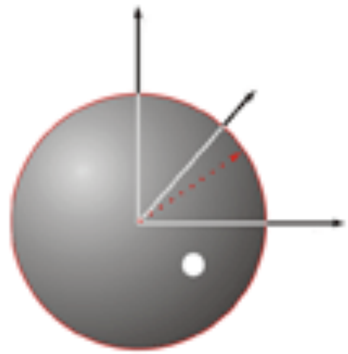
How Much Energy Does it Cost to Make a Hole in the Fermi Sea?

Robert Seiringer
Department of Mathematics and Statistics
McGill University

Joint work with
Rupert Frank, Mathieu Lewin and Elliott Lieb

Phys. Rev. Lett. **106**, 150402 (2011)
arXiv:1108.4246



Spectral Days, Munich, April 10, 2012

Lieb-Thirring Inequalities

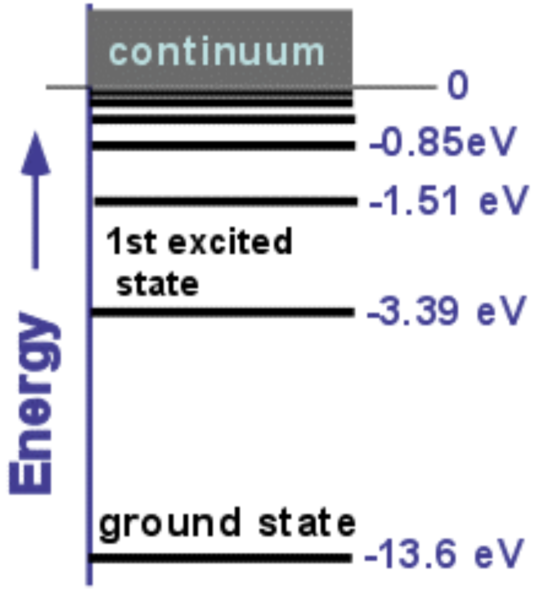
We consider the Schrödinger operator on $L^2(\mathbb{R}^d)$

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

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 $\sum_j |\lambda_j|^\kappa = \mathrm{Tr}\,\big(-\Delta + V(x)\big)_-^\kappa$. A **semiclassical approximation** of the trace yields the phase space integral

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

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

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

- $L_{\kappa,d} = L_{\kappa,d}^{\mathrm{scl}}$ for all $\kappa \geq 3/2$ and $d = 1$ (LT, Aizenman-Lieb), $d \geq 2$ (Laptev, Weidl)
- $L_{1/2,1} = 1/2$ while $L_{1/2,1}^{\mathrm{scl}} = 1/4$ (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 $L_{1,3} = L_{1,3}^{\mathrm{scl}}$)

Kinetic Energy Inequality

For $\kappa = 1$, the LT Inequality has the dual formulation

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

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 $\rho(x)$.

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

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

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

Stability of Matter refers to the fact that

$$\inf_{\{R_k\}} \inf \operatorname{spec} H \ge -\mathrm{const.}\,(N+K)$$

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,

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

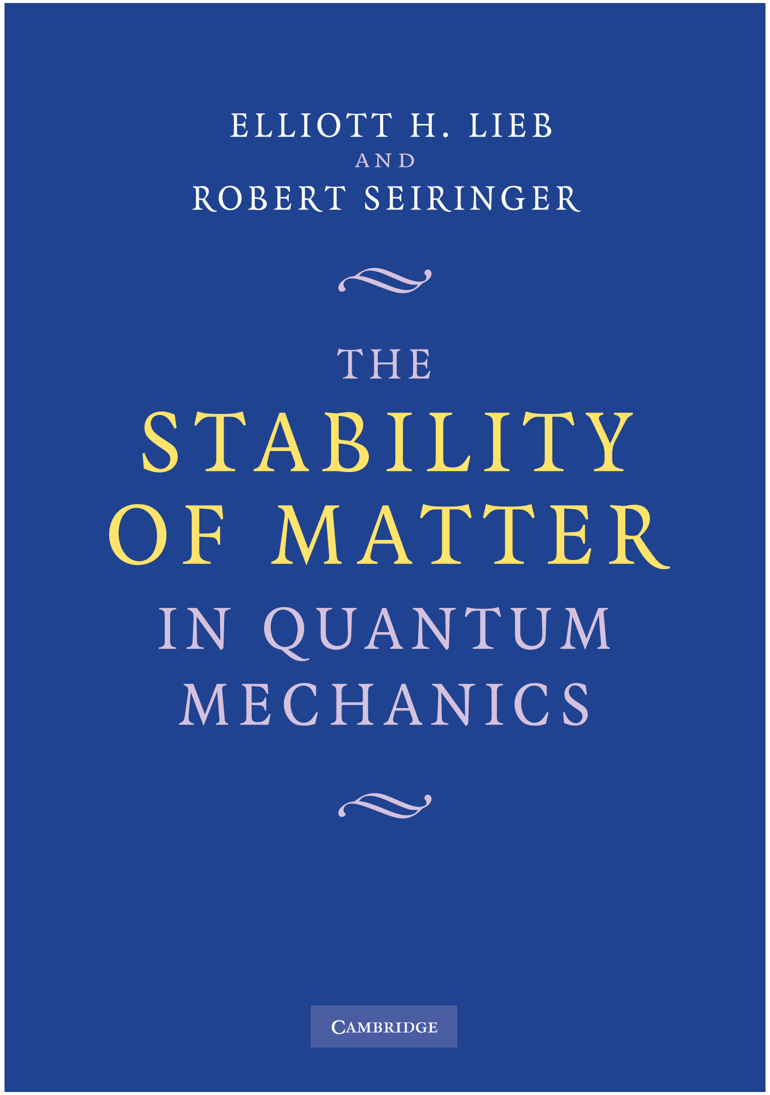
The reduction of the many-body Coulomb potential to a one-body potential is achieved via an **electrostatic inequality** due to Baxter (and refined later by Lieb and Yau):

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 $\lambda > 0$.

Commercial Break



Particle System at Positive Density

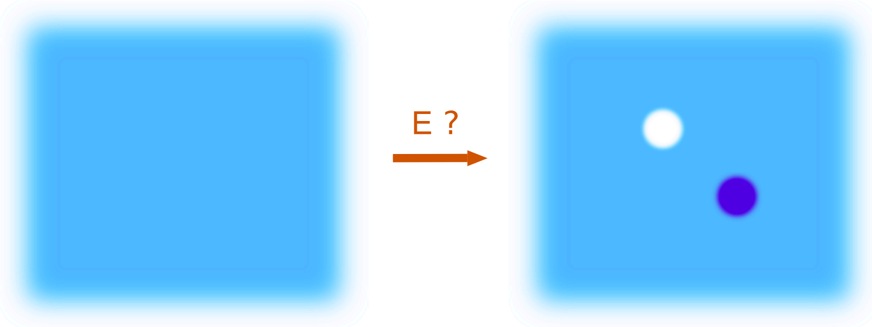
Imagine an infinite system of non-interacting fermions at some **density** $\rho > 0$. It is described by the projection

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

We seek a lower bound on the **energy difference**

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

in terms of its **semiclassical approximation**



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

Note that the integrand behaves like $(\rho_\gamma(x) - \rho)^2$ for $\rho_\gamma(x)$ close to ρ, 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 $0 \leq \gamma \leq 1$*

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

Remarks.

1. For $\rho = 0$ this reduces to the usual Lieb-Thirring Inequality
2. By scaling, K_d is independent of ρ.
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

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

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

$$-\mathrm{Tr}\,(-\Delta-\mu+V)\left(\mathbb{1}(-\Delta+V\leq\mu)-\mathbb{1}(-\Delta\leq\mu)\right)$$

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

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

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

where

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

Note that ψ_1 diverges logarithmically at $|k|=2$, while ψ_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

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

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

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

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

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

and

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

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

$$\mathrm{Tr}\,(-\Delta-\mu)Q^{++} = \mathrm{Tr}\,|-\Delta-\mu|Q^{++} = \int_0^\infty dE\,\mathrm{Tr}\,Q_E^{++} = \int_{\mathbb{R}^3} dx \int_0^\infty dE\,\rho_E^{++}(x)$$

where $Q_E^{++} = P_{\geq E} Q^{++} P_{\geq E}$, $\rho_E^{++}(x) = Q_E^{++}(x,x)$, and $P_{\geq E} = \mathbb{1}(|-\Delta-\mu| \geq E)$.
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

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

The Off-Diagonal Terms

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

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

with

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

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

$$\left| \int_{\mathbb{R}^d} V \rho_{Q^{-+}} \right| = |\mathrm{Tr}\, V \Pi_\mu Q (1 - \Pi_\mu)| \leq \left\| \frac{1-\Pi_\mu}{|\Delta + \mu|^{1/4}} V \frac{\Pi_\mu}{|\Delta + \mu|^{1/4}} \right\|_{\mathfrak{S}_2} \left[\mathrm{Tr}\,(-\Delta - \mu) Q \right]^{1/2}$$

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**