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A simple approach to Lieb–Thirring type inequalities ★

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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 γ 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 uncertainly principle, and reads

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

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 \(\text{Tr}(-\Delta) \gamma\) 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 \(\eta : \mathbb{R}_+ \to \mathbb{R}\) be a function with

\[
\int_0^\infty \eta(t)^2 \frac{dt}{t} = 1 = \int_0^\infty \eta(t)^2 t \, dt
\] (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 \(\rho\),

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

\[
\eta(t) = (\pi \varepsilon)^{-1/4} \exp \left(-\frac{\varepsilon}{2 + \ln t}^2/(2\varepsilon)\right)
\] (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)
with
\[
R_d = \sup_{\eta} \frac{1}{\int \eta(t)^2 t^{d+1} dt} \frac{1}{\int \eta'(t)^2 t dt}
\]
(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 $f : \mathbb{R}^d \to \mathbb{R}_+$,
\[
\Delta = \int_0^\infty \eta(t/f(x)) \Delta(\eta(t/f(x)) \frac{dt}{t} + \frac{|\nabla f(x)|^2}{f(x)^2} \int_0^\infty \eta'(t)^2 t dt
\]
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

\[
\text{Tr}(-\Delta) \gamma = -\int_\mathbb{R}^d f^2 \left( \left( \frac{\nabla f}{f} \right)^2 \right) \int_0^\infty \eta(t)^2 t \, dt + \int_\mathbb{R}^d \int_0^\infty p^2 \langle \psi_{p,t} | \gamma | \psi_{p,t} \rangle \frac{dt}{t} \, dp
\]

where \( \psi_{p,t}(x) = (2\pi)^{-d/2} e^{ipx} \eta(t/f(x)) \). Note also that

\[
\int_\mathbb{R}^d \int_0^\infty (p^2 - t^2) \langle \psi_{p,t} | \gamma | \psi_{p,t} \rangle \frac{dt}{t} \, dp \geq \int_\mathbb{R}^d \int_0^\infty (p^2 - t^2) - \| \psi_{p,t} \|^2 \frac{dt}{t} \, dp
\]

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

\[
\int_\mathbb{R}^d \int_0^\infty (p^2 - t^2) - \| \psi_{p,t} \|^2 \frac{dt}{t} \, dp = -\frac{1}{(2\pi)^d} \int_0^{\infty} (1 - p^2) dp \int_0^d f^{d+2} \int_0^\infty \eta(t)^2 t^{d+1} \, dt
\]

Altogether, we have thus shown that
\[
\text{Tr}(-\Delta) \gamma \geq -\int_\mathbb{R}^d \rho \frac{\|\nabla f\|^2}{f^2} \int_0^\infty \eta'(t)^2 t \, dt + \int_\mathbb{R}^d \rho f^2 \int_0^\infty \eta(t)^2 t^{d+1} \, dt - \frac{1}{(2\pi)^d} \int_{|p|\leq 1} (1 - p^2) dp \int_\mathbb{R}^{d+2} \eta(t)^2 t^{d+1} \, dt
\]

We now choose \( f = \rho^{1/d} \) 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

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

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

where \( \|\eta\|_2 \) denotes the \( L^2(\mathbb{R}_+, t \, dt) \) norm, and we used the simple identity \( ab^x = \frac{x^x}{(1+x)^{1+x}} \inf_{\lambda > 0} \lambda^{-x}(a + \lambda b)^{1+x} \) 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 \( d = 1 \), once 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

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

Data availability

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