How Much Energy Does it Cost to Make a Hole in the Fermi Sea?

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Lieb-Thirring Inequalities

We consider the Schrödinger operator on $L^2(\mathbb{R}^d)$

$$H = -\Delta + V(x)$$

The LT inequalities bound power sums of the negative eigenvalues of $H$ in terms of some $L^p$-norms of the negative part of the potential, $V(x)_- = \max\{0, -V(x)\}$.

If $\lambda_1, \lambda_2, \ldots$ are the negative eigenvalues of $H$ then

$$\sum_j |\lambda_j|^\kappa \leq L_{\kappa,d} \int_{\mathbb{R}^d} V(x)^{\kappa + d/2} \, dx$$

The (sharp) values of $\kappa \geq 0$ for which the inequality holds are

- for $d = 1$, $\kappa \geq 1/2$ (Lieb, Thirring, Weidl)
- for $d = 2$, $\kappa > 0$ (LT)
- for $d \geq 3$, $\kappa \geq 0$ (Cwikel, Lieb, Rozenblum, LT)
**The Constants** $L_{\kappa,d}$

Note that one can write $\sum_j |\lambda_j|^\kappa = \text{Tr} \left(-\Delta + V(x)\right)_-^\kappa$. A *semiclassical approximation* of the trace yields the phase space integral

$$(2\pi)^{-d} \int_{\mathbb{R}^d \times \mathbb{R}^d} (p^2 + V(x))_-^\kappa dp \, dx = L_{\kappa,d}^\text{scl} \int_{\mathbb{R}^d} V(x)_{-}^{\kappa + d/2} \, dx$$

It is always true that $L_{\kappa,d} \geq L_{\kappa,d}^\text{scl}$

Some *sharp values* for $L_{\kappa,d}$ are known:

- $L_{\kappa,d} = L_{\kappa,d}^\text{scl}$ for all $\kappa \geq 3/2$ and $d = 1$ (LT, Aizenman-Lieb), $d \geq 2$ (Laptev, Weidl)

- $L_{1/2,1} = 1/2$ while $L_{1/2,1}^\text{scl} = 1/4$ (Hundertmark, Lieb, Thomas)

**Open problem:** The optimal constant in the physically most interesting case, $\kappa = 1$ and $d = 3$, remains unknown (and is conjectured to be $L_{1,3} = L_{1,3}^\text{scl}$)
For $\kappa = 1$, the LT Inequality has the dual formulation

$$\text{Tr} \ ( -\Delta )\gamma \geq K_d \int_{\mathbb{R}^d} \rho_\gamma(x)^{1+2/d} \, dx$$

for trace class operators $0 \leq \gamma \leq 1$, with $\rho_\gamma(x) = \gamma(x, x)$. Alternatively,

$$\left\langle \Psi \left| - \sum_{i=1}^N \Delta_i \right| \Psi \right\rangle \geq K_d \int_{\mathbb{R}^d} \rho_\Psi(x)^{1+2/d} \, dx$$

for anti-symmetric functions $\Psi(x_1, \ldots, x_N)$, with

$$\rho_\Psi(x) = N \int_{\mathbb{R}^{d(N-1)}} |\Psi(x, x_2, \ldots, x_N)|^2 \, dx_2 \cdots dx_N$$

The LT Inequality can thus be viewed as giving a lower bound on the minimal kinetic energy needed to assemble a system of fermions at density $\rho(x)$. 

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**Application: Stability of Matter**

A system of charged particles ($N$ electrons and $K$ fixed nuclei) is described by the Hamiltonian

$$H = -\frac{1}{2m} \sum_{j=1}^{N} \Delta_i + e^2 V_{N,K}(x_1, \ldots, x_N; R_1, \ldots, R_K)$$

The Pauli exclusion principle dictates that $H$ acts on anti-symmetric functions in $L^2(\mathbb{R}^{3N})$. The Coulomb potential is

$$V_{N,K} = \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|} - \sum_{j=1}^{N} \sum_{k=1}^{K} \frac{Z_k}{|x_j - R_k|} + \sum_{1 \leq k < l \leq K} \frac{Z_k Z_l}{|R_k - R_l|}.$$  

(electron-electron, electron-nuclei, nuclei-nuclei, respectively).

**Stability of Matter** refers to the fact that

$$\inf_{\{R_k\}} \inf \text{spec } H \geq -\text{const.} \ (N + K)$$
Stability of non-relativistic matter was first proved by Dyson and Lenard in 1967. In 1975, Lieb and Thirring gave a much shorter proof using their inequalities: On the subspace of antisymmetric functions,

$$\sum_{i=1}^{N} (-\Delta_i + V(x_i)) \geq -2 L_{1,d} \int_{\mathbb{R}^d} V(x)^{1+d/2} \, dx$$

The reduction of the many-body Coulomb potential to a one-body potential is achieved via an electrostatic inequality due to Baxter (and refined later by Lieb and Yau):

In the case $Z_k = Z$ for $1 \leq k \leq K$,

$$V_{N,K}(x_1, \ldots, x_N; R_1, \ldots, R_K) \geq - \sum_{i=1}^{N} \frac{2Z + 1}{\min_k |x_i - R_k|}$$

Stability of Matter follows using $V(x) = \lambda - (2Z + 1)/\min_k |x - R_k|$ for some $\lambda > 0$. 

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Imagine an infinite system of non-interacting fermions at some density $\rho > 0$. It is described by the projection

$$\Pi_\mu = 1(-\Delta \leq \mu) \quad \text{with} \quad \mu = 4\pi^2 \left(\frac{\rho}{|\mathbb{B}^d|}\right)^{2/d}$$

We seek a lower bound on the energy difference

$$\text{Tr} \, (-\Delta - \mu)(\gamma - \Pi_\mu)$$

in terms of its semiclassical approximation

$$K^\text{scl}_d \int_{\mathbb{R}^d} \left(\rho_\gamma(x)^{1+2/d} - \rho^{1+2/d} - \frac{2 + d}{d} \rho^{2/d} (\rho_\gamma(x) - \rho)\right) dx$$

Note that the integrand behaves like $(\rho_\gamma(x) - \rho)^2$ for $\rho_\gamma(x)$ close to $\rho$, and like $\rho_\gamma(x)^{1+2/d}$ for large $\rho_\gamma(x)$.
**Lieb-Thirring Inequalities at Positive Density**

**Main result:**

**Theorem 1.** For $d \geq 2$ there exist constants $K_d > 0$ such that for all $0 \leq \gamma \leq 1$

$$\text{Tr} \left( -\Delta - \mu \right) (\gamma - \Pi_\mu) \geq K_d \int_{\mathbb{R}^d} \left( \rho_\gamma(x)^{1+2/d} - \rho^{1+2/d} - \frac{2 + d}{d} \rho^{2/d} (\rho_\gamma(x) - \rho) \right) dx$$

**Remarks.**

1. For $\rho = 0$ this reduces to the usual Lieb-Thirring Inequality

2. By scaling, $K_d$ is independent of $\rho$.

3. No such inequality can hold, in general, for $d = 1$. This can be verified using second-order perturbation theory and is related to the **Peierls instability**.

4. The inequality quantifies the **energy cost** to make a local change in the density of particles.
**Lieb-Thirring Inequality; Potential version**

Via a **Legendre transform**, the theorem leads to the statement that

\[
\text{Tr} \left( (-\Delta - \mu + V)_- - (-\Delta - \mu)_- \right) + \rho \int_{\mathbb{R}^d} V(x) dx \\
\leq L_d \int_{\mathbb{R}^d} \left( (V(x) - \mu)_-^{1+d/2} - \mu^{1+d/2} + \frac{2 + d}{d} \mu^{d/2} V(x) \right) dx
\]

for \( d \geq 2 \). Here, it is only necessary to assume that \( V \in L^2 (\mathbb{R}^d) \cap L^{1+d/2} (\mathbb{R}^d) \), the left side is really equal to

\[-\text{Tr} (-\Delta - \mu + V) \left( 1 (-\Delta + V \leq \mu) - 1 (-\Delta \leq \mu) \right)\]

which is well-defined even if \( V \notin L^1 (\mathbb{R}^d) \).

The right side estimates the **validity of first-order perturbation theory**. The integrand is quadratic in \( V(x) \) for small \( V(x) \), and grows like \(|V(x)|^{1+d/2}\) for large (negative) \( V(x) \).
Comparison with Second-Order Perturbation Theory

For nice enough $V$, one can compute the limit

$$
\lim_{t \to 0} \frac{\text{Tr} \left( -\Delta - \mu + tV \right) \left( 1 \left( -\Delta + tV \leq \mu \right) - 1 \left( -\Delta \leq \mu \right) \right)}{t^2}
$$

$$
= -\mu^{d/2-1} \int_{\mathbb{R}^d} \psi_d \left( \frac{k}{\sqrt{\mu}} \right) |\hat{V}(k)|^2 dk
$$

where

$$
\psi_d(k) = \frac{1}{(2\pi)^d} \int_{\frac{|p| \leq 1}{|p-k| \geq 1}} \frac{dp}{|p-k|^2 - |p|^2}
$$

Note that $\psi_1$ diverges logarithmically at $|k| = 2$, while $\psi_d$ is bounded for $d \geq 2$.

This shows that our Lieb-Thirring inequality fails for $d = 1$! A suitable modified version, with an integrand of the form above, does hold, however.
Ideas in the Proof

Let $Q = \gamma - \Pi_\mu$. Since the right side

$$\int_{\mathbb{R}^d} \left( \rho_\gamma(x)^{1+2/d} - \rho^{1+2/d} - \frac{2 + d}{d} \rho^{2/d} (\rho_\gamma(x) - \rho) \right) dx$$

is convex in $\rho_Q(x) = \rho_\gamma(x) - \rho$, it suffices to consider separately the contributions of

$$Q^{-\gamma} = \Pi_\mu Q \Pi_\mu, \quad Q^{++} = (1 - \Pi_\mu)Q(1 - \Pi_\mu), \quad Q^{-+} = \Pi_\mu Q(1 - \Pi_\mu)$$

Note that $\text{Tr} (-\Delta - \mu)Q = \text{Tr} (-\Delta - \mu)(Q^{++} + Q^{-\gamma})$ with

$$\text{Tr} (-\Delta - \mu)Q^{++} = \text{Tr} (-\Delta - \mu)(1 - \Pi_\mu)^\gamma(1 - \Pi_\mu)$$

and

$$\text{Tr} (-\Delta - \mu)Q^{-\gamma} = \text{Tr} (-\Delta - \mu)|\Pi_\mu(1 - \gamma)\Pi_\mu$$

To bound these terms, we use a recent method of Rumin (for any $d \geq 1$).
Rumin’s Method

The starting point is the representation

$$\text{Tr} (-\Delta - \mu) Q^{++} = \text{Tr} (-\Delta - \mu | Q^{++} = \int_0^\infty dE \text{Tr} Q^{++}_E = \int_{\mathbb{R}^3} dx \int_0^\infty dE \rho^{++}_E(x)$$

where $Q^{++}_E = P_{\geq E} Q^{++} P_{\geq E}$, $\rho^{++}_E(x) = Q^{++}_E(x, x)$, and $P_{\geq E} = 1(| - \Delta - \mu | \geq E)$. By the triangle inequality and $Q^{++} \leq 1$,

$$\sqrt{\rho^{++}(x)} \leq \sqrt{\rho^{++}_E(x)} + \sqrt{r(E)}$$

where $r(E)$ is the density of $P_{\leq E} = 1 - P_{\geq E}$, which is easily found to be

$$r(E) = (2\pi)^{-d} |\mathbb{B}^d| \left( (\mu + E)^{d/2} - (\mu - E)^{d/2}_+ \right)$$

This gives

$$\text{Tr} (-\Delta - \mu) Q^{++} \geq \int_{\mathbb{R}^3} F_d(\rho^{++}(x)) \, dx \quad \text{with} \quad F(y) = \int_0^\infty dE \left( \sqrt{|y|} - \sqrt{r(E)} \right)_+^2.$$
**The Off-Diagonal Terms**

To **conclude the proof** of the theorem, we shall show that

\[
\int_{\mathbb{R}^3} |\rho^{-+}(x)|^2 \, dx \leq \mu^{d/2-1} \|\phi_d\|_{\infty} \text{Tr} (-\Delta - \mu)Q
\]

with

\[
\phi_d(k) = \frac{1}{(2\pi)^d} \int_{|p-k|\geq 1} \frac{dp}{\sqrt{|p-k|^2 - 1} \sqrt{1 - |p|^2}}
\]

which is bounded for \(d \geq 2\). In fact, by **Schwarz’s inequality** and \(Q^2 \leq Q^{++} - Q^{--}\),

\[
\left| \int_{\mathbb{R}^d} V \rho_{Q^{--}} \right| = \left| \text{Tr} \, V \Pi_{\mu} Q (1 - \Pi_{\mu}) \right| \leq \left| \frac{1 - \Pi_{\mu}}{|\Delta + \mu|^{1/4}} V \frac{\Pi_{\mu}}{|\Delta + \mu|^{1/4}} \right| \left[ \text{Tr} (-\Delta - \mu)Q \right]^{1/2}
\]

which implies the statement since the square of the Hilbert-Schmidt norm equals

\[
\mu^{d/2-1} \int_{\mathbb{R}^d} |\hat{V}(k)|^2 \phi_d(k/\sqrt{\mu}) \, dk.
\]
Conclusions

- We have presented a positive density analogue of the Lieb-Thirring Inequalities.
- The bound estimates the energy cost to make a local change in the density of a free electron gas, in terms of the corresponding semiclassical approximation.
- Our inequality concerns the behavior of both the discrete and the continuous spectrum of the Laplacian under local perturbations.
- A similar bound can be proved at positive temperature.
- The method can be generalized in various ways, e.g., to particles in a periodic background potential.