Crystallization in Lieb-Thirring inequalities

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Theorem (Lieb-Thirring inequality, '75-76)

Let $d \geq 1$ (dimension), and let $\gamma > \max(0, 1 - d/2)$. There exists (an optimal -smallest- constant) $L_{\gamma,d} > 0$ so that, for all $V \in L^{\gamma + \frac{d}{2}}(\mathbb{R}^d)$

$$\boxed{\sum_{n=1}^{\infty} |\lambda_n(-\Delta + V)|^{\gamma} \leq L_{\gamma,d} \int_{\mathbb{R}^d} V(x)_-^{\gamma + \frac{d}{2}} \mathrm{d}x} \qquad \text{(Lieb-Thirring inequality).}$$

Similar results hold in the critical cases $\gamma = 0$ in dimensions $d \geq 3$ (Cwikel-Lieb-Rozenblum (CLR) inequality, '72-77), and $\gamma = \frac{1}{2}$ in dimension $d = 1$ (Weidl '96).

First remarks

- In the case $\gamma = 0$, $d \geq 3$ (CLR), bound the **number** of negative eigenvalues.
- The right-hand side is **extensive**.

Main application: Large fermionic systems (simple proof of the stability of matter by Lieb-Thirring '75).

Finite rank Lieb-Thirring.

$$\boxed{\sum_{n=1}^{N} |\lambda_n(-\Delta + V)|^\gamma \leq L_{\gamma,d}^{(N)} \int_{\mathbb{R}^d} V(x)_-^{\gamma+\frac{d}{2}}.}$$

Remark: The case $N = 1$ is equivalent to **Gagliardo-Nirenberg-Sobolev** inequality.

Semi-classical limit. For all $V \in L^{\gamma+\frac{d}{2}}(\mathbb{R}^d)$, in the limit $\hbar \to 0$,

$$\sum_{n=1}^{\infty} |\lambda_n(-\Delta + V(\hbar\cdot))|^\gamma \approx L_{\gamma,d}^{\mathrm{sc}} \int_{\mathbb{R}^d} V(\hbar\cdot)_-^{\gamma+\frac{d}{2}}.$$

Facts:

$$L_{\gamma,d} = \lim \uparrow L_{\gamma,d}^{(N)}, \quad \text{and} \quad \boxed{L_{\gamma,d} \geq \max\left\{L_{\gamma,d}^{(N)}, L_{\gamma,d}^{\mathrm{sc}}\right\}.}$$

Main questions:

- What is the value of the best constant $L_{\gamma,d}$?
- Is there an optimal potential for $L_{\gamma,d}$, or for the finite-rank version $L_{\gamma,d}^{(N)}$?
- Do we have equality $L_{\gamma,d} = L_{\gamma,d}^{(N)}$ for some (finite) N?

Lieb-Thirring (first) conjecture: $L_{\gamma,d} \stackrel{?}{=} \max\{L_{\gamma,d}^{(1)}, L_{\gamma,d}^{\mathrm{sc}}\}$.

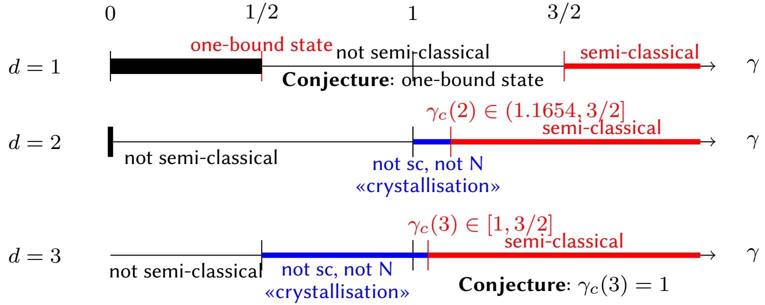
The optimal scenario is either the one-bound state, or the semi-classical one = fluid phase.

Known facts about Lieb-Thirring

- $\gamma \mapsto L_{\gamma,d}/L^{\rm sc}_{\gamma,d}$ is decreasing (Aizenmann-Lieb, 1978), and ≥ 1.
  There is a unique point $\gamma_c(d) > 0$ so that $L_{\gamma,d} = L^{\rm sc}_{\gamma,d}$ iff $\gamma \geq \gamma_c(d)$.
- $\gamma = 3/2$ in dimension $d = 1$. $L_{\gamma,d} = L^{(N)}_{\gamma,d} = L^{\rm sc}_{\gamma,d} = \frac{3}{16}$. (Lieb-Thirring 1976).
- $\gamma \geq 3/2$ is semi-classical: $L_{\gamma,d} = L^{\rm sc}_{\gamma,d}$ for all $\gamma \geq \frac{3}{2}$. (Laptev-Weidl 2000) .
- $\gamma = 1/2$ in dimension $d = 1$. $L_{\frac{1}{2},1} = L^{(1)}_{\frac{1}{2},1}$. (Hundertmark-Lieb-Thomas, 1998).
- $\gamma < 1$ is not semi-classical. $L_{\gamma,d} > L^{\rm sc}_{\gamma,d}$ for all $\gamma < 1$. (Hellfer-Robert, 2010).

Theorem (R.L. Frank, DG, M. Lewin, 2021)

For all $\gamma > \max\left\{0, 2 - \frac{d}{2}\right\}$*, and all* $N \in \mathbb{N}$*, we have* $L^{(2N)}_{\gamma,d} > L^{(N)}_{\gamma,d}$*. In particular,* $L_{\gamma,d} > L^{(N)}_{\gamma,d}$*.*
The N-th bound state scenario is never optimal.



Idea of the proof ($L^{(2)}_{\gamma,d} > L^{(1)}_{\gamma,d}$)

Fact: $L^{(1)}_{\gamma,d} \sim$ Gagliardo-Niremberg-Sobolev inequality, for which we know the optimizer.
Let $p := (\gamma + \frac{d}{2})'$ and Q be the (unique) radial decreasing solution to

$$-\Delta Q - Q^{2p-1} = -Q,$$

Then $V := -Q^{2(p-1)}$ is an optimizer for $L^{(1)}_{\gamma,d}$.

Idea: Consider the following *test potential* for $L^{(2)}_{\gamma,d}$:

$$\boxed{\widetilde{V}(x) := -\left[Q^2(x - Re_1) + Q^2(x + Re_1)\right]^{p-1}.}$$

We add the **densities**, not the **potentials**!

- $Q(x) \underset{x\to\infty}{\sim} C|x|^{-\frac{d-1}{2}} \mathrm{e}^{-|x|}$.
- The «interaction» between the two *bubbles* is exponentially small (*tunnelling effect*).
- A computation reveals that

$$L^{(2)}_{\gamma,d} \geq L^{(1)}_{\gamma,d}\left(1 + \alpha \mathrm{e}^{-2pR} + O\left(\mathrm{e}^{-4R}\right)\right), \quad \alpha > 0.$$

- We have $L^{(2)}_{\gamma,d} > L^{(1)}_{\gamma,d}$ if $p < 2$, which is our condition $\boxed{\gamma > 2 - d/2}$.

Remarks:

- This condition is optimal in $d = 1$, where we have $L^{(2)}_{3/2,1} = L^{(1)}_{3/2,1}$.
- For $\gamma = 0$ in dimension $d \geq 3$ (finite rank CLR), we also have $L^{(2)}_{0,d} = L^{(1)}_{0,d}$.

Crystallization

- If $\gamma \geq \gamma_c(d)$, the «optimal» V is the semi-classical case $V = cst$.
- If $\gamma \geq \max(0, 2 - d/2)$, the «optimal» V must have infinitely many bound states.

Idea: Study the periodic Lieb-Thirring inequality.

Lemma

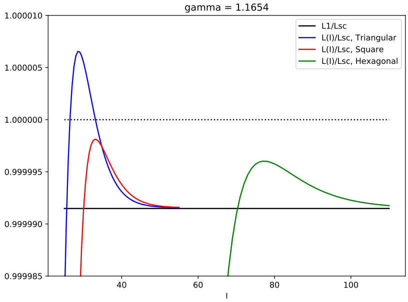
Let $\gamma > \max\{0, 1 - d/2\}$. Then, for all **periodic** $V \in L^{\gamma + \frac{d}{2}}_{\rm loc}(\mathbb{R}^d)$*, we have*

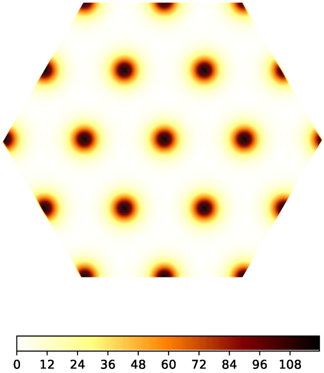
$$\boxed{\underline{\rm Tr}\left((-\Delta + V)_-^\gamma \right) \leq L_{\gamma,d} \fint V_-^{\gamma + \frac{d}{2}}.}$$

with the same best constant $L_{\gamma,d}$. In addition, $V = cst < 0$ is an optimizer iff $L_{\gamma,d} = L^{\rm sc}_{\gamma,d}$.

In the case where $L_{\gamma,d} > L^{\rm sc}_{\gamma,d}$, the constant potential is not optimal $\implies$ crystallization.

In dimension $d = 2$, we numerically found periodic potentials which beat both $L^{\mathrm{sc}}_{\gamma,d}$ and $L^{(1)}_{\gamma,d}$.





	Triangular	Square	Hexagonal	$L^{(1)}_{\gamma,2}$
Critical γ	1.165417	1.165395	1.165390	1.165378

Table: Critical values of γ for different lattices.

Conclusions

- Lieb-Thirring inequality valid for $\gamma > \max\{0, 1 - d/2\}$.
- If $\gamma > \max\{0, 2 - d/2\}$, then there is no optimal potential with a finite number of bound states.

Lieb-Thirring conjectures (still open)

- Dimension $d = 1, \gamma \in (1/2, 3/2)$. $L_{\gamma,d} \stackrel{?}{=} L_{\gamma,d}^{(1)}$.
- Dimension $d = 3, \gamma = 1$d. $L_{1,3} \stackrel{?}{=} L_{1,3}^{\mathrm{sc}}$.