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An Invitation to Lieb-Thirring Inequalities

(following mostly [arXiv:2007.09326] by R.L. Frank)

Introduction to M. Lewin's MCQM Seminar
On some server, probably in Italy, February 8th, 2021

Outline

The starting point: an inequality for orthonormal functions

In 1975, Lieb and Thirring proved a Sobolev-type inequality for a set of orthonormal functions:

Theorem 1 (Lieb–Thirring 1975)

$\forall d \in \mathbb{N}^*$, $\exists K_d > 0$ (optimal) s.t. $\forall N \in \mathbb{N}^*$ and $\forall \{u_1, \ldots, u_N\} \subset H^1(\mathbb{R}^d)$ orthonormal in L^2:

$$\sum_{n=1}^{N} \int_{\mathbb{R}^d} |\nabla u_n|^2 \mathrm{d}x \geq K_d \int_{\mathbb{R}^d} \Big(\sum_{n=1}^{N} |u_n|^2 \Big)^{1+\frac{2}{d}} \mathrm{d}x \, .$$

Original motivation: a (by then) new (now classical) proof of the Stability of Matter

Corollary 1

Let $\{u_n\}_{n\in\mathbb{N}} \subset H^1(\mathbb{R}^d)$ *be a sequence of* L^2*-orthonormal functions, and let* $\{\nu_n\}_{n\in\mathbb{N}} \subset [0,1]$*. Then*

$$\sum_{n\in\mathbb{N}} \nu_n \int_{\mathbb{R}^d} |\nabla u_n|^2 \mathrm{d}x \geq K_d \int_{\mathbb{R}^d} \Big(\sum_{n\in\mathbb{N}} \nu_n |u_n|^2 \Big)^{1+\frac{2}{d}} \mathrm{d}x$$

where K_d *is the optimal constant of Theorem 1.*

Corollary 2

Let $d, N \in \mathbb{N}^*$, and let $\psi(x_1, \dots, x_N) \in H^1(\mathbb{R}^{dN})$ be antisymmetric in the exchange of any $x_i, x_j \in \mathbb{R}^d$, $i \neq j$. Then

$$\int_{\mathbb{R}^{dN}} |\nabla \psi|^2 \mathrm{d}x_1 \cdots \mathrm{d}x_N \geq K_d \|\psi\|_2^{-\frac{d}{2}} \int_{\mathbb{R}^d} \varrho_\psi(x)^{1+\frac{2}{d}} \mathrm{d}x \,,$$

where

$$\varrho_\psi(x) = \sum_{n=1}^{N} \int_{\mathbb{R}^{d(N-1)}} |\psi(x_1, \dots, x_{n-1}, x, x_{n+1}, \dots, x_N)|^2 \mathrm{d}x_1 \cdots \mathrm{d}\widehat{x}_n \cdots \mathrm{d}x_N$$

is the one-particle density of ψ, and K_d is the optimal constant of Theorem 1.

Remarks

- ¡ Both K_d and $1+\frac{2}{d}$ are *independent* of N !
- $\|\varrho_\psi\|_1 = N\|\psi\|_2^2$

Proof of Corollary 2 ($\|\psi\|_2 = 1$)

$$\gamma_\psi(x,y) := \sum_{n=1}^{N} \int_{\mathbb{R}^{d(N-1)}} \bar{\psi}(x_1,\dots,x_{n-1},y,x_{n+1},\dots,x_N)\psi(x_1,\dots,x_{n-1},x,x_{n+1},\dots,x_N)\mathrm{d}x_1\cdots\mathrm{d}\hat{x}_n\cdots\mathrm{d}x_N$$

$\therefore \forall f \in L^2(\mathbb{R}^d)$:

$$\langle f, \gamma_\psi f\rangle_2 \geq 0 ,$$

and

$$\mathrm{Tr}\,\gamma_\psi = \sum_{n=1}^{N} \|\psi\|_2^2 = N .$$

Proof of Corollary 2 (cont.)

Hence $\gamma_\psi \in \mathfrak{S}^1_+(L^2(\mathbb{R}^d))$, and thus

$$\gamma_\psi = \sum_{k\in\mathbb{N}} \nu_k |u_k\rangle\langle u_k| \,.$$

$$\therefore \boxed{\int_{\mathbb{R}^{dN}} |\nabla\psi|^2 \mathrm{d}x_1 \cdots \mathrm{d}x_N = -\operatorname{Tr}\nabla\gamma_\psi\nabla = \sum_{k\in\mathbb{N}} \nu_k \int_{\mathbb{R}^d} |\nabla u_k(x)|^2 \mathrm{d}x} \,,$$

$$\boxed{\varrho(x) = \sum_{k\in\mathbb{N}} |u_k(x)|^2 \qquad \forall x \in \mathbb{R}^d \text{ (Leb.-a.e.)}} \,.$$

The proof follows now immediately from Corollary 1, provided that $\forall k \in \mathbb{N}$, $\nu_k \leq 1$.

Proof of Corollary 2 (end)

However, $\nu_k \leq 1$ since $\|\gamma_\psi\|_{\mathscr{B}(L^2)} \leq 1$. To prove this, the antisymmetry of ψ is *crucial*. Let $\{e_n\}_{n\in\mathbb{N}}$ be an o.n.b. of $L^2(\mathbb{R}^d)$. Then

$$\psi = \sum_{\mathtt{j}\in\mathbb{N}^N} \lambda_{\mathtt{j}}\, e_{j_1} \otimes \cdots \otimes e_{j_N} \,,$$

and

$$\langle e_0, \gamma_\psi e_0 \rangle_2 = \sum_{n=1}^{N} \sum_{\mathtt{i},\mathtt{j}\in\mathbb{N}^N} \lambda_{\mathtt{i}} \bar{\lambda}_{\mathtt{j}}\, \delta_{i_1 j_1} \cdots \delta_{i_n 0} \delta_{j_n 0} \cdots \delta_{i_N j_N} = \sum_{n=1}^{N} \sum_{\mathtt{j}\in\mathbb{N}^N} |\lambda_{\mathtt{j}}|^2 \delta_{j_n 0} \,.$$

By antisymmetry $\lambda_{(\sigma(j_1),\dots,\sigma(j_N))} = (\operatorname{sgn}\sigma)\lambda_{\mathtt{j}}$, and therefore

$$\langle e_0, \gamma_\psi e_0 \rangle_2 = N! \sum_{0=j_1<j_2<\cdots<j_N} |\lambda_{\mathtt{j}}|^2 \leq \sum_{\mathtt{j}\in\mathbb{N}^N} |\lambda_{\mathtt{j}}|^2 = \|\psi\|_2^2 = 1 \,.$$

Since the choice of e_0 is arbitrary, $\|\gamma_\psi\|_{\mathscr{B}(L^2)} \leq 1$. ⊣

- We are now ready to prove that matter consisting of K fixed nuclei and N electrons (seen as nonrelativistic quantum particles) is **stable**, contrarily to its classical counterpart:
  - let $\psi \in L^2(\mathbb{R}^{3N})$ be the (antisymmetric) wavefunction of the N electrons;
  - let $\mathbf{R} = (R_1, \dots, R_K) \in \mathbb{R}^{3K}$ be the (*distinct*) positions of the K nuclei, and $\mathbf{Z} = (Z_1, \dots, Z_K) \in \mathbb{R}_+^K$ their charges;
  - let

$$V_{\mathbf{R},\mathbf{Z}}(x_1, \dots, x_N) = -\sum_{n=1}^{N}\sum_{k=1}^{K} \frac{Z_k}{|x_n - R_k|} + \sum_{1 \le n < m \le N} \frac{1}{|x_n - x_m|} + \sum_{1 \le k < \ell \le K} \frac{Z_k Z_\ell}{|R_k - R_\ell|}$$

    be the Coulomb potential acting on the electrons;
  - Then the energy of the system is given by

$$\mathcal{E}_{\mathbf{R},\mathbf{Z}}[\psi] := \int_{\mathbb{R}^{3N}} \left(|\nabla \psi(x_1, \dots, x_N)|^2 + V_{\mathbf{R},\mathbf{Z}}(x_1, \dots, x_N) |\psi(x_1, \dots, x_N)|^2 \right) \mathrm{d}x_1 \cdots \mathrm{d}x_N$$

Theorem 2 (Stability of Matter)

$\forall \mathbf{R} \in \mathbb{R}^{3K}$ *(such that* $\forall k \neq \ell$*,* $R_k \neq R_\ell$*)* *and* $\forall \mathbf{Z} \in \mathbb{R}_+^K$*:*

$$\mathcal{E}_{\mathbf{R},\mathbf{Z}}(N) := \inf_{\substack{\psi \in H^1(\mathbb{R}^{3N}), \|\psi\|_2 = 1 \\ \psi \text{ antisymm.}}} \mathcal{E}_{\mathbf{R},\mathbf{Z}}[\psi] \geq -\frac{3\pi^{\frac{4}{3}}}{2^{\frac{2}{3}}5} K_3^{-1}(2z+1)^2(N+K)\,,$$

where K_3 *is the optimal constant of Theorem 1 with* $d = 3$*, and* $z = \max_{1 \leq k \leq K} Z_k$*.*

Lemma 1 (Baxter 1980)

$\forall \mathbf{R} \in \mathbb{R}^{3K}$ *($R_k \neq R_\ell$) and* $\mathbf{Z} \in \mathbb{R}_+^K$*, as multiplication operators*

$$V_{\mathbf{R},\mathbf{Z}}(x_1, \dots, x_N) \geq -\sum_{n=1}^{N} \frac{2z+1}{\delta_{\mathbf{R}}(x_n)} ,$$

where $\delta_{\mathbf{R}}(x_n) = \mathtt{min}_{1 \leq k \leq K}\{|x_n - R_k|\}$.

Proof of Theorem 2

We use respectively Corollary 2 (Lieb–Thirring) and Lemma 1 (Baxter) to bound the kinetic and potential energy, obtaining for $\|\psi\|_2 = 1$:

$$\mathcal{E}_{\mathbf{R},\mathbf{Z}}[\psi] \geq K_3 \int_{\mathbb{R}^3} \varrho_\psi^{\frac{5}{3}}(x)\mathrm{d}x - \int_{\mathbb{R}^3} \frac{2z+1}{\delta_{\mathbf{R}}(x)} \varrho_\psi \mathrm{d}x \geq K_3 \int_{\mathbb{R}^3} \varrho_\psi^{\frac{5}{3}}(x)\mathrm{d}x - \int_{\mathbb{R}^3} \left[\frac{2z+1}{\delta_{\mathbf{R}}(x)} - \mu\right]_+ \varrho_\psi(x)\mathrm{d}x - \mu N.$$

Now Hölder's inequality yields, defining $T = \int_{\mathbb{R}^3} \varrho^{\frac{5}{3}}(x)\mathrm{d}x$,

$$\mathcal{E}_{\mathbf{R},\mathbf{Z}}[\psi] \geq K_3 T - \left\| \left[\frac{2z+1}{\delta_{\mathbf{R}}} - \mu\right]_+ \right\|_{\frac{5}{2}} T^{\frac{3}{5}} - \mu N \,.$$

Optimizing with respect to T, we get

$$\mathcal{E}_{\mathbf{R},\mathbf{Z}}[\psi] \geq -\frac{2 \cdot 3^{\frac{3}{2}}}{5^{\frac{5}{2}}} K_3^{-\frac{3}{2}} \left\| \left[\frac{2z+1}{\delta_{\mathbf{R}}} - \mu\right]_+ \right\|_{\frac{5}{2}}^{\frac{5}{2}} - \mu N \,.$$

Proof of Theorem 2 (end)

Let us now scale w.r.t. $\tilde{\mathbf{R}} = \frac{\mu}{2z+1}\mathbf{R}$ and optimize w.r.t. μ obtaining

$$\mathcal{E}_{\mathbf{R},\mathbf{Z}}[\psi] \geq -\frac{3^2}{5^{\frac{5}{3}}} K_3^{-1} (2z+1)^2 N^{\frac{1}{3}} \left\| \left[\frac{1}{\delta_{\tilde{\mathbf{R}}}} - 1 \right]_+ \right\|_{\frac{5}{2}}^{\frac{5}{3}}$$

Finally, observe that

$$\left[\frac{1}{\delta_{\tilde{\mathbf{R}}}(x)} - 1 \right]_+^{\frac{5}{2}} \leq \sum_{k=1}^{K} \left[\frac{1}{|x - \tilde{R}_k|} - 1 \right]_+^{\frac{5}{2}},$$

and

$$\int_{\mathbb{R}^3} \left[\frac{1}{|y|} - 1 \right]_+^{\frac{5}{2}} \mathrm{d}y = 4\pi \int_0^1 (r^{-1} - 1)^{\frac{5}{2}} r^2 \mathrm{d}r = \frac{5\pi^2}{4},$$

to conclude, noting that $K^{\frac{2}{3}} N^{\frac{1}{3}} \leq \frac{2^{\frac{2}{3}}}{3}(K+N)$. ⊣

A dual inequality for Schrödinger operators

Theorem 3 (Lieb-Thirring 1975)

$\forall d \in \mathbb{N}^*$, $\exists L_d \in \mathbb{R}_+$ *such that* $\forall V \in L^{1+\frac{d}{2}}(\mathbb{R}^d, \mathbb{R})$,

$$\boxed{\sum_n \left|E_n^-(-\Delta + V)\right| \leq L_d \int_{\mathbb{R}^d} [V(x)]_-^{1+\frac{d}{2}} \mathrm{d}x \, .}$$

In addition, $L_d = L_d(K_d)$ *by means of*

$$\boxed{\left((1+\tfrac{d}{2})L_d\right)^{1+\frac{2}{d}} \left((1+\tfrac{2}{d})K_d\right)^{1+\frac{d}{2}} = 1 \, .}$$

Remark

$\langle\cdot,(-\Delta+V)\cdot\rangle_2$ is closed and bounded from below on $H^1(\mathbb{R}^d)$ by Gagliardo-Niremberg inequality for any $V\in L^{1+\frac{d}{2}}(\mathbb{R}^d,\mathbb{R})$.

Proof of Theorem 3 $\iff$ Theorem 1

For any $\{u_1,\dots,u_N\}\subset H^1(\mathbb{R}^d)$ that are L^2-orthonormal,

$$\sum_{n=1}^N\int_{\mathbb{R}^d}(|\nabla u_n(x)|^2+V|u_n(x)|^2)\mathrm{d}x\geq\sum_{n=1}^N E_n^-(-\Delta+V)\,,$$

with the equality verified if $-\Delta+V$ has at least N negative eigenvalues (counting multiplicity), and the u_n are $E_n^-(-\Delta+V)$-eigenfunctions. Therefore, the inequality of Theorem 3 implies that for all $N\in\mathbb{N}^*$, and all L^2-orthonormal functions $\{u_1,\dots,u_N\}\subset H^1(\mathbb{R}^d)$:

Proof of Theorem 3 $\iff$ Theorem 1 (end)

$$\sum_{n=1}^{N} \int_{\mathbb{R}^d} |\nabla u_n|^2 \mathrm{d}x \geq -\int_{\mathbb{R}^d} V(x) \sum_{n=1}^{N} |u_n(x)|^2 \mathrm{d}x - L_d \int_{\mathbb{R}^d} [V(x)]_-^{1+\frac{d}{2}} \mathrm{d}x \,.$$

The optimal choice of $V \in L^{1+\frac{d}{2}}(\mathbb{R}^d)$ is given by

$$V(x) = -\left(\tfrac{2+d}{2} L_d\right)^{-\frac{2}{d}} \left(\sum_{n=1}^{N} |u_n|^2 \right)^{\frac{2}{d}}$$

thus proving Theorem 1, with $K_d \geq \frac{d}{d+2}\left(\frac{2+d}{2} L_d\right)^{-\frac{2}{d}}$. Conversely, let V be given. Then by Theorem 1:

$$\sum_{n=1}^{N} \left| E_n^-(-\Delta + V) \right| \leq -K_d \int_{\mathbb{R}^d} \varrho^{1+\frac{2}{d}}(x) \mathrm{d}x + \int_{\mathbb{R}^d} V_-(x) \varrho(x) \mathrm{d}x \,,$$

where $\varrho = \sum_{n=1}^{N} |u_n(x)|^2$. Optimizing over ϱ we conclude the proof, since $L_d \leq \frac{2}{2+d}\left(\frac{d+2}{d} K_d\right)^{-\frac{d}{2}}$. ⊣

An open problem

$$\boxed{K_d = ?}$$

$$\boxed{(L_d = ?)}$$

The one-particle constant

$\exists L_d^{(1)} \in \mathbb{R}_+$ such that $\forall V \in L^{1+\frac{d}{2}}(\mathbb{R}^d, \mathbb{R})$,

$$|E_1^-(-\Delta + V)| \leq L_d^{(1)} \int_{\mathbb{R}^d} [V(x)]_-^{1+\frac{d}{2}} \mathrm{d}x \, .$$

Clearly,

$$\boxed{L_d^{(1)} \leq L_d \, .}$$

In a dual fashion, defining $K_d^{(1)}$ by

$$\left((1+\tfrac{d}{2})L_d^{(1)}\right)^{1+\frac{2}{d}} \left((1+\tfrac{2}{d})K_d^{(1)}\right)^{1+\frac{d}{2}} = 1 \, ,$$

we have that

$$\boxed{K_d \leq K_d^{(1)} \, .}$$

The one particle constants are more convenient for *numerical investigation*.

The semiclassical constant

Weyl asymptotics can be used to evaluate $\mathrm{Tr}[-\hbar^2\Delta + V]_-$ in the limit $\hbar \to 0$, for suitably regular potentials V (in particular $V \in L^{1+\frac{d}{2}}$):

$$\lim_{\hbar\to 0} \hbar^d\,\mathrm{Tr}[-\hbar^2\Delta + V]_- = \int_{\mathbb{R}^{2d}} [|\xi|^2 + V(x)]_- \frac{\mathrm{d}x\mathrm{d}\xi}{(2\pi)^d}\,.$$

On the other hand,

$$\int_{\mathbb{R}^{2d}} [|\xi|^2 + V(x)]\_\mathrm{d}x\mathrm{d}\xi = \frac{2}{2+d}\omega_d \int_{\mathbb{R}^d} [V(x)]_-^{1+\frac{d}{2}}\mathrm{d}x\,,$$

where ω_d is the volume of the d-dimensional ball of radius one. This follows from an explicit calculation (**do it!**) of

$$\int_{\mathbb{R}^d} [|\xi|^2 + V(x)]\_\mathrm{d}\xi\,.$$

Therefore,

$$\lim_{\hbar\to 0} \hbar^{2+d}\,\mathrm{Tr}[-\Delta+\hbar^{-2}V]_- = L_d^{\mathrm{cl}} \int_{\mathbb{R}^d} [V(x)]_-^{1+\frac{d}{2}}\,\mathrm{d}x\,,$$

$$L_d^{\mathrm{cl}} = \frac{2}{2+d}\frac{\omega_d}{(2\pi)^d} \qquad (\textbf{explicit!})$$

Therefore,

$$\lim_{\beta\to\infty} \beta^{-(1+\frac{d}{2})}\,\mathrm{Tr}[-\Delta+\beta V]_- = L_d^{\mathrm{cl}} \int_{\mathbb{R}^d} [V(x)]_-^{1+\frac{d}{2}}\,\mathrm{d}x\,,$$

$$\boxed{L_d^{\mathrm{cl}} = \frac{2}{2+d}\frac{\omega_d}{(2\pi)^d} \quad (\textbf{explicit!})}$$

It follows that, defining $\beta=\hbar^{-2}$, for β large enough (possibly depending on V):

$$\boxed{\sum_n |E_n^-(-\Delta+\beta V)| = \mathrm{Tr}[-\Delta+\beta V]_- \leq L_d^{\mathrm{cl}} \int_{\mathbb{R}^d} [\beta V(x)]_-^{1+\frac{d}{2}}\,\mathrm{d}x\,.}$$

Hence,

$$\boxed{L_d^{\mathrm{cl}} \leq L_d\,.}$$

As before, we can thus define

$$K_d^{\mathrm{cl}} = \frac{d}{d+2} \frac{(2\pi)^2}{\omega_d^{\frac{2}{d}}}$$

by

$$\left((1 + \tfrac{d}{2}) L_d^{\mathrm{cl}} \right)^{1+\frac{2}{d}} \left((1 + \tfrac{2}{d}) K_d^{\mathrm{cl}} \right)^{1+\frac{d}{2}} = 1 \, ,$$

obtaining

$$K_d \leq K_d^{\mathrm{cl}} \, .$$

The Lieb–Thirring conjecture

$$\boxed{K_d = \mathtt{min}\{K_d^{(1)}, K_d^{\mathtt{cl}}\}}$$

$$\boxed{(L_d = \mathtt{max}\{L_d^{(1)}, L_d^{\mathtt{cl}}\})}$$

The current best bounds

$$\boxed{K_d \geq (0.4771851)^{\frac{1}{d}}\, K_d^{\mathrm{cl}}}$$

$$\boxed{L_d \leq 1.456\, L_d^{\mathrm{cl}}}$$

Numerical simulations suggest that $K_d(L_d) = K_d^{(1)}(L_d^{(1)})$ for $d = 1, 2$ and $K_d(L_d) = K_d^{\mathrm{cl}}(L_d^{\mathrm{cl}})$ for $d \geq 3$.

A generalization for Schrödinger operators

Theorem 4 (Lieb-Thirring 1976)

Let $\gamma \geq \frac{1}{2}$ *for* $d = 1$, $\gamma > 0$ *for* $d = 2$, *and* $\gamma \geq 0$ *if* $d \geq 3$. *Then* $\exists L_{\gamma,d} \in \mathbb{R}_+$ *such that* $\forall V \in L^{\gamma+\frac{d}{2}}(\mathbb{R}^d, \mathbb{R})$*:*

$$\boxed{\sum_n \left|E_n^-(-\Delta + V)\right|^\gamma \leq L_{\gamma,d} \int_{\mathbb{R}^d} [V(x)]_-^{\gamma+\frac{d}{2}} \mathrm{d}x \,.}$$

A (partially) open problem

$$\boxed{L_{\gamma,d} = ?}$$

Known results (due to Lieb–Thirring, Aizenman–Lieb, Laptev–Weidl, Benguria–Loss, Hundertmark–Lieb–Thomas, Helffer–Robert, Glaser–Grosse–Martin,…)

Theorem 5

- $L_{\gamma,d} = L^{\mathrm{cl}}_{\gamma,d}$ *if* $\gamma \geq \frac{3}{2}$ *and* $d \geq 1$;
- $L_{\frac{1}{2},1} = L^{(1)}_{\frac{1}{2},1}$.

Theorem 6

- $L_{\gamma,d} > L^{\mathrm{cl}}_{\gamma,d}$ *if* $\gamma < \frac{3}{2}$ *with* $d = 1$, *or* $\gamma < 1$ *with* $d \geq 2$;
- $L_{\gamma,d} > L^{(1)}_{\gamma,d}$ *if* $\gamma > \max\{2 - \frac{d}{2}, 0\}$ *for* $1 \leq d \leq 6$, *or* $\gamma \geq 0$ *for* $d \geq 7$.

The main tool in the proof of Theorem 4: the Birman-Schwinger principle (main ideas)

Definition (Birman-Schwinger operator)

Let $V \in L^{\gamma+\frac{d}{2}}(\mathbb{R}^d, \mathbb{R})$, $\gamma \geq 0$, $V \leq 0$. The Birman-Schwinger operator K_E, $E > 0$, is defined by

$$\boxed{K_E := \sqrt{-V}(-\Delta + E)^{-1}\sqrt{-V}\ .}$$

Properties of the Birman-Schwinger operator:

- $\boxed{K_E \geq 0}$
- $\boxed{K_E \in \mathscr{B}(L^2(\mathbb{R}^d))}$
- $\boxed{E' < E}$ implies $\boxed{K_{E'} \geq K_E}$ (K_E is monotonically decreasing in E)

Theorem 7 (Birman-Schwinger principle)

Let $V \in L^{\gamma+\frac{d}{2}}(\mathbb{R}^d, \mathbb{R})$, $\gamma \geq 0$, $V \leq 0$. In addition, let $n_E(V)$ be the number of eigenvalues of $-\Delta + V$ that are less than E, and let $N_1(K_E)$ be the number of eigenvalues of the Birman-Schwinger operator that are greater than 1. Then,

$$\boxed{n_E(V) = N_1(K_E)\,.}$$

Thank you for the attention