Journal of Functional Analysis 285 (2023) 110129

Contents lists available at ScienceDirect

Journal of Functional Analysis

journal homepage: www.elsevier.com/locate/jfa

Full Length Article

A simple approach to Lieb–Thirring type inequalities ☆

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ARTICLE INFO

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

Keywords:
Lieb-Thirring inequality
Semiclassics
Density functional theory

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.

Let γ be a positive trace-class operator on $L^2(\mathbb{R}^d)$ with density (i.e., diagonal) ρ. 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 γ, 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 $\mathrm{Tr}(-\Delta)\gamma$, where Δ 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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https://doi.org/10.1016/j.jfa.2023.110129

$$\mathrm{Tr}(-\Delta)\gamma \geq C_d^{\mathrm{LT}} \int_{\mathbb{R}^d} \rho^{1+2/d} \tag{1}$$

for some universal constant C_d^{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, $C_d^{\mathrm{TF}} = 4\pi \frac{d}{d+2}\Gamma(1+d/2)^{2/d}$. 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^{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 $\mathrm{Tr}(-\Delta)\gamma$ for given ρ). 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*

$$\int_0^\infty \eta(t)^2 \frac{dt}{t} = 1 = \int_0^\infty \eta(t)^2 t\, dt \tag{2}$$

and let $C_d^{\mathrm{TF}} = 4\pi \frac{d}{d+2}\Gamma(1+d/2)^{2/d}$. For any trace-class $0 \leq \gamma \leq 1$ on $L^2(\mathbb{R}^d)$ with density ρ,

$$\mathrm{Tr}(-\Delta)\gamma \geq \frac{C_d^{\mathrm{TF}}}{\left(\int_0^\infty \eta(t)^2 t^{d+1} dt\right)^{2/d}} \int_{\mathbb{R}^d} \rho^{1+2/d} - \frac{4}{d^2} \int_{\mathbb{R}^d} |\nabla \sqrt{\rho}|^2 \int_0^\infty \eta'(t)^2 t\, dt \tag{3}$$

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, η^2 needs to be close to a δ-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

$$\int_0^\infty \eta(t)^2 t^{1+x} dt = \exp\left(\varepsilon x(2+x)/4\right)$$

for any $x \in \mathbb{R}$. For this choice of η the bound (3) thus reads

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

for any $\varepsilon > 0$. A similar bound was proved by Nam in [10], but with the exponent -1 of ε 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]

$$\mathrm{Tr}(-\Delta)\gamma \geq \int_{\mathbb{R}^d} |\nabla\sqrt{\rho}|^2 \tag{5}$$

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 ρ, we have*

$$\mathrm{Tr}(-\Delta)\gamma \geq C_d^{\mathrm{TF}} R_d \int_{\mathbb{R}^d} \rho^{1+2/d} \tag{6}$$

with

$$R_d = \sup_\eta \frac{1}{\left(\int \eta(t)^2 t^{d+1} dt\right)^{2/d}} \frac{1}{1 + \frac{4}{d^2} \int \eta'(t)^2 t \, dt} \tag{7}$$

where the supremum is over functions η satisfying the normalization conditions (2).

We shall show below that for $d \leq 2$, R_d can be calculated explicitly. In fact, $R_1 = (-3/a)^3/2^4 \approx 0.132$, 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

$$\mathrm{Tr}(-\Delta)\gamma = -\int_{\mathbb{R}^d} \rho \frac{|\nabla f|^2}{f^2} \int_0^\infty \eta'(t)^2 t\, dt + \int_{\mathbb{R}^d} \int_0^\infty p^2 \langle \psi_{p,t}|\gamma|\psi_{p,t}\rangle \frac{dt}{t} dp$$

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

$$\int_{\mathbb{R}^d} \int_0^\infty t\langle \psi_{p,t}|\gamma|\psi_{p,t}\rangle dt\, dp = \int_{\mathbb{R}^d} \rho f^2 \int_0^\infty \eta(t)^2 t\, dt = \int_{\mathbb{R}^d} \rho f^2$$

where we used the second normalization condition in (2). Hence

$$\mathrm{Tr}(-\Delta)\gamma = -\int_{\mathbb{R}^d} \rho \frac{|\nabla f|^2}{f^2} \int_0^\infty \eta'(t)^2 t\, dt + \int \rho f^2 + \int_{\mathbb{R}^d} \int_0^\infty (p^2 - t^2) \langle \psi_{p,t}|\gamma|\psi_{p,t}\rangle \frac{dt}{t} dp$$

Since $0 \le \gamma \le 1$ by assumption, we can get a lower bound on the last term as

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

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

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

Altogether, we have thus shown that

$$\mathrm{Tr}(-\Delta)\gamma \geq -\int_{\mathbb{R}^d} \rho \frac{|\nabla f|^2}{f^2} \int_0^\infty \eta'(t)^2 t\, dt + \int_{\mathbb{R}^d} \rho f^2$$
$$- \frac{1}{(2\pi)^d} \int_{|p|\leq 1} (1-p^2) dp \int_{\mathbb{R}^d} f^{d+2} \int_0^\infty \eta(t)^2 t^{d+1} dt$$

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

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 $-\Delta + |x|^d$ on $L^2(\mathbb{R}^{d+2})$). We claim that

$$R_d = \frac{d}{2} \left(\frac{d+2}{2e_d} \right)^{1+2/d} \tag{8}$$

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

$$\begin{aligned} \frac{1}{R_d} &= \frac{4}{d^2} \inf_{\|\eta\|_2=1} \left(\int \eta(t)^2 t^{d+1} dt \right)^{2/d} \int \left(\frac{d^2}{4t^2} \eta(t)^2 + \eta'(t)^2 \right) t\, dt \\ &= \frac{4}{d^2} \inf_{\|\eta\|_2=1} \inf_{\lambda>0} \left(\frac{2}{d\lambda} \right)^{2/d} \left[\frac{d}{d+2} \int \left(\frac{d^2}{4t^2} \eta(t)^2 + \lambda t^d \eta(t)^2 + \eta'(t)^2 \right) t\, dt \right]^{1+2/d} \end{aligned} \tag{9}$$

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 η for fixed λ 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 $t^{-1/2}\mathrm{Ai}(t + a)$ with a the largest real zero of the Airy function 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 ε, one finds

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

Data availability

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

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).

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