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A simple approach to Lieb–Thirring type inequalities

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\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.

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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

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\[ \text{Tr}(-\Delta)\gamma \geq C_d^{\text{LT}} \int_{\mathbb{R}^d} \rho^{1+2/d} \]

for some universal constant \( C_d^{\text{LT}} \) depending only on the space dimension \( d \). The optimal value of this constant is not known, and for \( d \geq 3 \) was conjectured by Lieb and Thirring to equal the semi-classical Thomas–Fermi value, \( C_d^{\text{TF}} = 4\pi \frac{d}{d+2} \Gamma(1 + d/2)^{2/d} \). We refer to [3] for the currently best known lower bounds, as well as to [2] for further information on Lieb–Thirring and related inequalities. We note that Lieb and Thirring proved (1) by first proving a dual inequality on the sum of the negative eigenvalues of Schrödinger operators, but direct proofs of (1) have since also been derived [11,9,3].

In [10] Nam proved a Lieb–Thirring inequality with constant arbitrarily close to \( C_d^{\text{TF}} \), at the expense of a gradient correction term. In this paper we present an improved version of Nam’s inequality, with a much simpler proof. Our proof is inspired by [5, Thm. 3], where an analogous upper bound is proved (on the kinetic energy density functional, i.e., the infimum of Tr\((-\Delta)\gamma \) for given \( \rho \)). Interestingly, the method can also be used for a lower bound, in a similar spirit as the method of coherent states, which can also be applied to give bounds in both directions [6], but seems to be more useful for the study of the dual problem, however.

Our main result is the following.

**Theorem 1.** Let \( \eta : \mathbb{R}_+ \rightarrow \mathbb{R} \) be a function with

\[ \int_0^\infty \eta(t)^2 dt = 1 = \int_0^\infty \eta(t)^2 t^2 dt \]

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 \( \rho \),

\[ \text{Tr}(-\Delta)\gamma \geq \frac{C_d^{\text{TF}}}{(\int_0^\infty \eta(t)^2 t^{d+1} dt)^{2/d}} \int_{\mathbb{R}^d} \rho^{1+2/d} - \frac{4}{d^2} \int_{\mathbb{R}^d} |\nabla \sqrt{\rho}|^2 \int_0^\infty \eta'(t)^2 t^2 dt \]

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

\[ \eta(t) = (\pi \varepsilon)^{-1/4} \exp \left( - (\varepsilon/2 + \ln t)^2 / (2\varepsilon) \right) \]

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)

with

\[
R_d = \sup_{\eta} \frac{1}{(\int \eta(t)^{2d+1} \, dt)^{2/d}} \left( \frac{1}{1+\frac{4}{d^2} \int \eta'(t)^2 \, dt} \right)
\]

(7)

where 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 \( f : \mathbb{R}^d \to \mathbb{R}_+ \),

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

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

\[
\frac{1}{R_d} = \frac{4}{d^2} \inf_{||\eta||_2 = 1} \left( \int \eta(t)^2 t^{d+1} \, dt \right)^{2/d} \int \left( \frac{d^2}{4t^2} \eta(t)^2 + \eta'(t)^2 \right) t \, dt
\]

\[
= \frac{4}{d^2} \inf_{||\eta||_2 = 1} \inf_{\lambda > 0} \left( \frac{2}{d \lambda} \right)^{2/d} \left[ \frac{d}{d + 2} \int \left( \frac{d^2}{4t^2} \eta(t)^2 + \lambda t^d \eta(t)^2 + \eta'(t)^2 \right) t \, dt \right]^{1+2/d}
\]

where \( ||\eta||_2 \) denotes the \( L^2(\mathbb{R}_+, t \, dt) \) norm, and we used the simple identity \( ab^x = \frac{a^x}{(1+x)^{1+x}} \inf_{\lambda > 0} \lambda^{-x}(a + \lambda b)^{1+x} \) for positive numbers \( a, b \) and \( x \). Taking first the infimum over \( \eta \) for fixed \( \lambda \) leads to the ground state energy of \(-\partial_t^2 - t^{-1} \partial_t + d^2/(4t^2) + \lambda t^d\), 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 \( te^{-t^2/2} \).

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

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

**Data availability**

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