A simple approach to Lieb–Thirring type inequalities

Seiringer, Robert; Solovej, Jan Philip

Published in:
Journal of Functional Analysis

DOI:
10.1016/j.jfa.2023.110129

Publication date:
2023

Document version
Publisher's PDF, also known as Version of record

Document license:
CC BY

Citation for published version (APA):
A simple approach to Lieb–Thirring type inequalities

Robert Seiringer \( ^a \), Jan Philip Solovej \( ^b \)

\( ^a \) IST Austria, Am Campus 1, 3400 Klosterneuburg, Austria
\( ^b \) Department of Mathematics, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen \( \emptyset \), Denmark

\textbf{Article info}

\textbf{Article history:}
Received 21 March 2023
Accepted 3 August 2023
Available online 18 August 2023
Communicated by Laszlo Erdos

\textbf{Keywords:}
Lieb-Thirring inequality
Semiclassics
Density functional theory

\textbf{Abstract}

In [10] Nam proved a Lieb–Thirring Inequality for the kinetic energy of a fermionic quantum system, with almost optimal (semi-classical) constant and a gradient correction term. We present a stronger version of this inequality, with a much simplified proof. As a corollary we obtain a simple proof of the original Lieb–Thirring inequality.

© 2023 The Author(s). Published by Elsevier Inc. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).

Let \( \gamma \) be a positive trace-class operator on \( L^2(\mathbb{R}^d) \) with density (i.e., diagonal) \( \rho \). Such operators naturally arise as reduced density matrices of many-particle quantum systems. In the case of fermions, the Pauli principle dictates a bound on the eigenvalues of \( \gamma \), which in the simplest (spinless) case reads \( \gamma \leq 1 \). In this case, Lieb and Thirring [7,8] proved a powerful lower bound on the kinetic energy \( \text{Tr}(-\Delta)\gamma \), where \( \Delta \) is the Laplacian on \( \mathbb{R}^d \), and the trace should really be interpreted as the one of the positive operator \( -\nabla \gamma \nabla \). This bound is one of the key ingredients in their elegant proof of the stability of matter, first proved by Dyson and Lenard in [1]. It can be interpreted as a many-body uncertainty principle, and reads

\[ \text{Tr}(-\Delta)\gamma \leq C \]
Theorem 1. Let \( \eta : \mathbb{R}_+ \to \mathbb{R} \) be a function with
\[
\int_0^\infty \eta(t)^2 \frac{dt}{t} = 1 = \int_0^\infty \eta(t)^2 dt \tag{2}
\]
and let \( C_d^{\text{TF}} = 4\pi \frac{d}{d+2} \Gamma(1+d/2)^{2/d} \). For any trace-class \( 0 \leq \gamma \leq 1 \) on \( L^2(\mathbb{R}^d) \) with density \( \rho \),
\[
\text{Tr}(-\Delta) \gamma \geq \frac{C_d^{\text{TF}}}{(\int_0^\infty \eta(t)^2 t^{d+1} dt)^{2/d}} \int_{\mathbb{R}^d} \rho^{1+2/d} - 4 \frac{d}{d^2} \int_{\mathbb{R}^d} |\nabla \sqrt{\rho}|^2 \int_0^\infty \eta'(t)^2 t dt \tag{3}
\]

We note that under the normalization conditions (2) we have \( \int_0^\infty \eta(t)^2 t^{d+1} dt > 1 \) by Jensen’s inequality. In order for this integral to be close to 1, \( \eta^2 \) needs to be close to a \( \delta \)-distribution at 1, in which case the final factor in (3) necessarily becomes large, however. A possible concrete choice is
\[
\eta(t) = (\pi \varepsilon)^{-1/4} \exp \left(-\varepsilon (2+\ln t)^2/(2\varepsilon)\right) \tag{4}
\]
for \( \varepsilon > 0 \). Then \( \int_0^\infty \eta'(t)^2 t dt = (2\varepsilon)^{-1} \) and
\[
\int_0^\infty \eta(t)^2 t^{1+x} dt = \exp (\varepsilon x (2+x)/4)
\]
for any $x \in \mathbb{R}$. For this choice of $\eta$ the bound (3) thus reads

$$\text{Tr}(-\Delta) \gamma \geq C_d^{\text{TF}} e^{-\varepsilon(1+d/2)} \int_{\mathbb{R}^d} \rho^{1+2/d} - \frac{2}{d^2 \varepsilon} \int_{\mathbb{R}^d} |\nabla \sqrt{\rho}|^2$$

for any $\varepsilon > 0$. A similar bound was proved by Nam in [10], but with the exponent $-1$ of $\varepsilon$ in the gradient term replaced by $-3 - 4/d$. We don’t expect the exponent $-1$ to be optimal, however. In fact, according to the Lieb–Thirring conjecture no correction term to the semiclassical expression should be needed at all for $d \geq 3$. Some correction term is needed for $d \leq 2$, but possibly the divergence of the prefactor as $\varepsilon \to 0$ could be slower than in our bound.

As already pointed out in [10], one can combine an inequality of the form (3) with the Hoffmann-Ostenhof inequality [4]

$$\text{Tr}(-\Delta) \gamma \geq \int_{\mathbb{R}^d} |\nabla \sqrt{\rho}|^2$$

(5)

to obtain a Lieb–Thirring inequality without gradient correction. The following is an immediate consequence of (3) and (5).

**Corollary 2.** For any trace-class $0 \leq \gamma \leq 1$ on $L^2(\mathbb{R}^d)$ with density $\rho$, we have

$$\text{Tr}(-\Delta) \gamma \geq C_d^{\text{TF}} R_d \int_{\mathbb{R}^d} \rho^{1+2/d}$$

(6)

where $R_d = \sup_{\eta} \frac{1}{(\int \eta(t)^2 t^d + 1) \int \eta(t)^2 t dt} \frac{1}{1 + \frac{4}{d^2} \int \eta(t)^2 t dt}$

(7)

and the supremum is over functions $\eta$ satisfying the normalization conditions (2).

We shall show below that for $d \leq 2$, $R_d$ can be calculated explicitly. In fact, $R_1 = (-3/a)^2/2^4 \approx 0.132$, where $a \approx -2.338$ is the largest real zero of the Airy function, and $R_2 = 1/4$. We were not able to compute $R_d$ for $d \geq 3$, but it can easily be obtained numerically. For $d = 3$, we find $R_d \approx 0.331$. In all these cases, our result is weaker than the best known one in [3], however, and also weaker than the one obtained in [11] where (6) was proved with $R_d = d/(d+4)$.

**Proof of Theorem 1.** The starting point is the following IMS type formula for any positive function $f: \mathbb{R}^d \to \mathbb{R}_+$,

$$\Delta = \int_0^\infty \xi(t/f(x)) \Delta \xi(t/f(x)) \frac{dt}{t} + \frac{|\nabla f(x)|^2}{f(x)^2} \int_0^\infty \eta(t)^2 t dt$$
where we used the first normalization condition in (2). This follows from
\[
\frac{1}{2} \theta^2 \Delta + \frac{1}{2} \Delta \theta^2 = \theta \Delta \theta + (\nabla \theta)^2
\]
applied to \(\theta(x) = \eta(t/f(x))\). As a consequence, we have
\[
\text{Tr}(\Delta) \gamma = - \int \frac{|\nabla f|^2}{f^2} \int_0^\infty \eta'(t)^2 t \, dt + \int \int p^2 \langle \psi_{p,t} | \gamma | \psi_{p,t} \rangle \frac{dt}{t} \, dp
\]
where \(\psi_{p,t}(x) = (2\pi)^{-d/2} e^{ipx} \eta(t/f(x))\). Note also that
\[
\int \int t \langle \psi_{p,t} | \gamma | \psi_{p,t} \rangle \, dt \, dp = \int \rho f^2 \int_0^\infty \eta(t)^2 t \, dt = \int \rho f^2
\]
where we used the second normalization condition in (2). Hence
\[
\text{Tr}(\Delta) \gamma = - \int \frac{|\nabla f|^2}{f^2} \int_0^\infty \eta'(t)^2 t \, dt + \int \rho f^2
\]
\[
+ \int \int (p^2 - t^2) \langle \psi_{p,t} | \gamma | \psi_{p,t} \rangle \frac{dt}{t} \, dp
\]
Since \(0 \leq \gamma \leq 1\) by assumption, we can get a lower bound on the last term as
\[
\int \int (p^2 - t^2) \langle \psi_{p,t} | \gamma | \psi_{p,t} \rangle \frac{dt}{t} \, dp \geq \int \int (p^2 - t^2) - \| \psi_{p,t} \|^2 \frac{dt}{t} \, dp
\]
where \((\cdot)_- = \min\{0, \cdot\}\) denotes the negative part. Since
\[
\| \psi_{p,t} \|^2 = \frac{1}{(2\pi)^d} \int \eta(t/f(x))^2 \, dx
\]
we have
\[
\int \int (p^2 - t^2) - \| \psi_{p,t} \|^2 \frac{dt}{t} \, dp = - \frac{1}{(2\pi)^d} \int (1 - p^2) dp \int f^{d+2} \int_0^\infty \eta(t)^2 t^{d+1} \, dt
\]
Altogether, we have thus shown that
\[
\text{Tr}(-\Delta) \gamma \geq - \int_\mathbb{R}^d \rho \frac{\nabla f}{f^2} \int_0^\infty \eta'(t)^2 t \, dt + \int_\mathbb{R}^d \rho f^2 t \, dt + \frac{1}{(2\pi)^d} \int_{|p| \leq 1} (1 - p^2) dp \int_0^\infty \eta(t)^2 t^{d+1} \, dt
\]

We now choose \( f = c \rho^{1/d} \) and optimize over \( c > 0 \). This gives (3). \( \square \)

Finally, we shall analyze the optimization problem in (7). Let \( e_d > 0 \) denote the ground state energy of \(-\partial_t^2 - t^{-1} \partial_t + d^2/(4t^2) + t^d \) on \( L^2(\mathbb{R}_+, t \, dt) \) (or, equivalently, of \(-\Delta + |x|^2 \) on \( L^2(\mathbb{R}^{d+2}) \)). We claim that

\[
R_d = \frac{d}{2} \left( \frac{d + 2}{2e_d} \right)^{1+2/d}
\]

To see this, let us note that by a straightforward scaling argument we can rewrite \( R_d^{-1} \) as

\[
\frac{1}{R_d} = 4 \frac{\inf_{\parallel \eta \parallel_2 = 1} \left( \int_\mathbb{R} \eta(t)^2 t^{d+1} \, dt \right)^{2/d} }{ \inf_{\parallel \eta \parallel_2^2} \left( \frac{d}{d+2} \int_\mathbb{R} \eta(t)^2 + \lambda \frac{d^2}{4t^2} \eta(t)^2 + \lambda^d \eta(t)^2 + \lambda'(t)^2 \right) t \, dt }^{1+2/d}
\]

where \( \parallel \eta \parallel_2 \) denotes the \( L^2(\mathbb{R}_+, t \, dt) \) norm, and we used the simple identity \( ab^x = \frac{x^x}{(1+x)^{1+x}} \inf_{b > 0} \lambda^{-x} (a + \lambda b)^{1+x} \) for positive numbers \( a, b \) and \( x \). Taking first the infimum over \( \eta \) for fixed \( \lambda \) leads to the ground state energy of \(-\partial_t^2 - t^{-1} \partial_t + d^2/(4t^2) + \lambda^d \), which a change of variables shows to be equal to \( \lambda^{2/(d+2)} e_d \). Hence we arrive at (8).

For \( d = 1 \), one readily checks that the ground state of \(-\partial_t^2 - t^{-1} \partial_t + 1/(4t^2) + t \) equals \( t^{-1/2} \text{Ai}(t + a) \) with \( a \) the largest real zero of the Airy function \( \text{Ai} \). In particular, \( e_1 = -a \). For \( d = 2 \) we find \( e_2 = 4 \) (the ground state energy of \(-\Delta + |x|^2 \) on \( \mathbb{R}^4 \)), and the ground state of \(-\partial_t^2 - t^{-1} \partial_t + 1/t^2 + t^2 \) is given by \( t e^{-t^2/2} \).

One can also check that \( R_d \to 1 \) as \( d \to \infty \). In fact, using (4) as a trial state and optimizing over the choice of \( \varepsilon \), one finds

\[
R_d \geq \sqrt{1 + \frac{2d^2}{1+d/2}} \frac{1 - \exp \left( \frac{1}{1 + \frac{2d^2}{1+d/2}} \left( \frac{\sqrt{1 + \frac{2d^2}{1+d/2}} - 1}{1 + \frac{2d^2}{1+d/2} + 1} \right) \right)}{1 - O(d^{-1/2})}.
\]

Data availability

No data was used for the research described in the article.
Acknowledgments

J.P.S. thanks the Institute of Science and Technology Austria for the hospitality and support during a visit where this work was done. J.P.S. was also partially supported by the VILLUM Centre of Excellence for the Mathematics of Quantum Theory (QMATH) (grant No. 10059).

References