Cristallisation in the Lieb-Thirring inequality

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Lieb-Thirring inequality

Let $\gamma \geq 0$ satisfy

$$\begin{cases} \gamma \geq \frac{1}{2} & \text{in dimension} \quad d = 1, \\ \gamma > 0 & \text{in dimension} \quad d = 2, \\ \gamma \geq 0 & \text{in dimension} \quad d = 3. \end{cases}$$

There exists (an optimal -smallest- constant) $L_{\gamma,d} > 0$ so that, for all $V \in L^{\gamma+\frac{d}{2}}(\mathbb{R}^d)$

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

where λ_n is the n-th min-max eigenvalue of $-\Delta + V$ if exists, 0 otherwise ($\lambda_n \leq 0$), and where $V_- := \max\{0, -V\}$.

References

Case $\gamma > \dots$ (strict inequality)

- E. H. Lieb, W. E. Thirring, *Bound on kinetic energy of fermions which proves stability of matter*, Phys. Rev. Lett., 35 (1975).
- E. H. Lieb, W. E. Thirring, Studies in Mathematical Physics, 1976.

Case $\gamma = 0$ for $d \geq 3$ (Cwikel-Lieb-Rozenblum (CLR) inequality)

- M. Cwikel, Ann. of Math., 106 (1977).
- E.H. Lieb, Bull. Amer. Math. Soc., 82 (1976).
- G. V. Rozenblum, Dokl. Akad. Nauk SSSR, 202 (1972).

Case $\gamma = \frac{1}{2}$ for $d = 1$

- T. Weidl, Comm. Math. Phys., 178 (1996).
- D. Hundertmark, E.H. Lieb, and L.E. Thomas, Adv. Theor. Math. Phys., 2 (1998).

Let $\gamma \geq 0$ satisfy

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First remarks:

- If $\gamma = 0$ (CLR), bound the **number** of negative eigenvalues.
- The right-hand side is **extensive**.
- Invariant by translations, and by scaling $V \mapsto t^2 V(tx)$.

In this presentation, we study the «optimisers» of the Lieb-Thirring inequality.

Two important regimes

The N-bound state case. We have $L_{\gamma,d} \geq L_{\gamma,d}^{(N)}$, where $L_{\gamma,d}^{(N)}$ is the best constant in the inequality

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

Example (the $N=1$ case).
$$\boxed{L_{\gamma,d}^{(1)} := \sup_{V \in L^{\gamma+\frac{d}{2}}} \max_{\substack{u \in H^1(\mathbb{R}^d) \\ \|u\|_{L^2}=1}} \frac{-|\langle u, (-\Delta+V)u\rangle|^\gamma}{\int_{\mathbb{R}^d} V_-^{\gamma+\frac{d}{2}}}.}$$

Switching the sup/max, and optimising first in V gives the usual Gagliardo-Niremberg inequality

$$\forall u \in H^1(\mathbb{R}^d), \quad K_{p,d}^{\mathrm{GN}} \|u\|_{L^{2p}(\mathbb{R}^d)}^{\frac{2}{d(p-1)}} \leq \|\nabla u\|_{L^2(\mathbb{R}^d)} \|u\|_{L^2(\mathbb{R}^d)}^{\frac{(2-d)p+d}{d(p-1)}}, \quad p = \left(\gamma + \frac{d}{2}\right)'.$$

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

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

with

$$\boxed{L_{\gamma,d}^{\mathrm{sc}} := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} (|p|^2 - 1)^\gamma \mathrm{d}p.}$$

Facts: $L_{\gamma,d} = \lim \uparrow L_{\gamma,d}^{(N)}$ and $L_{\gamma,d} \geq \max\{L_{\gamma,d}^{(1)}, L_{\gamma,d}^{\mathrm{sc}}\}$.

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

LT conjecture: 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.
  For $d \leq 8$, there is a unique point $\gamma_{\rm c}(d) > 0$ so that $L_{\gamma,d} = L^{\rm sc}_{\gamma,d}$ iff $\gamma \geq \gamma_c(d)$.
- $\gamma \mapsto L^{(1)}_{\gamma,d}/L^{\rm sc}_{\gamma,d}$ is decreasing, and cross 1 at a unique point $\gamma_{1\cap{\rm sc}}(d)$ if $d \leq 8$.

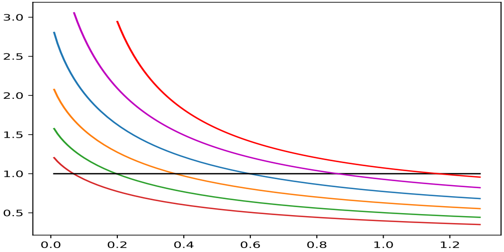


Figure: The curves $L^{(1)}_{\gamma,d}/L^{\rm sc}_{\gamma,d}$ as a function of γ, for $d = 2$ (red) to $d = 8$ (brown).

d	1	2	3	4	5	6	7	$d \geq 8$
$\gamma_{1\cap{\rm sc}}(d)$	$= 3/2$	1.1654	0.8627	0.5973	0.3740	0.1970	0.0683	no crossing

- $\gamma \geq 3/2$ is semi-classical: $L_{\gamma,d} = L^{\rm sc}_{\gamma,d}$ for all $\gamma \geq \frac{3}{2}$. (Lieb-Thirring 1976 (d = 1), Laptev-Weidl 2000 (all d)).
- $\gamma = 1/2$ in dimension 1. $L_{\frac{1}{2},1} = L^{(1)}_{\frac{1}{2},1}$ (Weidl, 1996).
- $\gamma < 1$ is not semi-classical. For all $\gamma < 1$, $L_{\gamma,d} > L^{\rm sc}_{\gamma,d}$ (Hellfer-Robert, 2010).

Theorem (R.L. Frank, DG, M.Lewin, 2020)

For all

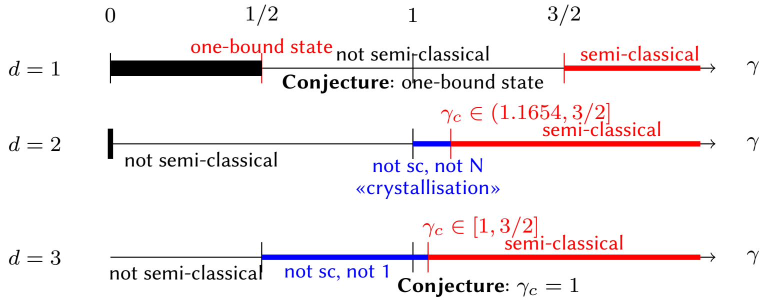
$$\gamma > \max\left\{0, 2 - \frac{d}{2}\right\} = \begin{cases} 3/2 & \text{in dimension} \quad d = 1 \\ 1 & \text{in dimension} \quad d = 2 \\ 1/2 & \text{in dimension} \quad d = 3 \\ 0 & \text{in dimension} \quad d > 4, \end{cases}$$

we have $L_{\gamma,d}^{(2)} > L_{\gamma,d}^{(1)}$. *In particular, the one bound state scenario is not optimal.*

If in addition, $\gamma > 1$, *we have* $L_{\gamma,d} > L_{\gamma,d}^{(N)}$ *for all* N: *the* N*-th bound state scenario is not optimal.*

In dimension $d = 2$, for all $\gamma \in (1, 1.1654]$, the «optimal» potential V has an infinity of bound states, but is not semi-classical (= Crystallisation).

Current knowledge in low dimensions:



Idea of the proof

Fact: There is an optimal potential V for $L^{(1)}_{\gamma,d}$.

Let $p := (\gamma + \frac{d}{2})'$ and Q be the (unique) radial decreasing solution to (Gagliardo-Niremberg)

$$-\Delta Q - Q^{2p-1} = -Q, \quad \text{and set} \quad m := \int_{\mathbb{R}^d} Q^2. \qquad (*)$$

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

$$\lambda_1(-\Delta + V) = -1, \quad \text{and} \quad \int_{\mathbb{R}^d} V_-^{\gamma+\frac{d}{2}} = \int_{\mathbb{R}^d} Q^{2p}, \quad \text{so} \quad L^{(1)}_{\gamma,d} = \frac{1}{\int_{\mathbb{R}^d} Q^{2p}}.$$

Idea: Consider the *test potential*

$$\boxed{\widetilde{V}(x) := -\left(Q_+^2(x) + Q_-^2(x)\right)^{p-1},} \quad \text{where} \quad Q_\pm(x) := Q\left(x \pm \frac{R}{2} e_1\right).$$

We add the **densities**, not the **potentials**! See [Gontier, Lewin, Nazar, 2020] for similar ideas in NLS.
We have

$$L^{(2)}_{\gamma,d} \geq \frac{|\lambda_1(-\Delta + \widetilde{V})|^\gamma + |\lambda_2(-\Delta + \widetilde{V})|^\gamma}{\int_{\mathbb{R}^d} |\widetilde{V}|^{\gamma+\frac{d}{2}}}.$$

Remark: $Q(x) \approx C|x|^{-\frac{d-1}{2}} \mathrm{e}^{-|x|}$ for x large. The «interaction» between the two *bubbles* is exponentially small. All quantities are expressed with

$$A := A(R) := \frac{1}{2} \int_{\mathbb{R}^d} (Q_+^2 + Q_-^2)^p - Q_+^{2p} - Q_-^{2p} \quad \geq 0, \quad \text{since} \quad p \geq 1.$$

Key Remark: Evaluating around 0, we obtain that $A(R) \geq cst \cdot \mathrm{e}^{-p|R|} \cdot R^{-(d-1)}$.

Computation of the numerator

We can bound from below the numerator by looking at $(-\Delta + \widetilde{V})$ projected on $\mathrm{Ran}\{Q_+, Q_-\}$. We find

$$|\lambda_1(-\Delta + \widetilde{V})|^\gamma + |\lambda_2(-\Delta + \widetilde{V})|^\gamma \geq 2 + \frac{2\gamma}{m} A + \underbrace{O(\mathrm{e}^{-2R})}_{= o(A) \text{ if } p<2} .$$

Computation of the denominator

Since $p = (\gamma + \frac{d}{2})'$, we get

$$\int_{\mathbb{R}^d} |\widetilde{V}|^{\gamma + \frac{d}{2}} = \int_{\mathbb{R}^d} (Q_+^2 + Q_-^2)^p = 2 \int_{\mathbb{R}^d} Q^{2p} + 2A.$$

Estimate. This gives, if $p < 2$, *i.e.* if $\gamma \geq 2 - \frac{d}{2}$, that

$$L_{\gamma,d}^{(2)} \geq \underbrace{\frac{1}{\int_{\mathbb{R}^d} Q^{2p}}}_{= L_{\gamma,d}^{(1)}} \left(1 + \left(\gamma - \frac{m}{\int_{\mathbb{R}^d} Q^{2p}} \right) A + o(A) \right).$$

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Pozhoev's identities. $\int (*) \times Q$ and $\int (*) \times x \cdot \nabla Q$ give

$$\begin{cases} \int_{\mathbb{R}^d} |\nabla Q|^2 - \int_{\mathbb{R}^d} Q^{2p} = - \int_{\mathbb{R}^d} Q^2 = -m, \\ \left(\frac{d}{2} - 1\right) \int_{\mathbb{R}^d} |\nabla Q|^2 - \frac{d}{2p} \int_{\mathbb{R}^d} Q^{2p} = -\frac{d}{2} m, \end{cases}$$

which implies

$$\left(\gamma - \frac{m}{\int_{\mathbb{R}^d} Q^{2p}} \right) = \frac{\gamma}{pm} \geq 0.$$

Periodic Lieb-Thirring

Facts:

- If $\gamma \geq \gamma_c(d)$, the «optimal» V is the semi-classical case $V = cst$.
- If $\gamma \geq 1$, the «optimal» V must have infinitely many bound states.

Idea: Study the periodic Lieb-Thirring inequality.

Lemma

Let γ be as before. Then, for all **periodic** $V \in L^{\gamma+\frac{d}{2}}_{\rm loc}(\mathbb{R}^d)$, *we have*

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

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

Here, if $\mathcal{L}$ is **any** periodic lattice of V, with cell Γ, then

Trace per unit volume:

$$\underline{\rm Tr}\left((-\Delta + V)_-^\gamma\right) := \lim_{L\to\infty} \frac{1}{|L\Gamma|} {\rm Tr}_{L^2(\mathbb{R}^d)}\left(\mathbb{1}_{L\Gamma}(-\Delta + V)^\gamma \mathbb{1}_{L\Gamma}\right).$$

Integral per unit volume:

$$\fint V_-^{\gamma+\frac{d}{2}} := \lim_{L\to\infty} \frac{1}{|L\Gamma|} \int_{L\Gamma} V_-^{\gamma+\frac{d}{2}} = \frac{1}{|\Gamma|}\int_\Gamma V_-^{\gamma+\frac{d}{2}}.$$

Conjecture: We have

- **either** there is $N \in \mathbb{N}$ and $V_N \in L^{\gamma+\frac{d}{2}}(\mathbb{R}^d)$ so that $L_{\gamma,d} = L^{(N)}_{\gamma,d}$, with optimal potential V_N;
- **or** $L_{\gamma,d} > L^{(N)}_{\gamma,d}$ for all $N \in \mathbb{N}$, in which case there is periodic optimiser. This minimiser can be constant ($L = L^{\rm sc}$) or not (crystallisation).

The case $\gamma = 3/2$ in dimension $d = 1$.

In the original article by Lieb-Thirring 1976, they proved

$$\boxed{L_{3/2,1} = L_{3/2,1}^{(1)} = L_{3/2,1}^{(N)} = L_{3/2,1}^{\rm sc} = \frac{3}{16}.}$$

Idea of the proof. Consider the Korteweg-de-Vries equation in $W = W(t,x)$ defined by

$$\partial_t W := 6W\partial_x W - \partial_{xxx}^3 W, \quad W(t=0,x) = V(x).$$

Then,

- the norm $\int_{\mathbb{R}} W^2$ is independent of t (here, $2 = 3/2 + 1/2 = \gamma + \frac{d}{2}$);
- the general KdV theory shows that the profile of W splits into non-interacting bubbles (= *solitons*) as $t \to \infty$;
  In addition, each soliton must be of the form

$$V_1(x) := \frac{-2c^2}{\cosh^2(cx)}.$$

- the spectrum of $-\Delta + W(t,\cdot)$ is independent of t (Lax' theory).

Can we have a periodic superposition of solitons?

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

For all $0 < k < 1$, *the potential*

$$\boxed{V_k(x) := 2k^2 \mathrm{sn}\,(x|k)^2 - 1 - k^2}, \quad \textit{with minimal period} \quad 2K(k),$$

is an optimiser for the periodic problem at $\gamma = 3/2$ *and* $d = 1$. *Here,* $\mathrm{sn}(\cdot|k)$ *is the Jacobi elliptic function, and* $K(\cdot)$ *is the complete elliptic integral of the first kind. In addition,*

$$\lim_{k \to 0} V_k(x) = -1 \quad \textit{and} \quad \lim_{k \to 1} V_k(x) = \frac{-2}{\cosh^2(x)}.$$

This potential is sometime called the periodic Lamé potential, or the cnoidal wave.
It interpolates between the semi-classical constant and the $N = 1$ soliton.
The operator $-\Delta + V_k$ has a single negative Bloch band, and a spectral gap of size k^2.

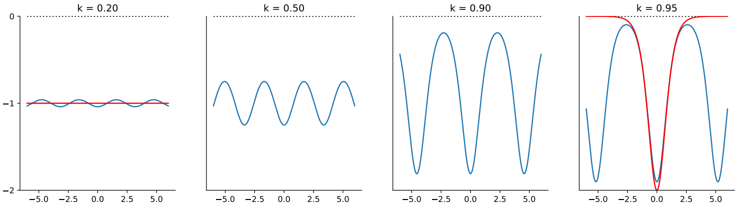


Figure: The potential V_k for some values of k.

How to distinguish these solutions?

Recall that the inequality is invariant by scaling $V \mapsto t^2 V(tx)$.

Let $\widetilde{V_k}$ be the 1-periodic version of V_k.

Fact: the map $(0,1) \ni k \mapsto \displaystyle\int_0^1 \widetilde{V_k}^2$ is increasing from π^2 to ∞.

Idea: Study the problem at $\mathcal{I}^{\gamma+\frac{d}{2}} := \displaystyle\fint V_-^{\gamma+\frac{d}{2}}$ fixed. Let $\mathcal{L}$ be a lattice with unit cell $|\Gamma| = 1$, and set

$$L_{\gamma,d,\mathcal{L}}(\mathcal{I}) := \frac{1}{\mathcal{I}^{\gamma+\frac{d}{2}}} \sup \left\{ \fint_{B.Z.} \varepsilon_1(-\Delta_q + V)_-^\gamma \, \mathrm{d}q, \; V \in L_{\rm per}^{\gamma+\frac{d}{2}}(\Gamma), \fint V^{\gamma+\frac{d}{2}} = \mathcal{I}^{\gamma+\frac{d}{2}} \right\}.$$

- B.Z. is the Brillouin zone, q is the Bloch quasi-momentum, $-\Delta_q := |-\mathrm{i}\nabla + q|^2$ acts on $L^2(\Gamma)$;
- we only consider the first band (variant with K bands possible), so

$$\fint_{B.Z.} \varepsilon_1(-\Delta_q + V)_-^\gamma \, \mathrm{d}q \leq \underline{\mathrm{Tr}} \left((-\Delta + V)_-^\gamma \right)$$

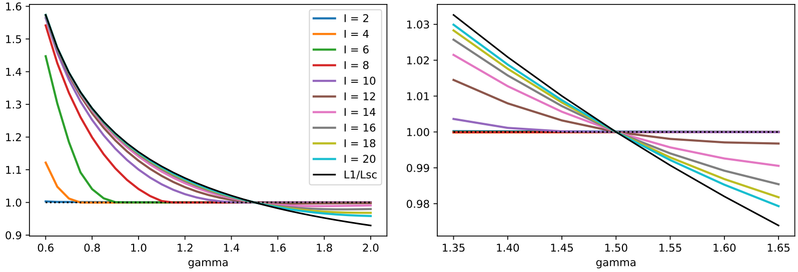
  with equality iff $-\Delta + V$ has a single negative Bloch band.

Remark: In the $\gamma = 3/2$ and $d = 1$ case,

- For $\mathcal{I} \leq \pi^2$, the constant potential $V = -\mathcal{I}$ has a single negative Bloch band, so $V = -\mathcal{I}$ is an optimiser (there is no spectral gap: semi-classical/fluid case, metallic system);
- At $\mathcal{I} = \pi^2$, the second Bloch band of $V = -\mathcal{I}$ touches 0;
- For $\mathcal{I} > \pi^2$, $V = -\mathcal{I}$ is no longer an optimiser. But there is $0 < k < 1$, so that $\widetilde{V_k}$ is an optimiser (there is a spectral gap of size k^2: solid phase, insulating system).

Numerical results in dimension $d = 1$

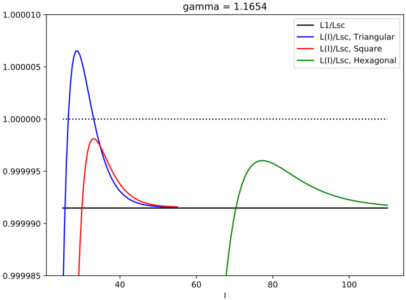
We plot $\gamma \mapsto L_{\gamma,1}(\mathcal{I})/L^{\rm sc}_{\gamma,1}$ for different values of $\mathcal{I}$.

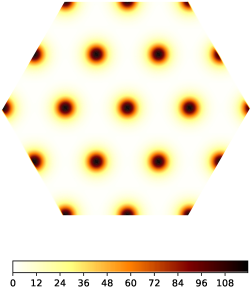


- All curves cross at $\gamma = 3/2$, *as expected.*
- If $\mathcal{I} < \pi^2$, the corresponding curve hits 1 (semi-classical) for some $\gamma < 3/2$.
- If $\gamma < 3/2$, the curves are increasing with $\mathcal{I}$. The potentials concentrate as $\mathcal{I} \to \infty$.
  Lieb-Thirring conjecture in dimension $d = 1$: $L_{\gamma,1} = L^{(1)}_{\gamma,1}$: optimisers are not periodic.

Numerical results in dimension $d = 2$

We fix $\gamma = 1.1654 > \gamma_{1\cap \mathrm{sc}}(d=2)$, and plot $\mathcal{I} \mapsto L_{\gamma,2,\mathcal{L}}(\mathcal{I})/L^{\mathrm{sc}}_{\gamma,2}$ for different lattices.





- The black curve represents the value $L^{(1)}_{\gamma,2}/L^{\mathrm{sc}}_{\gamma,2}$, which is less than 1 since $\gamma = 1.1654 > \gamma_{1\cap \mathrm{sc}}(2)$.
- For $\mathcal{I} \approx 30$, the triangular lattice gives a better bound than the fluid phase: crystallisation.
- We need very precise computations: precision to the order 10^{-7}.
- We believe that the previous *exponentially small attraction scenario* indeed happens.

	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.