = 2$,
 $\gamma \ge 0$ for $d \ge 3$. (2)

Otherwise, there is V that violates (1) for any finite choice of $L_{\gamma,d}$.

History - Recent development

We are interesting in

$$R_{\gamma,d} = L_{\gamma,d} / L_{\gamma,d}^{\text{cl}} \tag{1}$$

where

$$L_{\gamma,d}^{\text{cl}} = (2\pi)^d \int_{|p| \le 1} (1 - |p|^2)^{\gamma} dp = \frac{2(2\pi)^{-d} |S^{d-1}|}{d(d+2)}$$
(2)
Find the surface area of the unit ball in \mathbb{R}^d

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

Dolbeault, Laptev and Loss (2008)

$$R_{1,d} \le \pi/\sqrt{3} = 1.81...$$

Rumin (2011), Solovej (2011)

$$R_{1,d} \le \left(\frac{d+4}{d}\right)^{d/2}$$

Cut-off wavefunction in momentum space

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

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

where ${\mathscr F}$ stands for Fourier transform and χ denotes the characteristic function defined by

$$\chi_{[0,\varepsilon)}(|p|^2) = \begin{cases} 1 & \text{if } 0 \le |p|^2 < \varepsilon \\ 0 & \text{if } \varepsilon \le |p|^2 \end{cases} . \tag{2}$$

Lemma 1

For every $\phi \in H^1$

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

Lemma 2

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

$$\left(\sum_{j} |\phi_{j}(x) - \phi_{j}^{\ell}(x)|^{2}\right)^{1/2} \ge \left[\left(\sum_{j} |\phi_{j}(x)|^{2}\right)^{1/2} - \left(\sum_{j} |\phi_{j}^{\ell}(x)|^{2}\right)^{1/2}\right]_{+},$$

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

Lemma 3

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

$$\sum_{j} |\phi_{j}^{\epsilon}(x)|^{2} \leq (2\pi)^{-d} d^{-1} |S^{d-1}| \varepsilon^{d/2},$$

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

Proposition for kinetic energy [Solovej]

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

$$\sum_{j} \int_{\mathbb{R}^{d}} |\nabla \phi_{j}(x)|^{2} dx \geq \frac{(2\pi)^{2} d^{2+2/d} |S^{d-1}|^{-2/d}}{(d+2)(d+4)} \int_{\mathbb{R}^{d}} (\sum_{j} |\phi_{j}(x)|^{2})^{1+2/d} dx.$$

Solovej's approach

$$\sum_{j} \int_{\mathbb{R}^{d}} |\nabla \phi_{j}(x)|^{2} dx \ge \int_{\mathbb{R}^{d}} \int_{0}^{\infty} \left[A_{0} - B \varepsilon^{d/4} \right]_{+}^{2} d\varepsilon dx \tag{1}$$

where

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

and

$$B = (2\pi)^{-d/2} d^{-1/2} |S^{d-1}|^{1/2}.$$
 (3)

Proposed idea

$$\int_0^\infty \left[\left(\sum_j |\phi_j(x)|^2 \right)^{1/2} - \left(\sum_j |\phi_j^{\varepsilon}(x)|^2 \right)^{1/2} \right]_+^2 d\varepsilon \ge \sum_{n=0}^\infty \int_{\varepsilon_n}^{\varepsilon_{n+1}} \{A_n - B(\varepsilon - \varepsilon_n)^{d/4} \}^2 d\varepsilon,$$

where

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

and $\varepsilon_{n+1} - \varepsilon_n = (A_n/B)^{4/d}$ with $\varepsilon_0 = 0$. Then

$$\int_{\epsilon_n}^{\epsilon_{n+1}} \{A_n - B(\epsilon - \epsilon_n)^{d/4}\}^2 d\epsilon = \frac{d^2}{(d+2)(d+4)} B^{-4/d} A_n^{2+4/d}.$$

Conjecture

There is $\kappa > 0$ independent of x and n such that

$$(1 - \kappa^n)^2 \sum_{j} |\phi_j^{\ell_n}(x)|^2 \le \sum_{j} |\phi_j(x)|^2. \tag{1}$$

for any $x \in \mathbb{R}^d$ and n = 0, 1, 2,

Expected results

$$\sum_{j} E_{j} = \sum_{j} (\phi_{j}, H\phi_{j})$$

$$\geq -\frac{2(2\pi)^{-d}|S^{d-1}|}{d(d+2)} \left(\frac{(d+4)(1-\kappa)}{d}\right)^{d/2} \int_{\mathbb{R}^{d}} V_{-}(x)^{1+d/2} dx$$
(1)

with $0 \le \kappa \le 4/(d+4)$. We have just obtained the new estimate in the Lieb-Thirring inequalities for $\gamma = 1$, and

$$R_{1,d} \le \left(\frac{(d+4)(1-\kappa)}{d}\right)^{d/2}.$$
 (2)

Application

- 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 Navier-Stokes equations
 - Lieb (1984)
 - to prove geometrical problem for ovals in the plane
 - Benguria and Loss (2004)

Concluding Remarks

- Lieb-Thirring inequalities play an essential role in stability of quantum systems
- Solovej's previous approach is effective in proof of the inequalities
- If the proposed conjecture is true, we have an improvement of the inequalities