ELEMENTARY SPECTRAL THEORY OF SOME SCHRÖDINGER OPERATORS

Abstract. We prove some elementary properties regarding Schrödinger operators of the form $-\Delta + V$. In particular we prove for a certain class of potentials V that the spectrum of $-\Delta + V$ has only eigenvalues below 0. We also prove a basic Lieb-Thirring inequality for large sums of eigenvalues for Schrödinger operators and show that this inequality is dual to a type of Sobolev inequality for fermionic particles.

1. Solutions of the Schrödinger equation

The time independent Schrödinger equation (TISE) for a particle interacting with a potential $V(x)$ in $\mathbb{R}^n$ is given by

$$-\Delta\psi(x) + V(x)\psi(x) = E\psi(x) \tag{1}$$

where Δ is the (distributional) Laplacian. Here, $V : \mathbb{R}^n \to \mathbb{R}$ is some real valued measureable function. ψ is a wave function and the physical interpretation is that $|\psi(x)|^2\mathrm{d}x$ is the probability density associated with finding a particle at the point x. We therefore require the normalization condition,

$$\|\psi\|_2 = 1, \tag{2}$$

with $\|\cdot\|_p$ denoting the L^p norm on $\mathbb{R}^n$ as usual. We are interested in the eigenfunctions and eigenvalues for which (1) holds. Formally associated with the equation (1) and the operator $-\Delta + V$ is the quadratic form given by

$$\mathcal{E}(\psi) = T_\psi + V_\psi \tag{3}$$

where

$$T_\psi = \int_{\mathbb{R}^n} |\nabla\psi(x)|^2\mathrm{d}x, \qquad V_\psi = \int_{\mathbb{R}^n} V(x)|\psi(x)|^2\mathrm{d}x. \tag{4}$$

Physically, T_ψ is the kinetic energy of the particle, and V_ψ is the potential energy. One of our tasks is to find a class of wave functions and assumptions on V so that the above definitions make sense. It is natural to assume that ψ has finite kinetic energy, i.e., that $\psi \in H^1(\mathbb{R}^n)$, where $H^1(\mathbb{R}^n)$ is the space of square integrable wave functions with square integrable weak first derivatives. We will later see that in the case $n = 3$, a suitable assumption on the potential is that $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$.

Supposing that the definition of $\mathcal{E}(\psi)$ makes sense, we define the ground state energy

$$E_0 = \inf\left\{\mathcal{E}(\psi) : \|\psi\|_2 = 1, \psi \in H^1(\mathbb{R}^n)\right\}. \tag{5}$$

We would also like to find assumptions under which $E_0 > -\infty$. Minimizers of $\mathcal{E}(\psi)$, i.e. functions ψ_0 so that $\mathcal{E}(\psi_0) = E_0$ will turn out to be solutions to (1) with eigenvalue E_0. We will also define and investigate higher eigenvalues and obtain a complete description of the part of the spectrum of $-\Delta + V$ (under suitable assumptions on V) that lies below 0. Note that physically the negative part of the spectrum corresponds to bound states. They are stationary with respect to the dynamics induced by the semigroup $t \to e^{it(-\Delta+V)}$. However, this is unimportant for us and we will not mention this in the remainder of the paper.

From now on we will consider the physical case $n = 3$. We comment that the situations for $n > 3$ are relatively similar to the situation described below, as the nature of the Sobolev inequalities in dimensions $n \geq 3$ are similar. Similar statements for $n = 1$ and $n = 2$ can be made, and in general, less regularity can be assumed on the potentials. In $n = 1$, the potential can be any bounded Borel measure.

Lemma 1. *Let $\mathcal{E}(\psi)$ be as in (3) and assume that the potential satisfies $V(x) \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Then there exists a constant C so that $\forall \psi \in H^1(\mathbb{R}^3)$,*

$$\mathcal{E}(\psi) \geq \frac{1}{2} T_\psi - C \|\psi\|_2 \tag{6}$$

Proof. For $\psi \in H^1(\mathbb{R}^3)$ the Sobolev inequality

$$\int_{\mathbb{R}^3} |\nabla \psi(x)|^2 \mathrm{d}x \geq S_3 \left(\int_{\mathbb{R}^3} |\psi(x)|^6 \mathrm{d}x \right)^{1/3} \tag{7}$$

holds, with $S_3 = 3(2\pi^3)^{2/3}/4$. By assumption, we can write $V(x) = w(x) + h(x)$ with $w \in L^{3/2}(\mathbb{R}^3)$ and $h \in L^\infty(\mathbb{R}^3)$. Define for $\lambda > 0$,

$$w_\lambda(x) = \begin{cases} w(x), & |w(x)| \leq \lambda \\ 0, & \text{else.} \end{cases} \tag{8}$$

By dominated convergence, $\lim_{\lambda \to \infty} \|w - w_\lambda\|_{3/2} = 0$. Since $V(x) = (w(x) - w_\lambda(x)) + (w_\lambda(x) + h(x))$, for any $\delta > 0$ we can write $V(x) = v_\delta(x) + v(x)$, where $\|v_\delta\|_{3/2} < \delta$ and $v \in L^\infty(\mathbb{R}^3)$. Take $\delta = S_3/2$. Then,

$$\begin{aligned} |V_\psi| &\leq \int_{\mathbb{R}^3} |v_\delta(x)||\psi(x)|^2 \mathrm{d}x + \int_{\mathbb{R}^3} |v(x)||psi(x)|^2 \mathrm{d}x \\ &\leq \left(\int_{\mathbb{R}^3} |v_\delta(x)|^{3/2} \mathrm{d}x \right)^{2/3} \left(\int_{\mathbb{R}^3} |\psi(x)|^6 \mathrm{d}x \right)^{1/3} + \|v\|_\infty \|\psi\|_2^2 \\ &\leq \frac{1}{2} T_\psi + \|v\|_\infty \|\psi\|_2^2 . \end{aligned} \tag{9}$$

In the second line we have applied Hölder's inequality. In the last line we have applied the Sobolev inequality (7) and our bound on the $L^{3/2}$ norm of v_δ. Note that the above argument also shows that under the assumption that $V(x) \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, the function $\psi \to V_\psi$ is well defined whenever $\psi \in H^1(\mathbb{R}^3)$. Therefore,

$$\mathcal{E}(\psi) = T_\psi + V_\psi \geq T_\psi - |V_\psi| \geq \frac{1}{2} T_\psi - \|v\|_\infty \|\psi\|_2^2 . \tag{10}$$

□

In particular, Lemma 1 implies that $E_0 > -\infty$. We will now turn to establishing the existence of a minimizer ψ_0. The main technical element is the following, in which we establish weak semicontinuity of the potential.

Lemma 2. *Assume the potential $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Additionally, assume that V vanishes at infinity, that is, for any $a > 0$,*

$$|\{x : |V(x)| > a\}| < \infty, \tag{11}$$

where $|\cdot|$ denotes the Lebesgue measure of a set. Then the function $\psi \to V_\psi$ is weakly (sequentially) continuous on $H^1(\mathbb{R}^3)$. That is, if $\psi_j \rightharpoonup \psi$ in $H^1(\mathbb{R}^3)$, then $V_{\psi_j} \to V_\psi$.

Proof. Let $\psi_j \rightharpoonup \psi$ in $H^1(\mathbb{R}^3)$. By the uniform boundedness principle and the fact that $H^1(\mathbb{R}^3)$ is a Hilbert space the $H^1(\mathbb{R}^3)$ norms of the ψ_j are uniformly bounded. For $\delta > 0$, define

$$V_\delta(x) = \begin{cases} V(x), & |V(x)| \leq \delta^{-1} \\ 0, & \text{else.} \end{cases} \tag{12}$$

Note that $\lim_{\delta\to 0}\|V - V_\delta\|_{3/2} = 0$. Since,

$$\begin{aligned}|V_{\psi_j} - V_\psi| &\le \int_{\mathbb{R}^3} |V_\delta(x) - V(x)||\psi_j(x)|^2 \mathrm{d}x + \int_{\mathbb{R}^3} |V_\delta(x) - V(x)||\psi|^2 \mathrm{d}x + \int_{\mathbb{R}^3} |V_\delta(x)| \left||\psi_j|^2 - |\psi|^2\right| \mathrm{d}x \\ &\le \|V_\delta - V\|_{3/2}\, 2S_3 \times \sup_j \|\psi_j\|_{H^1} + \int_{\mathbb{R}^3} |V_\delta(x)| \left||\psi_j(x)|^2 - |\psi(x)|^2\right| \mathrm{d}x, \end{aligned} \tag{13}$$

we have that

$$\limsup_{j\to\infty} |V_{\psi_j} - V_\psi| \le C_\delta + \limsup_{j\to\infty} \int_{\mathbb{R}^3} |V_\delta(x)| \left||\psi_j(x)|^2 - |\psi(x)|^2\right| \mathrm{d}x, \tag{14}$$

where C_δ is a constant independent of j that goes to 0 as $\delta \to 0$. Note we have used that $\|\psi\|_{H^1} \le \sup_j \|\psi_j\|_{H^1}$. We are therefore left with proving that for any $\delta > 0$, $\limsup_{j\to\infty} \int_{\mathbb{R}^3} |V_\delta(x)|\left||\psi_j(x)|^2 - |\psi(x)|^2\right|\mathrm{d}x = 0$.

Let $\varepsilon > 0$, and define $A_\varepsilon = \{x : |V_\delta| > \varepsilon\}$. By our assumptions on V we have $|A_\varepsilon| < \infty$. By Theorem 8.6 of [LL], we have $\psi_j \to \psi$ strongly in $L^r(A_\varepsilon)$, for $2 \le r < 6$ (this follows from the fact that $\psi_j \rightharpoonup \psi$ in $H^1(\mathbb{R}^3)$ and A_ε is of finite measure). By the elementary inequality,

$$\left||\psi_j|^2 - |\psi|^2\right| = ||\psi_j| - |\psi|| \times ||\psi_j| + |\psi|| \le |\psi_j - \psi| \times ||\psi_j| + |\psi||, \tag{15}$$

we have that $|\psi_j|^2 \to |\psi|^2$ strongly in $L^{r/2}(A_\varepsilon)$. Let $1 \le s \le \infty$ be a number so that $1/s + 2/r = 1$. Since $V_\delta \in L^\infty(\mathbb{R}^3)$, we have that $V_\delta \in L^s(A_\varepsilon)$. It follows that,

$$\begin{aligned}\int_{\mathbb{R}^3} |V_\delta(x)| \left||\psi_j(x)|^2 - |\psi(x)|^2\right| \mathrm{d}x &\le \int_{A_\varepsilon} |V_\delta(x)| \left||\psi_j(x)|^2 - |\psi(x)|^2\right| \mathrm{d}x \\ &\quad + \int_{\mathbb{R}^3\setminus A_\varepsilon} |V_\delta(x)| \left||\psi_j(x)|^2 - |\psi(x)|^2\right| \mathrm{d}x \\ &\le \|V_\delta\|_s \left\||\psi_j|^2 - |\psi|^2\right\|_{r/2}^2 + 2\varepsilon \times \sup_j \|\psi_j\|_2^2 \end{aligned} \tag{16}$$

In the last line we have applied Hölder's inequality. Taking lim sup on both sides and then $\varepsilon \to 0$ yields the claim. □

We record here the following Corollary of the above proof, which will be useful later.

Corollary 1. *Let U be a nonnegative potential satisfying the conditions of Lemma 2. Then, multiplication by $\sqrt{U}(x)$ is a compact operator from $H^1(\mathbb{R}^3)$ to $L^2(\mathbb{R}^3)$. That is, if $\psi_j \rightharpoonup \psi$ weakly in $H^1(\mathbb{R}^3)$, then $\sqrt{U}\psi_j \to \sqrt{U}\psi$ strongly in $L^2(\mathbb{R}^3)$.*

Proof. Applying the Sobolev and Hölder inequalities as before, we see that multiplication by $\sqrt{U}$ is indeed a bounded operator from $H^1(\mathbb{R}^3)$ to $L^2(\mathbb{R}^3)$. To see that it is compact, we need to prove that if $\psi_j \rightharpoonup \psi$ weakly then

$$\lim_{j\to\infty} \int_{\mathbb{R}^3} U(x)|\psi_j(x) - \psi(x)|^2 \mathrm{d}x = 0. \tag{17}$$

However, this precisely the content of the proof of Lemma 2. □

We are now in position to prove the existence of a minimizer for $\mathcal{E}(\psi)$.

Theorem 1. *Let $V(x)$ be a real valued function satisfying $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Assume furthermore that V vanishes at infinity. Let $\mathcal{E}(\psi) = T_\psi + V_\psi$ as before and assume that*

$$E_0 = \inf\left\{\mathcal{E}(\psi) : \psi \in H^1(\mathbb{R}^3), \|\psi\|_2 = 1\right\} < 0. \tag{18}$$

Then there exists a $\psi_0 \in H^1(\mathbb{R}^3)$ satisfying $\|\psi_0\|_2 = 1$ and $\mathcal{E}(\psi_0) = E_0$. Furthermore, ψ_0 satisfies the TISE,

$$-\Delta\psi_0(x) + V(x)\psi_0(x) = E_0\psi(x), \tag{19}$$

in the sense of distributions.

Proof. By Lemma 1, $E_0 > -\infty$. Let ψ_j be a minimizing sequence of $H^1(\mathbb{R}^3)$ functions with $\|\psi_j\|_2 = 1$ so that $\mathcal{E}(\psi_j) \to E_0$. By (6), the $H^1(\mathbb{R}^3)$ norms of the ψ_j are uniformly bounded, since the $\mathcal{E}(\psi_j)$ are a converging sequence of real numbers. Since $H^1(\mathbb{R}^3)$ is weakly compact, there exists a subsequence, which we continue to denote by ψ_j, that converges weakly to some $H^1(\mathbb{R}^3)$ function ψ_0. By the fact that norms are weakly lower semicontinuous,

$$\liminf_{j\to\infty} \int_{\mathbb{R}^3} |\psi_j(x)|^2 \mathrm{d}x \geq \int_{\mathbb{R}^3} |\psi_0(x)|^2 \mathrm{d}x \tag{20}$$

$$\liminf_{j\to\infty} \int_{\mathbb{R}^3} |\nabla\psi_j(x)|^2 \mathrm{d}x \geq \int_{\mathbb{R}^3} |\nabla\psi_0(x)|^2 \mathrm{d}x. \tag{21}$$

By (20), $\|\psi_0\|_2 \leq 1$. By (21) and Lemma 2 the function $\psi \to \mathcal{E}(\psi)$ is weakly lower semicontinuous, i.e.,

$$\liminf_{j\to\infty} \mathcal{E}(\psi_j) \geq \liminf_{f\to\infty} T_{\psi_j} + \liminf_{j\to\infty} V_{\psi_j} \geq T_{\psi_0} + V_{\psi_0} = \mathcal{E}(\psi_0). \tag{22}$$

Therefore, $E_0 \geq \mathcal{E}(\psi_0)$. Since $E_0 < 0$ by assumption, ψ_0 cannot be the zero function, i.e., $\|\psi_0\|_2 > 0$. We have

$$0 > E_0 \geq \mathcal{E}(\psi_0) = \mathcal{E}\left(\psi_0/\|\psi_0\|_2\right) \|\psi_0\|_2^2 \geq E_0 \|\psi_0\|_2^2, \tag{23}$$

and so $\|\psi_0\|_2 \geq 1$. But since we already had that $\|\psi_0\|_2 \leq 1$, we must have $\|\psi_0\|_2 = 1$ and so $\mathcal{E}(\psi_0) = E_0$.

We now prove that ψ_0 satisfies (19). For functions $H^1(\mathbb{R}^3)$ functions ϕ and φ define

$$\mathcal{E}(\phi, \varphi) = \int_{\mathbb{R}^3} \overline{\nabla}\phi(x) \cdot \nabla\varphi(x) \mathrm{d}x + \int_{\mathbb{R}^3} V(x)\bar{\phi}(x)\varphi(x)\mathrm{d}x. \tag{24}$$

Obviously, $\mathcal{E}(\phi, \varphi)$ is well defined and $\mathcal{E}(\psi, \psi) = \mathcal{E}(\psi)$. Let $\varepsilon > 0$ and $f \in C_c^\infty(\mathbb{R}^3)$ any infinitely differentiable function of compact support. Let $\psi^\varepsilon(x) = \psi_0(x) + \varepsilon f(x)$. Define for ε small enough the function,

$$R(\varepsilon) = \frac{\mathcal{E}(\psi^\varepsilon)}{(\psi^\varepsilon, \psi^\varepsilon)} = \frac{\mathcal{E}(\psi_0) + \varepsilon\mathcal{E}(\psi_0, f) + \varepsilon\mathcal{E}(f, \psi_0) + \varepsilon^3\mathcal{E}(f, f)}{(\psi_0, \psi_0) + \varepsilon(\psi_0, f) + \varepsilon(f, \psi_0) + \varepsilon^2(f, f)}, \tag{25}$$

where $(\cdot, \cdot)$ is the inner product on $L^2(\mathbb{R}^3)$. Clearly $R(\varepsilon)$ is differentiable at $\varepsilon = 0$ and since ψ_0 is a minimizer, the derivative must be 0 there. We compute,

$$0 = \frac{\mathrm{d}}{\mathrm{d}\varepsilon} R(\varepsilon)\bigg|_{\varepsilon=0} = \mathcal{E}(\psi_0, f) + \mathcal{E}(f, \psi_0) - \mathcal{E}(\psi_0)\left[(\psi_0, f) + (f, \psi_0)\right] \tag{26}$$

Integrating by parts we have

$$(-\Delta f + Vf, \psi_0) + (\psi_0, -\Delta f + Vf) = E_0\left[(f, \psi_0) + (\psi_0, f)\right]. \tag{27}$$

Because we take f to be purely imaginary or purely real, we see that the real and imaginary parts of ψ_0 satisfy the TISE separately, and therefore all of ψ_0 satisfies the TISE. □

We have shown that minimizers of the functional $\mathcal{E}(\phi)$ satisfy the TISE. The converse also holds:

Lemma 3. *Let the potential V be as in Theorem 1, and let $\psi \in H^1(\mathbb{R}^3)$ satisfy*

$$-\Delta\psi(x) + V(x)\psi(x) = E\psi(x) \tag{28}$$

in the sense of distributions for $E \in \mathbb{R}$. Then,

$$\mathcal{E}(\psi) = E\|\psi\|_2^2 \tag{29}$$

In particular, if ψ satisfies (28) with eigenvalue E_0, then ψ minimizes the functional $\mathcal{E}(\phi)$.

Proof. Let ϕ_j be a sequence of $C_c^\infty(\mathbb{R}^3)$ functions converging to ψ in $H^1(\mathbb{R}^3)$ norm. By the Sobolev inequalities they also converge in $L^6(\mathbb{R}^3)$ norm. For every j we have by taking the conjugate of (28),

$$-\int_{\mathbb{R}^3} \bar{\psi}(x)\Delta\phi_j(x)\mathrm{d}x + \int_{\mathbb{R}^3} V(x)\bar{\psi}(x)\phi_j(x)\mathrm{d}x = E\int_{\mathbb{R}^3} \bar{\psi}(x)\phi_j(x)\mathrm{d}x. \tag{30}$$

Let us take $j \to \infty$ on both sides. Integrating by parts (which we may do because ψ is an H^1 function) we obtain

$$\lim_{j\to\infty} -\int_{\mathbb{R}^3} \bar{\psi}(x)\Delta\phi_j(x)\mathrm{d}x = \lim_{j\to\infty}\int_{\mathbb{R}^3} \nabla\bar{\psi}(x)\cdot\nabla\phi_j(x)\mathrm{d}x = \int_{\mathbb{R}^3} |\nabla\psi(x)|^2\mathrm{d}x. \tag{31}$$

The last equality follows from Cauchy-Schwarz. Also by Cauchy-Schwarz, $\lim_{j\to\infty}(\psi,\phi_j) = (\psi,\psi)$. Let $V(x) = w(x) + h(x)$, with $w \in L^{3/2}(\mathbb{R}^3)$ and $h \in L^\infty(\mathbb{R}^3)$. By Hölder's inequality,

$$\left|\int_{\mathbb{R}^3} V(x)\bar{\psi}(x)\phi_j(x)\mathrm{d}x - \int_{\mathbb{R}^3} V(x)|\psi(x)|^2\mathrm{d}x\right| \le \|w\|_{3/2}\|\psi\|_6\|\psi-\phi_j\|_6 + \|h\|_\infty\|\psi\|_2\|\psi-\phi_j\|_2 \tag{32}$$

Therefore,

$$E\|\psi\|_2^2 = \lim_{j\to\infty} E(\psi,\phi_j) = \lim_{j\to\infty} -\int_{\mathbb{R}^3}\bar{\psi}(x)\Delta\phi_j(x)\mathrm{d}x + \int_{\mathbb{R}^3} V(x)\bar{\psi}(x)\phi_j(x)\mathrm{d}x = \mathcal{E}(\psi). \tag{33}$$

□

Remark. We did not require that V vanishes at infinity.

We have shown that under suitable assumptions on V that the ground state energy E_0 is attained if it is negative. We would now like to turn to the definition of higher eigenvalues. Before, doing so we should make a comment on our choice of terminology. In the remainder of the paper, we will use the term **orthogonal** to refer to two functions that are orthogonal in $L^2(\mathbb{R}^3)$, even though the Hilbert space we are considering is $H^1(\mathbb{R}^3)$. We will also use **orthonormal** to denote a set of functions which are pairwise orthogonal in $L^2(\mathbb{R}^3)$ and have $L^2(\mathbb{R}^3)$ norms equal to 1.

Let us now proceed with our discussion of higher eigenvalues. We define the first higher eigenvalue as

$$E_1 = \inf\left\{\mathcal{E}(\psi) : \psi \in H^1(\mathbb{R}^3), \|\psi\|_2 = 1, (\psi_0,\psi) = 0\right\}. \tag{34}$$

Again, $(\cdot,\cdot)$ is the inner product on $L^2(\mathbb{R}^3)$. We are minimizing the functional $\mathcal{E}(\psi)$ over the part of $L^2(\mathbb{R}^3)$ that is orthogonal to the minimizer ψ_0. This leads us to a natural inductive definition. If the eigenvalue E_1 is attained by some function ψ_1 (that is normalized to have L^2 norm 1 and is orthogonal to ψ_0), then we can define the second higher eigenvalue E_2 by the same formula as in (34) but also require that the functions are orthogonal to ψ_1. If this eigenvalue is attained, then we can define E_3, and so on and so forth.

To make this precise, suppose that the first k eigenvalues have been defined and are attained. What we mean is that for each $0 \le j \le k$ there is an $H^1(\mathbb{R}^3)$ function ψ_j with $\|\psi_j\|_2 = 1$ so that $(\psi_j,\psi_l) = 0$ for any $0 \le l < j$, and $\mathcal{E}(\psi_j) = E_j$ where

$$E_j = \inf\left\{\mathcal{E}(\psi) : \psi \in \mathcal{H}^1(\mathbb{R}^3), \|\psi\|_2 = 1, (\psi_l,\psi) = 0, 0 \le l < j\right\}. \tag{35}$$

Then we define the $(k+1)$th eigenvalue E_{k+1} by

$$E_{k+1} = \inf\left\{\mathcal{E}(\psi) : \psi \in \mathcal{H}^1(\mathbb{R}^3), \|\psi\|_2 = 1, (\psi_l,\psi) = 0, 0 \le l < k+1\right\}. \tag{36}$$

We continue to define eigenvalues until one is not attained. If an eigenvalue E_k is not attained by some wave function ψ_k with the required orthogonality properties, then we stop this definition.

Obviously we have $E_0 \le E_1 \le$ ..... The following theorem says this process does not stop until we hit $E_k = 0$.

Theorem 2. *Let V be as in Theorem 1 and assume that the $(k+1)$th eigenvalue is negative. This includes the assumption that the first k eigenfunctions exist and attain the first k eigenvalues. Then the $(k+1)$th eigenfunction also exists and satisfies*

$$-\Delta\psi_k(x) + V(x)\psi_k(x) = E_k\psi_k(x) \tag{37}$$

in the sense of distributions (note that the $(k+1)$th eigenvalue is E_k since the first eigenvalue is E_0).

Proof. The proof is nearly identical to that of Theorem 1. We take a minimizing sequence of normalized H^1 functions ϕ_j so that $\mathcal{E}(\phi_j) \to E_k$. By Lemma 1 the H^1 norms of the ϕ_l's are bounded and so we extract a subsequence (which we continue to denote by ϕ_j) converging weakly to some ψ_k. The same argument of Theorem 1 shows us that $E_k = \mathcal{E}(\psi_k)$ and $\|\psi_k\|_2 = 1$ *if* we can show that ψ_k is orthogonal to each ψ_j, $0 \le i < k$. But $\psi \to (\psi_i, \psi)$ defines a linear functional on $H^1(\mathbb{R}^3)$ and so $0 = \lim_{j\to\infty}(\psi_i, \phi_j) = (\psi_i, \psi_k)$.

Let us now prove that (37) holds. Let $f \in C_c^\infty(\mathbb{R}^3)$ be a function so that $(f, \psi_i) = 0$, for $0 \le i < k$. As in the proof of Theorem 1, define for ε small enough the function $\varepsilon \to R(\varepsilon) = \mathcal{E}(\psi_k + \varepsilon f)/\|\psi_k + \varepsilon f\|_2^2$. Arguing as in Theorem 1 by evaluating the derivative of $R(\varepsilon)$ at $\varepsilon = 0$, we see that the distribution $D := (-\Delta + V - E_k)\psi_k$ satisfies $D(f) = 0$ for every $C_c^\infty(\mathbb{R}^3)$ that is orthogonal to every ψ_i, for $i < k$. It follows from Theorem 6.14 in [LL] that

$$D = \sum_{i=0}^{k-1} c_i\psi_i, \tag{38}$$

where $c_0, ..., c_{k-1}$ are constants. We would like to show that every constant c_l is 0. Let ϕ_j be a sequence of $C_c^\infty(\mathbb{R}^3)$ functions converging to ψ_l in H^1 norm, for some $l < k$. Taking the conjugate of D, we have

$$\sum_{i=1}^{k-1}(\psi_i, \phi_j) = \int_{\mathbb{R}^3} \nabla\overline{\psi_k}(x)\cdot\nabla\phi_j(x)\mathrm{d}x + \int_{\mathbb{R}^3} V(x)\overline{\psi_k}(x)\phi_j(x)\mathrm{d}x - E_k(\psi_k, \phi_j). \tag{39}$$

Above, we have integrated by parts which is justifed because $\psi_k \in H^1(\mathbb{R}^3)$. Let us take $j \to \infty$ on both sides. The same arguments that appear in Lemma 3 show that we can pass the limit inside the integral on both sides of the above equality. We obtain

$$c_l = \int_{\mathbb{R}^3} \nabla\overline{\psi_k}(x)\cdot\nabla\psi_l(x)\mathrm{d}x + \int_{\mathbb{R}^3} V(x)\overline{\psi_k}(x)\psi_l(x)\mathrm{d}x \tag{40}$$

by the orthogonality of ψ_i's. Let now φ_j be a sequence of $C_c^\infty(\mathbb{R}^3)$ functions converging to ψ_k in H^1 norm. Since ψ_l satisfies the Schrödinger equation (37) with the eigenvalue E_l, we have, after an integration by parts,

$$\int_{\mathbb{R}^3} \nabla\overline{\varphi_j}(x)\cdot\nabla\psi_l(x)\mathrm{d}x + \int_{\mathbb{R}^3} V(x)\overline{\varphi_j}(x)\psi_l(x)\mathrm{d}x = E_l(\varphi_j, \psi_l). \tag{41}$$

Again, we may take the limit $j \to \infty$ on both sides and pass the limit inside the integral. We obtain,

$$\int_{\mathbb{R}^3} \nabla\overline{\psi_k}(x)\cdot\nabla\psi_l(x)\mathrm{d}x + \int_{\mathbb{R}^3} V(x)\overline{\psi_k}(x)\psi_l(x)\mathrm{d}x = E_l(\psi_k, \psi_l) = 0. \tag{42}$$

Comparing with (40) we see that each $c_l = 0$. The claim follows. □

Let us now prove some elementary properties of the eigenfunctions:

Lemma 4. *Consider our sequence of eigenvalues $E_0 \le E_1$... and our sequence of orthonormal eigenfunctions ψ_0, ψ_1.... Then each eigenvalue has finite multiplicity. That is any number $E_k < 0$ occurs only finitely many times in our list of eigenvalues. Furthermore, let ψ be any H^1 function satisfying (37) with eigenvalue E_k. Then ψ is a linear combination of the eigenfunctions that have an eigenvalue equal to E_k.*

Proof. Assume that there is some E_k that occurs in our list of eigenvalues infinitely many times with $E_k < 0$ (i.e., $E_k = E_{k+1} = ...$). By the theorem just proved, there are then infinitely many orthonormal eigenfunctions ψ_j, $j \geq k$, each with eigenvalue $E_j = E_k$. Since any sequence of orthonormal functions converges weakly to 0 in L^2, we have that $\psi_j \rightharpoonup 0$ in L^2.

By Lemma 1 the H^1 norms of the ψ_j's are uniformly bounded, and so we may pass to a subsequence converging weakly in H^1. But this subsequence must have the same weak limit in L^2 as the entire sequence does, so this subsequence, which we continue denote by ψ_j, must converge to 0 weakly in H^1. By Lemma 2 we must have that $\lim_{j\to\infty} V_{\psi_j} = 0$. But,

$$0 > E_k = \lim_{j\to\infty} \mathcal{E}(\psi_j) = \lim_{j\to\infty} \left(T_{\psi_j} + V_{\psi_j}\right) \geq 0. \tag{43}$$

we therefore have a contradiction and the first claim is proven.

Let now ψ be an $H^1(\mathbb{R}^3)$ function satisfying the TISE with eigenvalue $E_k < 0$. Say that E_k has multiplicty l, so that $\psi_k, ..., \psi_{k+l-1}$ are the l orthonormal eigenfunctions with eigenvalue E_k. WLOG, assume that $E_{k-1} < E_k$. Let ϕ_j be a sequence of $C_c^\infty(\mathbb{R}^3)$ functions converging to ψ_i in H^1 norm, with $i < k$. Since ψ satisfies the TISE with eigenvalue E_k we have that

$$\begin{aligned} E_k(\psi, \psi_i) = \lim_{j\to\infty} E_k(\psi, \phi_j) &= \lim_{j\to\infty} \int_{\mathbb{R}^3} \nabla\bar{\psi}(x) \cdot \nabla\phi_j(x)\ dx + \int_{\mathbb{R}^3} V(x)\bar{\psi}(x)\phi_j(x)\mathrm{d}x \\ &= \int_{\mathbb{R}^3} \nabla\bar{\psi}(x) \cdot \nabla\psi_i(x)\ dx + \int_{\mathbb{R}^3} V(x)\bar{\psi}(x)\psi_i(x)\mathrm{d}x. \end{aligned} \tag{44}$$

The integration by parts and passing the limits through the integrals is justifed by the same argument appearing in Lemma 3. However, since ψ_i satisfies the TISE with eigenvalue E_i, the same argument shows that

$$E_i(\psi, \psi_i) = \int_{\mathbb{R}^3} \nabla\bar{\psi}(x) \cdot \nabla\psi_i(x)\ dx + \int_{\mathbb{R}^3} V(x)\bar{\psi}(x)\psi_i(x)\mathrm{d}x. \tag{45}$$

Since $E_i \neq E_k$, $(\psi, \psi_i) = 0$. Therefore ψ is orthogonal to each ψ_i, with $i < k$. Assume that $\psi(x) - \sum_{i=k}^{k+l-1}(\psi_i, \psi)\psi_i(x)$ is not the 0 function (if it is, then we are done - note that this the sum is just the projection of ψ onto the eigenspace of E_k). Let now,

$$\widehat{\psi}(x) = \frac{\psi(x) - \sum_{i=k}^{k+l-1}(\psi_i, \psi)\psi_i(x)}{\left\|\psi(x) - \sum_{i=k}^{k+l-1}(\psi_i, \psi)\psi_i(x)\right\|_2} \tag{46}$$

Then $\widehat{\psi}$ is a normalized wave function that is orthogonal to each ψ_i, for $i \leq k + l - 1$. Therefore, $\mathcal{E}(\widehat{\psi}) \geq E_{k+l} > E_k$. However, $\widehat{\psi}$ clearly satisfies the TISE with eigenvalue E_k and so by Lemma 3, $\mathcal{E}(\widehat{\psi}) = E_k$. This is a contradiction, and so

$$\psi(x) = \sum_{i=k}^{k+l-1} (\psi_i, \psi)\psi_i(x). \tag{47}$$

□

With a bit more work regarding defining the operator $-\Delta + V$ as an unbounded operator on L^2, what we have proven can be turned into a statement about its spectrum. What we have shown is that the spectrum of $-\Delta + V$ that lies below 0 consists purely of eigenvalues. The general picture is that above 0 one expects continuous spectrum which is related to scattering.

2. Lieb-Thirring Inequalities

We turn now to a slightly different, however related, topic regarding the operator $-\Delta + V$, specifically that of bounds on large sums of its negative eigenvalues. We begin with a heuristic discussion which will hopefully motivate the topic. The semiclassical approach to quantum mechanics goes back to some of the earliest days of its development. The main idea was to literally quantize the classical phase space (i.e. the $2d$-dimensional space consisting of pairs (p, x), with p the momentum of a particle in n dimensions and x its position) by saying that every allowed unit of $(2\pi)^n$ of phase space volume can support a single quantum state.

This prescription allows one to 'calculate' the number of negative eigenvalues by integration as follows:

$$\sum_j |E_j|^0 \approx (2\pi)^{-n} \int_{\mathbb{R}^n \times \mathbb{R}^n} \Theta(-p^2 - V(x)) \mathrm{d}p \mathrm{d}x. \tag{48}$$

Here, $\Theta(t)$ is the step function which is 0 for $t < 0$ and 1 otherwise. The heuristic justification of (48) is as follows. The RHS is the volume of phase space where the classical energy of the particle, $p^2 + V(x)$, is negative. Dividing this volume by the normalization $(2\pi)^n$ we obtain the number of quantum states that this part of phase space can support. This is equal to the LHS, the number of nonpositive eigenvalues (here $0^0 = 1$).

It is easy to do the p integral first; for every fixed x, the p integration just gives the volume of the d dimensional ball of radius $\sqrt{V_-(x)}$, where $V_-(x) = \max\{0, -V(x)\}$ is the negative part of the potential. Hence,

$$\sum_j |E_j|^0 = \frac{1}{(4\pi)^{n/2}\Gamma(n/2+1)} \int_{\mathbb{R}^n} V_-(x)^{n/2} \mathrm{d}x. \tag{49}$$

Above, $\Gamma(t)$ is the gamma function. One can go further and compute moments of the negative eigenvalues, $\sum_j |E_j|^\gamma$ for $\gamma \geq 0$. Now every volume $(2\pi)^n$ of phase space where $p^2 + V(x) < 0$ contributes $|p^2 + V(x)|^\gamma$ to this sum. By this reasoning,

$$\sum_j |E_j|^\gamma \approx \int_{p^2+V(x)<0} |p^2 + V(x)|^\gamma \mathrm{d}p \mathrm{d}x. \tag{50}$$

Again, one can do the p integration first and arrive at

$$\sum_j |E_j|^\gamma \approx L^{\mathrm{cl}}_{\gamma,n} \int_{\mathbb{R}^n} V_-(x)^{\gamma+n/2} \mathrm{d}x, \tag{51}$$

where $L^{\mathrm{cl}}_{\gamma,n}$ is the 'classical' constant

$$\begin{aligned} L^{\mathrm{cl}}_{\gamma,n} &= (2\pi)^{-n} \int_{\mathbb{R}^n : |p| \leq 1} (1-p^2)^\gamma \mathrm{d}p \\ &= \frac{\Gamma(\gamma+1)}{(4\pi)^{n/2}\Gamma(\gamma+1+n/2)}. \end{aligned} \tag{52}$$

The interesting fact is that under suitable assumptions on V, the formula (51) is actually asymptotically correct in the semiclassical limit, where we scale $V \to \lambda V$ and send $\lambda \to \infty$ (see Theorem 12.12 in [LL] for the case $\gamma = 1$). In physics, this corresponds to taking the value of Planck's constant $\hbar \to 0$.

We will not be interested in this semiclassical limit, but we will be interested in whether or not the equality in (51) can be turned into an inequality for the sums of moments of negative eigenvalues which holds for any potential V. Our next theorem says that this can, in fact, be achieved. We record here suitable assumptions on the potential $V(x)$, which generalize the assumptions we made in the case $n = 3$. "Suitable assumptions" on $V : \mathbb{R}^n \to \mathbb{R}$ will from now on mean:

$$V \in \begin{cases} L^{n/2}(\mathbb{R}^n) + L^\infty(\mathbb{R}^n), & n \geq 3, \\ L^{1+\varepsilon}(\mathbb{R}^2) + L^\infty(\mathbb{R}^2), & n = 2, \\ L^1(\mathbb{R}^1) + L^\infty(\mathbb{R}^1), & n = 1 \end{cases} \tag{53}$$

Theorem 3. *Fix $\gamma \geq 0$. Assume that the potential $V = V_+ - V_-$ satisfies (53) and that $V_- \in L^{\gamma+d/2}(\mathbb{R}^n)$. Let $E_0 < E_1 \leq E_2 \ldots$ be the negative eigenvalues, if there are any. Then, for suitable n, there is a constant $L_{\gamma,n}$ so that*

$$\sum_{j\geq 0} |E_j|^\gamma \leq L_{\gamma,n} \int_{\mathbb{R}^n} V_-(x)^{\gamma+n/2} \mathrm{d}x. \tag{54}$$

By suitable n, we mean that the inequality holds for the following pairs of γ and n:

$$\begin{aligned} \gamma &\geq \frac{1}{2} \quad \text{for } n = 1, \\ \gamma &> 0 \quad \text{for } n = 2, \\ \gamma &\geq 0 \quad \text{for } n = 3. \end{aligned} \tag{55}$$

For any other pair, there is a choice of potential V_- that violates (54). We can take the constants to be

$$L_{\gamma,n} = (4\pi)^{-n/2} 2^\gamma \gamma \times \begin{cases} (n+\gamma)\Gamma(\gamma/2)^2\Gamma(\gamma+1+n/2), & \text{if } n > 1, \gamma > 0 \\ & \text{or } n = 1, \gamma \geq 1, \\ \sqrt{\pi}/(\gamma^2 - 1/4), & \text{if } n = 1, \gamma > 1/2 \end{cases} \tag{56}$$

Note that our assumptions on the potential here are weaker than the assumptions of Theorem 2, and so we are not guaranteed discrete spectra below 0. However, our definition of the eigenvalues is still valid: we define inductively each higher eigenvalue only if the previous eigenvalues are achieved by requiring that the functions we are minimizing over are orthogonal to the previous eigenfunctions. Note, however, that through an application of the min-max principle (i.e., Theorem 12.1 in [LL]), it is easy to see that the operator $\Delta + V$ can only have eigenvalues below 0, by the assumptions on V_-.

The proof of (54) in all cases *except* $n \geq 3, \gamma = 0$ and $n = 1, \gamma = 1/2$ is due to E.H. Lieb and W. Thirring [LT]. The inequalities in the case of $\gamma = 0, n \geq 3$ were proven independently in [C], [L] and [R], each by completely different methods and are known as the CLR bounds (for an amusing anecdote of B. Simon regarding the three almost simultaneuous proofs see [Si]. For a correction to this anecdote see [SRY]). The proof in the case $\gamma = 1/2, n = 1$ came much later in [1]. It is also one of the few cases where the sharp constant is currently known [HLT].

It is an open (if not as active as it once was) area of research to compute the sharp constants in (54). It is known in some cases that $L_{\gamma,n} = L^{\mathrm{cl}}_{\gamma,n}$, while in other cases that $L_{\gamma,n} > L^{\mathrm{cl}}_{\gamma,n}$. Unfortunately the sharp constant is not known in the physically most interesting case, $\gamma = 1, n = 3$. It is conjectured that $L^{\mathrm{cl}}_{1,3} = L_{1,3}$ [LT]. It is also known that for $\gamma < 1$, $L_{\gamma,n} > L^{\mathrm{cl}}_{\gamma,n}$.

2.1. **The Birman-Schwinger Principle.** Birman [B] and Schwinger [Sch] independently discovered that the problem of computing the number of eigenvalues of $-\Delta + V$ that lie below some number can be recast as a problem of computing the number of eigenvalues of an integral kernal operator. For $U \geq 0, U \in L^{\gamma+n/2}(\mathbb{R}^n)$ consider the eigenvalue equation $(-\Delta - U)\psi = -E\psi$ with $\psi \in H^1(\mathbb{R}^n)$ and $E > 0$. Define $\phi(x) = \sqrt{U(x)}\psi(x)$. Our eigenvalue equation then says that $(-\Delta + E)\psi(x) = \sqrt{U(x)}\phi(x)$, or equivalently, $\psi = (-\Delta + E)^{-1}\sqrt{U(x)}\phi(x)$. Therefore if $\psi(x)$ is an eigenvalue of $-\Delta + E$, then ϕ satisfies

$$\phi = K_E \phi \tag{57}$$

where K_E (called the Birman-Schwinger kernal) is the integral kernal operator given by

$$K_E(x, y) = \sqrt{U(x)} \frac{1}{-\Delta + E}(x, y) \sqrt{U(y)} \tag{58}$$

where $(-\Delta+E)^{-1}(x,y)$ is the usual Green's function for $-\Delta+E$ (i.e., the Yukawa potential). Explicity,

$$\frac{1}{-\Delta-E}(x,y) = G_E(x-y),$$

$$G_E(x) = \int_0^\infty (4\pi t)^{-n/2}\exp\left[\frac{-|x|^2}{4t} - Et\right]\mathrm{d}t. \tag{59}$$

Elementary properties of the Yukawa potential are proven in Theorem 6.23 of [LL]. We record here a few facts that we will use in our study of the Birman-Schwinger kernel.

Proposition 1. *The Yukawa potential $G_E(x)$ is in $L^q(\mathbb{R}^n)$ if $1 \leq q \leq \infty$ if $n = 1$, $1 \leq q < \infty$, if $n = 2$, or $1 \leq q < n/(n = 2)$ if $n \geq 3$.*

If $f \in L^p(\mathbb{R}^n)$ for some $1 \leq p \leq \infty$, then $u(x) = G_E * f(x) \in L^s(\mathbb{R}^n)$ where, $p \leq s \leq \infty$ if $n = 1$; $p \leq s \leq \infty$ when $p > 1$ and $n = 2$; $1 \leq s \leq \infty$ when $p = 1$ and $n = 2$; $p \leq s \leq np/(n-2p)$ when $1 < p < n/2$ and $n \geq 3$; $p \leq s \leq \infty$ when $p \geq n/2$ and $n \geq 3$; $1 \leq s \leq n/(n-2)$ when $p = 1$ and $n \geq 3$.

Lastly, the Fourier transform of G_E is given by

$$\widehat{G_E}(k) = \frac{1}{(2\pi k)^2 + E} \tag{60}$$

We collect some elementary properties of the Birman Schwinger operator. Because we will not provide proofs of the $n = 1, \gamma = 1/2$ and $n \geq 3, \gamma = 0$ cases of the LT inequalities (54), we will always assume that $\gamma > 0$ and if $n = 1$ that $\gamma > 1/2$.

Lemma 5. *The Birman-Schwinger operator is a bounded operator from L_2 to L_2. It is positive; that is, it satisfies $(f, K_E f) \geq 0$ for every $f \in L^2$. It is compact; that is, if $f_j \rightharpoonup f$ weakly in $L^2(\mathbb{R}^n)$, then $K_E f_j \to K_E f$ strongly in $L^2(\mathbb{R}^n)$. It is monotonically decreasing in E; that is, if $E < E'$, then $(f, K_E f) \geq (f, K_{E'} f)$ for every f.*

Remark. That K_E is compact actually follows from the fact that it is Schatten class; that is, for m large enough, $\mathrm{tr}(K_E)^m < \infty$. The fact that this implies that K_E is compact requires quite a bit of functional analysis machinery, and we will therefore look for a different proof of the compactness of K_E.

Proof. Let us first prove boundedness. For any $L^2(\mathbb{R}^n)$ function f a straightforward calculation using Hölder's inequality shows that $\sqrt{U}f$ is in $L^r(\mathbb{R}^n)$ with

$$r = \frac{2(\gamma + n/2)}{1+\gamma+n/2}.. \tag{61}$$

Furthermore, the L^r norm of $\sqrt{U}f$ is bounded by a constant times the L^2 norm of f. Note that $1 < r < 2$. For $L^2(\mathbb{R}^n)$ functions f and g,

$$(K_E g, f) = \int_{\mathbb{R}^n\times\mathbb{R}^n} \bar{f}(x)\sqrt{U}(x)G_E(x-y)g(y)\sqrt{U}(y)\mathrm{d}x\mathrm{d}y, \tag{62}$$

if the functions on the RHS are integrable. However, Young's inequality (Theorem 4.2 in [LL]) states that,

$$\int_{\mathbb{R}^n\times\mathbb{R}^n} \left|(\bar{f}(x)\sqrt{U}(x))(G_E(x-y))(g(y)\sqrt{U}(y))\right|\mathrm{d}x\mathrm{d}y \leq C\left\|\sqrt{U}f\right\|_r \left\|\sqrt{U}g\right\|_r \|G_E\|_q \tag{63}$$

where $2/r + 1/q = 2$ and C a constant. It is straightforward but tedious to check that with r as in (61) and q as in Proposition 1 that this equality for r and q can be satisfied. Since the L^r norm of $\sqrt{U}f$ is bounded by a constant times the L^2 norm of f, we have $f \to (K_E g, f)$ is a bounded linear functional on L^2 with norm less than a constant times the L^2 norm of g, and so the mapping $g \to K_E g \in L^2$ is bounded.

Let us now prove positivity. First consider $f \in C_c^\infty(\mathbb{R}^n)$. Then, by our assumptions on U, $\sqrt{U}f \in L^2(\mathbb{R}^n)$, and by Proposition 1, $G_E * (\sqrt{U}f) \in L^2(\mathbb{R}^n)$, and $*$ denotes convolution as usual. By Plancherel's theorem,

$$(f, K_E f) = (\sqrt{U}f, G_E * \sqrt{U}f) = (\widehat{\sqrt{U}f}, \widehat{G_E * \sqrt{U}f}), \tag{64}$$

with $\widehat{h}$ denoting the Fourier transform of h. Because $\sqrt{U}f \in L^2(\mathbb{R}^n)$ and because of the regularity on G_E stated in Proposition 1 (i.e., which L^q spaces G_E is in), we may apply Theorem 5.8 of [LL] to turn the Fourier transform of a convolution into the product of the Fourier transforms:

$$\widehat{G_E * \sqrt{U}f} = \widehat{G_E}\widehat{\sqrt{U}f}. \tag{65}$$

Here, it is crucial which L^p spaces our functions are in. Since the Fourier transform of G_E is positive by Proposition 1, we have immediately by (64) and (65) that $(f, K_E f) \geq 0$ for $f \in C_c^\infty(\mathbb{R}^n)$. By density of $C_c^\infty(\mathbb{R}^n)$ in $L^2(\mathbb{R}^n)$, positivity of K_E for general $f \in L^2(\mathbb{R}^n)$ follows immediately.

Additionally, monotonicity also follows immediately from the Fourier characterization of G_E. For if $E < E'$, then $\widehat{G_E}(k) \geq \widehat{G_{E'}}(k)$. By our above argument, $(f, K_E f) \geq (f, K_{E'} f)$ for every $f \in C_c^\infty(\mathbb{R}^n)$ and by density this extends to all of $L^2(\mathbb{R}^n)$.

Lastly, we prove compactness. We first comment that Corollary 1 holds for our $U(x)$ because of our (stronger) assumption that $U \in L^{n/2+\gamma}(\mathbb{R}^n)$, even if $n \neq 3$ (Corollary 1 is stated only in the case $n = 3$). The proof in the case $n \neq 3$ is identical and is the content of Theorem 11.4 in [LL]. We take the result without proof.

Our claim will therefore follow if we can prove that $f \to G_E * \sqrt{U}f$ is a bounded mapping from $L^2(\mathbb{R}^n)$ to $H^1(\mathbb{R}^n)$. We already have argued that $f \to \sqrt{Uf}$ is a bounded mapping of $L^2(\mathbb{R}^n)$ to $L^r(\mathbb{R}^n)$ with r as in (61). We therefore need only show that $g \to G_E * g$ is a bounded mapping of $L^r(\mathbb{R}^n)$ into $H^1(\mathbb{R}^n)$. However, that $G_E * g$ is in $L^2(\mathbb{R}^n)$ follows from Proposition 1 (again, this is straightforward but tedious to check). By the Fourier characterization of $H^1(\mathbb{R}^n)$ (see, e.g., Theorem 7.9 of [LL]) we need only prove that $k\widehat{G_E * g}(k) \in L^2(\mathbb{R}^n)$ (i.e., that its first derivative is square integrable).

Again, the constant r and the regularity of G_E given in Proposition 1 are such that we may apply Theorem 5.8 of [LL] to write

$$\widehat{G_E * g}(k) = \widehat{G_E}(k)\widehat{g}(k). \tag{66}$$

Here, $\widehat{g}(k) \in L^{r'}(\mathbb{R}^n)$, with r' the dual index to r (here, we are applying the L^r Fourier transform which exists because $r \leq 2$). We have then that

$$\left\| k\widehat{G_E * g} \right\|_2^2 \leq (2\pi)^2 \int_{\mathbb{R}^n} \frac{|\widehat{g}(k)|^2}{(2\pi k)^2 + E} \mathrm{d}k \tag{67}$$

where we have used that $k^2/([2\pi k]^2 + E) \leq (2\pi)^2$. By Hölder's inequality, the RHS is bounded above by a power of the $L^{r'}$ norm of $\widehat{g}$ times a constant. By Hausdorff-Young inequality (Theorem 5.7 in [LL]), we have that $\|\widehat{g}\|_{r'} \leq C \|g\|_r$ for a constant C. We therefore conclude that $g \to G_E * g$ is indeed a bounded linear map of $L^r(\mathbb{R}^n)$ into $H^1(\mathbb{R}^n)$. This proves our claim. $\square$

We have now characterized K_E as a compact and positive integral kernal operator on $L^2(\mathbb{R}^n)$. By the spectral theorem, it therefore has a list of eigenvalues, where denote the jth eigenvalue of K_E by λ_E^j, which are nonnegative, decreasing in j, and converge to 0. With this in hand, we prove the Birman-Schwinger principle:

Lemma 6. *Let $N_E(U)$ denote the number of eigenvalues of $-\Delta - U$ that are less than $-E$. Then $N_E(U)$ equals the number of eigenvalues of K_E that are greater than 1.*

Proof. We have already seen that every solution of the Schrödinger equation ψ gives rise to an eigenfunction $\phi = \sqrt{U}\psi$ of the Birman Schwinger kernel. Note that ϕ cannot be 0. If it were, this would imply that $-\Delta\psi = -E\psi$ which is impossible for an $H^1(\mathbb{R}^n)$ function. Now, if ϕ is an $L^2(\mathbb{R}^n)$ function satisfying $K_E\phi = \phi$, then we define $\psi = (-\Delta + E)^{-1}\sqrt{U}\phi$. Our argument using the Fourier characterization of G_E to prove compactness of the Birman-Schwinger kernel in the proof of Lemma 5 shows that ψ is an $H^1(\mathbb{R}^n)$ function. We have then

$$(-\Delta + E)\psi = \sqrt{U}\phi = \sqrt{U}K_E\phi = U\psi \tag{68}$$

and so ψ is a solution of the Schrödinger equation with eigenvalue E. This one-to-one correspondence between ψ and ϕ implies that the multiplicities of the eigenvalue $-E$ of $-\Delta - U$ and the eigenvalue 1 of K_E are the same.

Since the Birman-Schwinger kernel is decreasing in E, we see that the function $E \to \lambda_E^j$, the jth eigenvalue of K_E, is monotonically decreasing. In particular, λ_E^1 (the first and largest eigenvalue of K_E) is a monotonically decreasing function of E. Now if E is very large, then every eigenvalue of K_E will lie below 1 because $K_E \to 0$ uniformly as $E \to \infty$ (this follows from the Fourier characterization of G_E used in the proof of Lemma 5) and we will also have that $N_E(U) = 0$ (our assumptions on U imply that $-\Delta - U$ is bounded below - Lemma 1).

Now as we start to decrease E, eventually we will have $\lambda_E^1 = 1$ for some E, when λ_E^1 crosses the threshold 1. At this point, we have $N_E(U) = 1$ (by our one-to-one correspondence between ϕ and ψ described above) and there is precisely one eigenvalue of K_E above 1 (here we assume that the ground state is unique - if it is not, then the first m functions $E \to \lambda_E^j$ all cross 1 simultaneously and so $N_E(U) = m$ too). Now we continue to decrease E. Each time that, for some j, the function $E \to \lambda_E^j$ crosses the threshold 1, we get another eigenvalue of $-\Delta - U$ at this value $-E$ and $N_E(U)$ increases by 1. On the other hand, everytime $N_E(U)$ increases by 1, we get another eigenvalue of K_E, and by monotonicty, this eigenvalue is larger than 1 for all larger E. This proves the claim. $\square$

Remark. We have implicitly assumed that the functions $E \to \lambda_E^j$ are continuous in E. However it is easy to see that this is the case. For $0 < E \le E'$, we have from the Fourier representation of G_E, the inequality $0 \le K_E - K_{E'} \le [(E' - E)/E']K_E$. By the min-max principle (see, e.g., Thm 12.1 of [LL]) the eigenvalues of K_E differ from the corresponding eigenvalues of $K_{E'}$ by at most $(E' - E)/E'$ times the norm of K_E. This proves continuity.

2.2. **Proof of the LT inequalities (54).** . By the min-max principle, the eigenvalues of $-\Delta + V$ are all larger than the eigenvalues of $-\Delta - V_-$ so it is no loss of generality to assume that $V = -V_-$. We continue to denote $U = V_-$.

Lemma 6 implies that

$$N_E(U) \le N_E^{(m)} := \sum_j (\lambda_E^j)^m, \tag{69}$$

where the RHS is possibly ∞. The RHS is just the trace of $(K_E)^m$. Note that $(K_E)^m$ is perfectly well defined as a (positive) operator through the functional calculus since $K_E \ge 0$. We therefore have

$$\begin{aligned} N_E(U) \le N_E^{(m)} &= \operatorname{tr}(\sqrt{U}G_E\sqrt{U})^m \\ &\le \operatorname{tr}(U)^{m/2}(G_E)^m(U)^{m/2} \\ &= \int_{\mathbb{R}^n} U(x)^m G_E(0)\mathrm{d}x \\ &= \left(\int_{\mathbb{R}^n} \frac{1}{((2\pi k)^2 + E)^m}\right) \int_{\mathbb{R}^n} U(x)^m \mathrm{d}x. \end{aligned} \tag{70}$$

Above we have used the operator trace inequality $\operatorname{tr}(B^{1/2}AB^{1/2})^m \le \operatorname{tr} B^{m/2}A^mB^{m/2}$ which holds for positive A and B. A proof of this inequality is in [LS]. Since $(U)^{m/2}(G_E)^m(U)^{m/2}$ is an integral kernel operator, its trace is just the integral over its diagonal entries, which we have applied in the third line. The fourth line follows by the Fourier characterization of G_E in Proposition 1. The integral over k is finite iff $2m > n$, in which case it is equal to

$$\int_{\mathbb{R}^n} \frac{1}{((2\pi k)^2 + E)^m} = (4\pi)^{-n/2} \frac{\Gamma(m - n/2)}{\Gamma(m)} E^{-m+n/2}. \tag{71}$$

We wish to employ the bound (70). We write

$$\sum_j |E_j|^\gamma = \gamma \int_0^\infty N_E(U) E^{\gamma-1} \mathrm{d}E, \tag{72}$$

which follows by integration by parts and noting that the derivative of $N_E(U)$ is just a sum of delta functions at the numbers $|E_j|$. We cannot however use (70) directly in (72) or we would be led to a divergent integral. We instead note that $N_E(U) \le N_{E/2}((U - E/2)_+)$ (where $(z)_+ := \max\{0, z\}$). This follows from the fact that the number of eigenvalues for $-\Delta - U$ below $-E$ must be the same as the number of eigenvalues below $-E/2$ for $-\Delta - U + E/2$, and so $N_E(U) = N_{E/2}(U - E/2)$. But by the min-max principle deleting the positive part of the potential only decreases the eigenvalues and so $N_{E/2}(U - E/2) \le N_{E/2}((U - E/2)_+)$. Using this bound in (72) and then using the bound (70) but with $(U - E/2)_+$ in place of U, we obtain

$$\sum_j |E_j|^\gamma \le (4\pi)^{-n/2} \gamma \frac{\Gamma(m - n/2)}{\Gamma(m)} \int_0^\infty \int_{\mathbb{R}^n} \left(U(x) - \frac{E}{2} \right)_+^m \left(\frac{E}{2} \right)^{-m+n/2} \mathrm{d}x E^{\gamma-1} \mathrm{d}E. \tag{73}$$

We do the E-integration first. A computation shows

$$\begin{aligned} \int_0^\infty (A - E)_+^s E^t \mathrm{d}E &= A^{s+t+1} \int_0^1 (1 - y)^s y^t \mathrm{d}y \\ &= A^{s+t+1} \Gamma(s + 1)\Gamma(t + 1)/\Gamma(s + t + 2) \end{aligned} \tag{74}$$

Therefore,

$$\sum_j |E_j|^\gamma \le (4\pi)^{-n/2} 2^\gamma \gamma m \frac{\Gamma(m - n/2)\Gamma(-m + \gamma + n/2)}{\Gamma(\gamma + 1 + n/2)} \int_{\mathbb{R}^n} U(x)^{\gamma+n/2} \mathrm{d}x. \tag{75}$$

In order for the E-integration in (73) to be finite, we require $-m + n/2 + \gamma > 0$. Recall that we also require $m > n/2$. We therefore require $\gamma + n/2 > m > n/2$.

By choosing $m = (\gamma + n)/2$ when $n > 1$ or $n = 1, \gamma \ge 1$ and $m = 1$ for other cases, we obtain the claims (54) except in the critical cases $n \ge 3, \gamma = 0$ and $n = 1, \gamma = 1/2$. □

3. Kinetic Energy Inequalities

We will now give a useful application of the LT inequalities (54). In the case $\gamma = 1$ we have,

$$\sum_j |E_j| \le L_{1,n} \int_{\mathbb{R}^n} V_-(x)^{1+n/2} \mathrm{d}x. \tag{76}$$

Our goal is to use (76) to obtain an upper bound on the kinetic energy of N quantum particles. More precisely, let $\psi \in H^1(\mathbb{R}^{Nn})$ be a function with L^2 norm 1. ψ is a wave function describing N quantum particles and the function

$$\rho_\psi(x) := \sum_{i=1}^n \int_{\mathbb{R}^{(N-1)n}} |\psi(x_1, ..., x_N)|^2 \mathrm{d}x_1 ... \widehat{\mathrm{d}x_i} ... \mathrm{d}x_N \tag{77}$$

(where the hat indicates that $\widehat{dx_i}$ is omitted in the integration) is the probability density associated with finding a particle at the point $x \in \mathbb{R}^n$. The kinetic energy of the N particles is just the sum of the kinetic energies of each of the individual particles:

$$T_\psi = \sum_{i=1}^{N} \int_{\mathbb{R}^{Nn}} |\nabla_{x_i} \psi(x_1, ..., x_N)|^2 \mathrm{d}x_1 ... \mathrm{d}x_N. \tag{78}$$

The single particle density matrix associated with ψ is given by

$$\gamma_\psi^{(1)}(x, x') = \sum_{i=1}^{N} \int \psi(x_1, ..., x_{i-1}, x, ..., x_N)\psi(x_1, ..., x_{i-1}, x', ..., x_N)\mathrm{d}x_1 ... \widehat{\mathrm{d}x_i} ... \mathrm{d}x_N. \tag{79}$$

It is easy to see that $\gamma_\psi^{(1)}$ is a positive integral kernal operator on $L^2(\mathbb{R}^n)$ satisfying $\mathrm{tr}\, \gamma_\psi^{(1)} = N$. Its largest eigenvalue is denoted $||\gamma_\psi^{(1)}||_\infty$. It is bounded above by N. If ψ is antisymmetric function (i.e. ψ describes fermions) then $||\gamma_\psi^{(1)}||_\infty$ is less than 1.

With these definitions we can state the following fundamental kinetic energy inequality:

Theorem 4. *With the kinetic energy and density defined above, the inequality (76) implies*

$$T_\psi \geq \frac{K}{||\gamma_\psi^{(1)}||_\infty^{p'/p}} \int_{\mathbb{R}^n} \rho_\psi(x)^{p'} \mathrm{d}x \tag{80}$$

where $p = 1 + n/2$ *(the power appearing in (76))* $p' = p/(p-1)$ *(the dual index to* p*) and* K *satisfying*

$$(pL_{1,n})^{p'}(p'K)^p = 1. \tag{81}$$

Proof. Consider now the operator $H = -\Delta + V$ acting on $H^1(\mathbb{R}^n)$, i.e., single particle wave functions, where V is a potential to be determined. We then consider the N-body operator

$$K_N = \sum_{i=1}^{N} H_i \tag{82}$$

with H_i acting as H on the ith particle. With the aid of the one particle density matrix $\gamma_\psi^{(1)}$ we can write

$$(\psi, K_N \psi) = \mathrm{tr}\left[H\gamma_\psi^{(1)}\right]. \tag{83}$$

Let us pause to comment on the above notation. Instead of worrying about defining $-\Delta$ as an unbounded operator on a dense domain, we are interpreting the expectation $(\psi, K_N\psi)$ by the formally associated quadratic form, i.e.,

$$(\psi, K_N\psi) = T_\psi + \sum_{i=1}^{N} \int_{\mathbb{R}^{Nn}} V(x_i)|\psi(x_1, ..., x_N)|^2 \mathrm{d}x_1 ... \mathrm{d}x_N. \tag{84}$$

Note that

$$\sum_{i=1}^{N} \int_{\mathbb{R}^{Nn}} V(x_i)|\psi(x_1, ..., x_N)|^2 \mathrm{d}x_1 ... \mathrm{d}x_N = \int_{\mathbb{R}^n} V(x)\rho_\psi(x)\mathrm{d}x \tag{85}$$

For positive trace class operators A on $L^2(\mathbb{R}^n)$ we interpret $\mathrm{tr}(HA)$ as follows. Since A has the decomposition $A = \sum_{i=1}^{\infty} \lambda_i \varphi_i(\varphi_i, \cdot)$ for orthonormal $\psi_i \in L^2(\mathbb{R}^n)$ and positive λ_i, we can define

$$\mathrm{tr}\,[HA] := \sum_{i=1}^{\infty} \lambda_i \mathcal{E}(\varphi_i) \tag{86}$$

with $\mathcal{E}(\phi)$ as before. We define the trace wherever the RHS makes sense (in particular, whever the sum is absolutely summable and every $\varphi_j \in H^1(\mathbb{R}^n)$.)

It is the content of Chapter 3 of [LS] that the equality (83) holds (see the footnote on page 45).

We now continue with the proof. The minimum of of tr $[HA]$ over all positive trace-class operators A with $||A||_\infty \le ||\gamma_\psi^{(1)}||_\infty$ is clearly given by the sum of the negative eigenvalues of H times $||\gamma_\psi^{(1)}||_\infty$. That is, the optimal choice of A is $||\gamma_\psi^{(1)}||_\infty$ times the projection onto the negative spectral subspace of H. Therefore,

$$(\psi, K_N\psi) \ge ||\gamma_\psi^{(1)}||_\infty \sum_j E_j. \tag{87}$$

We now apply (76):

$$T_\psi + \int_{\mathbb{R}^n} V(x)\rho_\psi(x)\mathrm{d}x = (\psi, K_N\psi) \ge -||\gamma_\psi^{(1)}||_\infty L_{1,n} \int_{\mathbb{R}^n} V_-(x)^p \mathrm{d}x. \tag{88}$$

We now make a choice for V. Let $V(x) = -C\rho_\psi(x)^{1/(p-1)}$ where $C > 0$ is a constant to be determined. We obtain the inequality

$$T_\psi \ge C \int_{\mathbb{R}^n} \rho_\psi(x)^{p'}\mathrm{d}x - ||\gamma_\psi^{(1)}||_\infty L_{1,n} C^p \int_{\mathbb{R}^n} \rho_\psi(x)^{p'}\mathrm{d}x. \tag{89}$$

We know optimize over C and choose $C = (p||\gamma_\psi^{(1)}||_\infty L_{1,n})^{-p'/p}$. This proves the claim. □

An interesting fact is that the kinetic energy inequality is equivalent to the LT inequality for $\gamma = 1$. This is captured by the following theorem:

Theorem 5. *Suppose that (80) holds for every N particle wave function ψ (for every N), with the constant K as in (81). Then (76) holds.*

Proof. Let ψ be the N particle wave function formed by the Slater determinant of the eigenfunctions for the N lowest eigenvalues of $-\Delta + V$. More precisely, if E_j are the negative eigenvalues of $-\Delta + V$ and $(-\Delta + V)\psi_j = E_j\psi_j$, then

$$\psi(x_1, ..., x_N) = (N!)^{-1/2} \det\{\psi_i(x_j)\}_{i,j}^N. \tag{90}$$

It is straightforward to check that

$$\sum_{j=0}^{N-1} E_j = T_\psi + \int_{\mathbb{R}^n} V(x)\rho_\psi(x)\mathrm{d}x. \tag{91}$$

For ψ of this form, we have that $||\gamma_\psi^{(1)}||_\infty \le 1$. Applying (80) we have

$$\begin{aligned} T_\psi + \int_{\mathbb{R}^n} V(x)\rho_\psi(x)\mathrm{d}x &\ge K \int_{\mathbb{R}^n} \rho_\psi(x)^{p'}\mathrm{d}x - \int_{\mathbb{R}^n} [(pL_{1,n})^{1/p}V_-(x)][(pL_{1,n})^{-1/p}\rho_\psi(x)]\mathrm{d}x \\ &\ge K \int_{\mathbb{R}^n} \rho_\psi(x)^{p'}\mathrm{d}x - \frac{1}{p'}\int_{\mathbb{R}^n} [(pL_{1,n})^{-1/p}\rho_\psi(x)]^{p'}\mathrm{d}x \\ &- \frac{1}{p}\int_{\mathbb{R}^n} [(pL_{1,n})^{1/p}V_-(x)]^p\mathrm{d}x = -L_{1,n}\int_{\mathbb{R}^n} V_-(x)^p\mathrm{d}x. \end{aligned} \tag{92}$$

The third equality comes from Hölder's inequality followed by $ab \le a^p/p + b^{p'}/p'$. The equality comes from the definition of the constants in 81. Taking $N \to \infty$ yields the claim. □

What these two theorems show are that the inequalities (in the case of antisymmetric ψ)

$$\mathrm{tr}\,(-\Delta + V)_\le \int V_-(x)^p\mathrm{d}x \tag{93}$$

and

$$(\psi, \sum_{i=1}^N -\Delta_{x_i}\psi) \ge K \int_{\mathbb{R}^n} \rho_\psi(x)^{p'}\mathrm{d}x \tag{94}$$

are dual to each other, in the sense that the integrands on the RHS are a certain Legendre transform of each other. The same holds for the LHS. For suitable convex functions, taking a double Legendre transform reproduces the original function. Thus, Theorems 4 and 5 represent an attractive method of computing sharp constants in the LT inequality in the physical case of interest, that is with $\gamma = 1$. If one can compute the sharp constant in the kinetic energy inequality (80), then one immediately obtains the sharp constant in (76).

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