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Improved sharp spectral inequalities for Schrödinger operators on the semi-axis

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Abstract. We prove a Lieb–Thirring inequality for Schrödinger operators $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$ on the semi-axis with Robin boundary condition at the origin. The result improves on a bound obtained by P. Exner, A. Laptev, and M. Usman [Commun. Math. Phys. 362 (2014), 531–541] albeit under the additional assumption $V \in L^1(\mathbb{R}_+)$. The main difference in our proof is that we use the double commutation method in place of the single commutation method. We also establish an improved inequality in the case of a Dirichlet boundary condition.

1. Introduction

In their proof of stability of matter, Lieb and Thirring [20, 21] introduced the bound

$$\sum_{j\geq 1} |\lambda_j|^\gamma \leq L_{\gamma,d} \int_{\mathbb{R}^d} V(x)_-^{\gamma+\frac{d}{2}}\, \mathrm{d}x$$

for the negative eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq 0$ of a Schrödinger operator $-\Delta + V$ on $L^2(\mathbb{R}^d)$ with real-valued potential V that decays sufficiently fast. Here and below, $a_- = (|a| - a)/2$ denotes the negative part of a real variable $a \in \mathbb{R}$. The bound was proved for any $\gamma > \max(0, 1 - \frac{d}{2})$ and was later extended to the endpoint cases $d = 1, \gamma = \frac{1}{2}$ and $d = 3, \gamma = 0$ in [27] and [5, 19, 23], respectively. The sharp constants $L_{\gamma,d}$, which importantly do not depend on V, have been subject of intense investigation over the last 45 years [25].

The case $d = 1$ and $\gamma = \frac{3}{2}$ has proved especially accessible to mathematical investigations due to its connection to trace formulae. The sharp constant $L_{\frac{3}{2},1} = \frac{3}{16}$ was established even before Lieb and Thirring's original papers by Gardner, Greene, Kruskal, and Miura [12]. The authors considered the Buslaev–Faddeev–Zaharov trace

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formula [3, 28]

$$\sum_{j\geq 1}|\lambda_j|^{\frac{3}{2}} + \frac{3}{\pi}\int\limits_{\mathbb{R}_+} k^2 \log|a(k)|\,\mathrm{d}k = \frac{3}{16}\int\limits_{\mathbb{R}} V(x)^2\,\mathrm{d}x$$

for the negative eigenvalues λ_j of $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$ on $L^2(\mathbb{R})$ and noted that the scattering coefficient satisfies $|a(k)| \geq 1$. This yields the sharp inequality

$$\sum_{j\geq 1}|\lambda_j|^{\frac{3}{2}} \leq \frac{3}{16}\int\limits_{\mathbb{R}} V(x)^2\,\mathrm{d}x. \tag{1}$$

An extension of (1) to matrix-valued potentials by Laptev and Weidl [17] was crucial in establishing the sharp Lieb–Thirring constants $L_{\gamma,d}$ for $\gamma \geq 3/2$ in all dimensions $d \geq 1$. Note that the trace formula also yields a bound on the integral involving the scattering coefficient, which has proved very useful in the investigation of the absolute continuity of the spectrum of the Schrödinger operator [8].

In this short note, we consider the Schrödinger operator

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$$

on $L^2(\mathbb{R}_+)$ with real-valued potential and Robin boundary condition

$$\varphi'(0) - \sigma_0\varphi(0) = 0,$$

where $\sigma_0 \in \mathbb{R}$. If the potential V is sufficiently smooth and decays sufficiently fast, the negative spectrum of H consists of discrete eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq 0$ with corresponding eigenfunctions φ_j. While trace formulae have also been established in this setting [10], there is no known analogue of $|a(k)| \geq 1$. Thus, Lieb–Thirring inequalities have to be proved by different means and could in turn be used to shed more light on the scattering coefficient. Our main result is the following Lieb–Thirring-type bound.

Theorem 1.1. *Let $V \in L^1(\mathbb{R}_+) \cap L^2(\mathbb{R}_+)$. The negative eigenvalues λ_j of $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$ with Robin boundary condition $\varphi'(0) - \sigma_0\varphi(0) = 0$ satisfy*

$$\sum_{j\geq 1}|\lambda_j|^{\frac{3}{2}} + \frac{1}{4}\sum_{j\geq 1}(\sigma_j^3 - \sigma_{j-1}^3) \leq \frac{3}{16}\int\limits_0^\infty V(x)^2\,\mathrm{d}x + \frac{3}{4}\sum_{j\geq 1}|\lambda_j|(\sigma_j - \sigma_{j-1})$$

where

$$\sigma_j = \sigma_{j-1} + \frac{|\varphi_j(0)|^2}{\|\varphi_j\|^2}, \quad j = 1, 2, \ldots$$

and φ_j denotes the eigenfunction to λ_j.

Remark 1.2. From the proof, it is clear that the bound also holds if each of the three sums only extends to $j \leq N$ for some cutoff $N \geq 1$ (with additional terms replaced by 0 if there are fewer than N negative eigenvalues). All four quantities in the inequality above are then non-negative and non-decreasing in N. Thus, the two sides of the inequality are also well defined in the case of infinitely many negative eigenvalues, though the theorem does not make any assertion about the finiteness of the two series involving σ_j. However, the difference of the fourth and second term is always bounded from above. Some explicit upper bounds that could be useful in applications will be discussed in Section 4. Note that finiteness of the discrete spectrum holds for example if $\int_0^\infty (1+x)|V(x)|\,\mathrm{d}x < \infty$ and in particular if $V \in \mathcal{C}_0^\infty([0,\infty))$.

In the special case of a Dirichlet boundary condition, we obtain the following.

Theorem 1.3. *Let $V \in L^1(\mathbb{R}_+) \cap L^2(\mathbb{R}_+)$. The negative eigenvalues λ_j of $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$ with Dirichlet boundary condition $\varphi(0) = 0$ satisfy*

$$\sum_{j \geq 1} |\lambda_j|^{\frac{3}{2}} \leq \frac{3}{16} \int_0^\infty V(x)^2\,\mathrm{d}x - \frac{3}{4} \sum_{j \geq 1} \frac{|\varphi_j'(0)|^2}{\|\varphi_j\|^2},$$

where φ_j denotes the eigenfunction to λ_j.

Remark 1.4. From the proof, it is again clear that the bound also holds if each of the two sums only extends to $j \leq N$ for some cutoff $N \geq 1$. Both sums are non-negative and non-decreasing in N. Letting $N \to \infty$, we can conclude that under the assumptions of the theorem the two series are both finite, even in the case of infinitely many eigenvalues.

Note that the inequality of Theorem 1.3 without the negative last term can be obtained from the whole line result (1). The inequality of Theorem 1.1 should be compared to the following result by Exner, Laptev, and Usman [11] which was established in the same setting but without the assumption $V \in L^1(\mathbb{R}_+)$.

Theorem 1.5 ([11, Theorem 1.1]). *Let $V \in L^2(\mathbb{R}_+)$, $V \leq 0$. The negative eigenvalues λ_j of $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$ with Robin boundary condition $\varphi'(0) - \sigma_0\varphi(0) = 0$ satisfy*

$$\frac{1}{2}|\lambda_1|^{\frac{3}{2}} + \sum_{j \geq 2} |\lambda_j|^{\frac{3}{2}} \leq \frac{3}{16} \int_0^\infty V(x)^2\,\mathrm{d}x - \frac{3}{4}|\lambda_1|\sigma_0 + \frac{1}{4}\sigma_0^3.$$

Theorem 1.5 shows that, compared to the whole line case (1), the boundary condition at zero leads to a change in the term corresponding to λ_1 in the Lieb–Thirring bound. Our result in Theorem 1.1 aims to further elaborate on the influence of the boundary condition. In Section 4 we will show that the additional terms in Theorem 1.1 strengthen the inequality. In particular, Theorem 1.5 can be obtained from our result. While the inequality in Theorem 1.1 may be difficult to use in applications due to the necessary knowledge of σ_j (and thus of $|\varphi_j(0)|/\|\varphi_j\|$) for $j \geq 1$, we will show in Section 4 how in some cases the bound can be weakened to a form that does not require this information. Some of these results cannot be obtained directly from Theorem 1.5. Before we prove the main result, it is worth pointing out the differences in our proof method compared to the existing literature.

For $d = 1$, the so-called *commutation method* has proved valuable in establishing sharp Lieb–Thirring inequalities. This method goes back to the idea of inserting eigenvalues into the spectrum of differential operators and was first discussed by Jacobi [16], Darboux [7], and Crum [4]. A rigorous characterisation can be found in [9, 13, 14]. For the purpose of proving Lieb–Thirring inequalities, the method is reversed and eigenvalues are successively removed from the spectrum, starting with the lowest, λ_1. To this end, one constructs a first-order differential operator D that factorises the original Schrödinger operator as $-\frac{d^2}{dx^2} + V = DD^* + \lambda_1$. Commuting D and D^* leads to a new operator $-\frac{d^2}{dx^2} + V_1 = D^*D + \lambda_1$, which has the same spectrum as the original operator with the exception of the eigenvalue λ_1. In order to obtain a spectral inequality, it is necessary to establish a connection between integrals of powers of the potentials V and V_1 (such as $\int V^2 \, dx$), and the eigenvalue λ_1. Assuming that there are only finitely many negative eigenvalues $\lambda_1, \ldots, \lambda_N$, repetition of this process removes all of these eigenvalues from the spectrum and one eventually obtains an identity that links $\lambda_1, \ldots, \lambda_N$ to integrals of V and some potential V_N that corresponds to a Schrödinger operator without negative eigenvalues. If this last term has a definite sign, an inequality can be obtained.

In the case of a Schrödinger operator on the real line, the commutation method was first used by Schmincke [26] to prove the lower bound

$$\sum_{j \geq 1} |\lambda_j|^{\frac{1}{2}} \geq -\frac{1}{4} \int_{\mathbb{R}} V(x) \, dx. \tag{2}$$

Subsequently, it has been applied to provide a new, direct proof of (1) in the case of matrix-valued potentials [1] (as first established by Laptev and Weidl [17]) and to prove similar inequalities for fourth-order differential operators [15] and Jacobi operators [24]. In a slight variation, this proof method has also been used to establish Theorem 1.5. Here, after removing the first eigenvalue, one obtains a Schrödinger operator with Dirichlet boundary condition at zero. The Lieb–Thirring inequality is then proved by continuing the problem to the whole line and applying (1). Our Theorem 1.3 shows that such an approach cannot yield a sharp inequality if the potential supports more than one eigenvalue (under the additional condition $V \in L^1(\mathbb{R}_+)$). Recently, the same variation of the commutation method has been applied to fourth-order operators on the semi-axis [6].

In all of theses results, the applied method is more precisely known as the *single commutation method.* In comparison, the so-called *double commutation method* [13, 14] involves an additional step where after commuting D, D^* the resulting operator is again factorised using a new first-order operator D_γ such that $-\frac{d^2}{dx^2} + V_1 = D^*D + \lambda_1 = D_\gamma^* D_\gamma + \lambda_1$. Applying a second commutation, one obtains yet another Schrödinger operator $-\frac{d^2}{dx^2} + V_{\gamma,1} = D_\gamma D_\gamma^* + \lambda_1$ that has the same spectrum as the original operator with the exception of the eigenvalue λ_1. This method has several advantages compared to the single commutation method. For example, it allows to remove eigenvalues in arbitrary order, as it does not require the corresponding eigenfunction to have no zeros. In our case, its main advantage is that after the first step, we do not obtain a Schrödinger operator with Dirichlet boundary condition, but rather one with a new Robin boundary condition. This leads to the additional terms in Theorem 1.1 compared to Theorem 1.5. To the best of our knowledge, the double commutation method has not been used previously in the context of Lieb–Thirring inequalities. In [2], the closely related Gelfand–Levitan method [18] was applied in the same setting as in this note to obtain the lower bound

$$\sum_{j\geq 1} |\lambda_j|^{\frac{1}{2}} \geq -\frac{1}{4}\int_{\mathbb{R}} V(x)\,dx - \frac{1}{4}\sigma_0 + \frac{1}{4}\sum_{j\geq 1} \frac{|\varphi_j(0)|^2}{\|\varphi_j\|^2}$$

for the operator $-\frac{d^2}{dx^2} + V$ on $L^2(\mathbb{R}_+)$ with Robin boundary condition. This result shows that the boundary condition at the origin influences Schmincke's inequality (2) in a similar way as it influences the Lieb–Thirring inequality (1) in Theorem 1.1.

In Section 2 we will introduce the double commutation method in more detail and subsequently we will use it in Section 3 to prove Theorem 1.1 and Theorem 1.3.

2. The double commutation method

For brevity, we restrict ourselves to the case at hand, i.e., a Schrödinger operator $H = -\frac{d^2}{dx^2} + V$ on $L^2(\mathbb{R}_+)$ with Robin boundary condition $\varphi'(0) - \sigma\varphi(0) = 0$. For comparison, we first state the single commutation method, details of which can be found in [9].

Theorem 2.1. *Let φ be an eigenfunction of $H = -\frac{d^2}{dx^2} + V$ to the lowest eigenvalue λ. Then, the operator $H_\lambda = -\frac{d^2}{dx^2} + V_\lambda$ with potential*

$$V_\lambda(x) = V(x) - 2\frac{d^2}{dx^2}\log\varphi(x)$$

and with Dirichlet boundary condition

$$\varphi(0) = 0$$

has spectrum $\sigma(H_\lambda) = \sigma(H) \setminus \{\lambda\}$.

Remark 2.2. As discussed in the introduction, the result is the consequence of the factorisation $H = DD^* + \lambda$ and $H_\lambda = D^*D + \lambda$, where, more precisely,

$$D = \frac{\mathrm{d}}{\mathrm{d}x} + \frac{\varphi'}{\varphi}.$$

The spectral characterisation of the double commutation method was first achieved in [13] for Schrödinger operators on $L^2(\mathbb{R})$ as well as on $L^2(\mathbb{R}_+)$ with Dirichlet boundary condition at the origin. The results were extended to Sturm–Liouville operators on arbitrary intervals with Robin boundary conditions in [14], from where we take the following result [14, Theorem 3.2] (see also [14, Remark 3.3 (i)]).

Theorem 2.3. *Let φ be an eigenfunction of $H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$ with eigenvalue λ and let $\gamma = -1/\|\varphi\|^2$. Then, the operator $H_\lambda = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_\lambda$ with potential*

$$V_\lambda(x) = V(x) - 2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\log\left(1 + \gamma\int_0^x |\varphi(t)|^2\,\mathrm{d}t\right)$$

and with Robin boundary condition

$$\psi'(0) - \sigma_\lambda\psi(0) = 0, \quad \sigma_\lambda = \sigma + \frac{|\varphi(0)|^2}{\|\varphi\|^2}$$

has point spectrum $\sigma_p(H_\lambda) = \sigma_p(H) \setminus \{\lambda\}$. Furthermore, ψ is an eigenfunction of H with eigenvalue $\eta \neq \lambda$ if and only if

$$\psi_\lambda(x) = \psi(x) - \gamma\tilde{\varphi}(x)\int_0^x \psi(t)\overline{\varphi(t)}\,\mathrm{d}t$$

is an eigenfunction of H_λ with eigenvalue $\eta \neq \lambda$ where the function $\tilde{\varphi}$ is defined as

$$\tilde{\varphi}(x) = \frac{\varphi(x)}{1 + \gamma\int_0^x |\varphi(t)|^2\,\mathrm{d}t}.$$

Remark 2.4. In the notation of [14], the boundary condition of H_λ is given by the vanishing Wronskian $\psi(0)\varphi'(0) - \psi'(0)\varphi(0) = 0$, which can easily be reduced to the one given above. As mentioned in the introduction, the double commutation method relies on a second factorisation $D^*D + \lambda = D_\gamma^* D_\gamma + \lambda$, where more precisely $D_\gamma = \frac{\mathrm{d}}{\mathrm{d}x} + \frac{\tilde{\varphi}'}{\tilde{\varphi}}$.

3. The proofs of Theorem 1.1 and Theorem 1.3

In many cases, proofs of Lieb–Thirring inequalities initially restrict to compactly supported potential V and then use an approximation argument to extend the result to more general $V \in L^{\gamma+d/2}(\mathbb{R}^d)$. Since the bound in Theorem 1.1 contains the terms σ_j, in our case such an approximation argument would necessarily have to establish the continuous dependence of the eigenfunctions on the potential in terms of the norm on $L^2(\mathbb{R}_+)$. To avoid this argument altogether, our proof will not restrict to compactly supported potentials. Establishing the required asymptotic behaviour of eigenfunctions is then more technical and relies on the additional assumption $V \in L^1(\mathbb{R}_+)$. This assumption is also necessary in the proof of the corresponding trace formula [10]. We do not know whether Theorem 1.1 holds true without it.

3.1. The proof of Theorem 1.1

Let φ_1 now be the eigenfunction for the eigenvalue λ_1 and let $\gamma_1 = -1/\|\varphi_1\|^2$. As a ground state, φ_1 does not vanish anywhere (see, e.g., [11] for a proof in this setting). It can thus be chosen to be strictly positive. Note that the behaviour of φ_1 at the origin is characterised by the boundary condition

$$\varphi_1'(0) - \sigma_0\varphi_1(0) = 0. \tag{3}$$

For large x, the asymptotic behaviour

$$\lim_{x\to\infty} \varphi_1(x)\mathrm{e}^{\sqrt{|\lambda_1|}x} = C_1, \quad \lim_{x\to\infty} \varphi_1'(x)\mathrm{e}^{\sqrt{|\lambda_1|}x} = -C_1\sqrt{|\lambda_1|} \tag{4}$$

holds with some $C_1 > 0$. This is a consequence of the additional assumption $V \in L^1(\mathbb{R}_+)$ (see, e.g., [2, Lemma 1] which uses [22, Theorem 8, Section 22]).

By Theorem 2.3, the operator $H_1 = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_1$ with potential

$$V_1(x) = V(x) - 2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\log\left(1 + \gamma_1\int_0^x |\varphi_1(t)|^2\,\mathrm{d}t\right)$$

and Robin boundary condition

$$\varphi'(0) - \sigma_1\varphi(0) = 0, \quad \sigma_1 = \sigma_0 + \frac{|\varphi_1(0)|^2}{\|\varphi_1\|^2}$$

has only the negative eigenvalues $\lambda_2 \le \lambda_3 \le \cdots \le 0$. The potential can be written as $V_1 = V - 2G'$ with

$$G(x) = \frac{\gamma_1\varphi_1(x)^2}{1 + \gamma_1\int_0^x |\varphi_1(t)|^2\,\mathrm{d}t}$$

which can be further decomposed into $G = F - \widetilde{F}$ with

$$F(x) = \frac{\varphi_1'(x)}{\varphi_1(x)}, \quad \widetilde{F}(x) = \frac{\tilde{\varphi}_1'(x)}{\tilde{\varphi}_1(x)}$$

and

$$\tilde{\varphi}_1(x) = \frac{\varphi_1(x)}{1 + \gamma_1 \int_0^x |\varphi_1(t)|^2 \, \mathrm{d}t}.$$

Lemma 3.1. *The functions F and $\widetilde{F}$ solve the first-order differential equations*

$$F^2 + F' = V - \lambda_1, \quad \widetilde{F}^2 - \widetilde{F}' + 2F' = V - \lambda_1$$

with boundary conditions

$$\begin{aligned} F(0) &= \sigma_0, & \widetilde{F}(0) &= \sigma_1, \\ \lim_{x\to\infty} F(x) &= -\sqrt{|\lambda_1|}, & \lim_{x\to\infty} \widetilde{F}(x) &= \sqrt{|\lambda_1|}. \end{aligned}$$

Proof. The differential equation for F can be found in several applications of the single commutation method. It is an immediate consequence of the eigenequation for φ_1

$$F(x)^2 + F'(x) = \frac{\varphi_1'(x)^2 + \varphi_1''(x) - \varphi_1'(x)^2}{\varphi_1(x)^2} = V(x) - \lambda_1.$$

The boundary conditions follow from (3) and (4). For $\widetilde{F}$, we compute that

$$\widetilde{F}(x)^2 - \widetilde{F}'(x) = F(x)^2 - F'(x) + G'(x) - 2F(x)G(x) + G(x)^2$$

and the differential equation can be proved by verifying that $G'(x) - 2F(x)G(x) + G(x)^2 = 0$. The boundary condition at the origin is a consequence of (3) while for $x \to \infty$ we use (4) and de l'Hôpital's rule to compute

$$\begin{aligned} \lim_{x\to\infty} \widetilde{F}(x) &= \lim_{x\to\infty} \left(\frac{\varphi_1'(x)}{\varphi_1(x)} - \frac{\gamma_1 |\varphi_1(x)|^2}{1 + \gamma_1 \int_0^x |\varphi_1(t)|^2 \, \mathrm{d}t} \right) \\ &= -\sqrt{|\lambda_1|} - \lim_{x\to\infty} \frac{2\varphi_1(x)\varphi_1'(x)}{\varphi_1(x)^2} = \sqrt{|\lambda_1|}. \end{aligned}$$ ■

We first note that

$$\int_0^\infty V_1(x)^2 \, \mathrm{d}x = \int_0^\infty V(x)^2 \, \mathrm{d}x + 4 \int_0^\infty G'(x)\big(G'(x) - V(x)\big) \, \mathrm{d}x.$$

The last term on the right-hand side can be computed explicitly by using Lemma 3.1:

$$\int_0^\infty G'(x)\big(G'(x) - V(x)\big) \, \mathrm{d}x$$

$$= \int_0^\infty F'(x)\big(F'(x) - V(x)\big)\,\mathrm{d}x - \int_0^\infty \widetilde{F}'(x)\big(2F'(x) - \widetilde{F}'(x) - V(x)\big)\,\mathrm{d}x$$

$$= -\int_0^\infty F'(x)\big(\lambda_1 + F(x)^2\big)\,\mathrm{d}x + \int_0^\infty \widetilde{F}'(x)\big(\lambda_1 + \widetilde{F}(x)^2\big)\,\mathrm{d}x$$

$$= \Big[|\lambda_1|F(x) - \frac{1}{3}F(x)^3 - |\lambda_1|\widetilde{F}(x) + \frac{1}{3}\widetilde{F}(x)^3\Big]_{x=0}^{x=\infty}$$

$$= -\frac{4}{3}|\lambda_1|^{\frac{3}{2}} + |\lambda_1|(\sigma_1 - \sigma_0) - \frac{1}{3}(\sigma_1^3 - \sigma_0^3).$$

Thus, we arrive at

$$\int_0^\infty V_1(x)^2\,\mathrm{d}x = -\frac{16}{3}|\lambda_1|^{\frac{3}{2}} + 4|\lambda_1|(\sigma_1 - \sigma_0) - \frac{4}{3}(\sigma_1^3 - \sigma_0^3) + \int_0^\infty V(x)^2\,\mathrm{d}x.$$

We aim to repeat the process and thus check whether V_1 satisfies the assumptions of Theorem 1.1. The identity above shows that $V_1 \in L^2(\mathbb{R}_+)$. In [2, Lemma 2], it is stated that $V_1 \in L^1(\mathbb{R}_+)$, arguing that $|G'| \in L^1(\mathbb{R}_+)$ since $G'(x) \geq 0$ for sufficiently large x. The latter is claimed to be a consequence of the asymptotics of φ_1. Unfortunately, we could not fill in all of the details of the argument. In particular, we could not rule out that G' oscillates as $x \to \infty$. We instead present an argument that avoids investigating the integrability of V_1 altogether. In the computations above, the property $V \in L^1(\mathbb{R}_+)$ was only used to prove the asymptotic behaviour of the ground state φ_1 of H. More generally, the condition $V \in L^1(\mathbb{R}_+)$ guarantees that the eigenfunctions φ_j of H satisfy

$$\lim_{x\to\infty} \varphi_j(x)\mathrm{e}^{\sqrt{|\lambda_j|}x} = C_j, \quad \lim_{x\to\infty} \varphi_j'(x)\mathrm{e}^{\sqrt{|\lambda_j|}x} = -C_j\sqrt{|\lambda_j|}$$

with $C_j \neq 0$. These results already imply similar asymptotics for the eigenfunctions ψ_j of H_1 without the need to establish $V_1 \in L^1(\mathbb{R}_+)$. To this end, we note that, by Theorem 2.3,

$$\psi_j(x) = \varphi_{j+1}(x) + \gamma_1\tilde{\varphi}_1(x)\int_x^\infty \varphi_{j+1}(t)\overline{\varphi_1(t)}\,\mathrm{d}t. \tag{5}$$

Using de l'Hôpital's rule, it is straightforward to compute the three limits

$$\lim_{x\to\infty} \tilde{\varphi}_1(x)\mathrm{e}^{-\sqrt{|\lambda_1|}x} = -\frac{2}{C_1\gamma_1}\sqrt{|\lambda_1|},$$

$$\lim_{x\to\infty} \tilde{\varphi}_1'(x)\mathrm{e}^{-\sqrt{|\lambda_1|}x} = -\frac{2}{C_1\gamma_1}|\lambda_1|,$$

$$\lim_{x\to\infty}\int_x^\infty \varphi_{j+1}(t)\overline{\varphi_1(t)}\,\mathrm{d}t\, \mathrm{e}^{\sqrt{|\lambda_1|}x}\mathrm{e}^{\sqrt{|\lambda_{j+1}|}x} = \frac{C_1 C_{j+1}}{\sqrt{|\lambda_1|}+\sqrt{|\lambda_{j+1}|}}.$$

From (5), we then obtain the desired asymptotics

$$\lim_{x\to\infty}\psi_j(x)\mathrm{e}^{\sqrt{|\lambda_j|}x} = D_j, \quad \lim_{x\to\infty}\psi_j'(x)\mathrm{e}^{\sqrt{|\lambda_j|}x} = -D_j\sqrt{|\lambda_j|}$$

with $D_j = C_{j+1}(\sqrt{|\lambda_{j+1}|}-\sqrt{|\lambda_1|})/(\sqrt{|\lambda_{j+1}|}+\sqrt{|\lambda_1|}) \neq 0$.

We can thus repeat the process for H_1 and remove λ_2 from its spectrum. While the eigenfunctions of H_1 are different to those of H, the relevant quantities in the definition of σ_2 importantly do not differ. More precisely, (5) allows us to conclude that $\psi_1(0) = \varphi_2(0)$ and furthermore that $\|\psi_1\|^2 = \|\varphi_2\|^2$, as shown in [14, Lemma 2.1]. Thus, σ_2 can be written as $\sigma_2 = \sigma_1 + |\psi_1(0)|^2/\|\psi_1\|^2 = \sigma_1 + |\varphi_2(0)|^2/\|\varphi_2\|^2$.

We can continue in this manner, noting that in each application of the double commutation method, the desired eigenfunction asymptotics inductively hold true. This yields the identity

$$\int_0^\infty V_N(x)^2\,\mathrm{d}x = -\frac{16}{3}\sum_{j=1}^N |\lambda_j|^{\frac{3}{2}} + 4\sum_{j=1}^N |\lambda_j|(\sigma_j-\sigma_{j-1}) - \frac{4}{3}(\sigma_N^3-\sigma_0^3) + \int_0^\infty V(x)^2\,\mathrm{d}x$$

after N steps. Since the left-hand side is non-negative, we obtain the inequality

$$\sum_{j=1}^N |\lambda_j|^{\frac{3}{2}} + \frac{1}{4}\sum_{j=1}^N (\sigma_j^3-\sigma_{j-1}^3) \leq \frac{3}{16}\int_0^\infty V(x)^2\,\mathrm{d}x + \frac{3}{4}\sum_{j=1}^N |\lambda_j|(\sigma_j-\sigma_{j-1}).$$

If the number of negative eigenvalues is finite, this is already the desired bound. In the case of infinitely many eigenvalues, we can let $N\to\infty$ as all four terms are positive and non-decreasing in N.

3.2. The proof of Theorem 1.3

We start with the following observation.

Remark 3.2. We recall that F and $\widetilde{F}$ in Lemma 3.1 were well defined, since under the assumptions of Theorem 1.1 the ground state φ_1 does not have any zeros. This fact was subsequently also used in the proof of the lemma. Note, however, that the decomposition $G = F - \widetilde{F}$ was only necessary in order to evoke similarities to the single commutation method and to simplify the computations. It can also be checked directly that the identity

$$\begin{aligned} &G'(x)\big(G'(x) - V(x)\big) \\ &\quad = \frac{\mathrm{d}}{\mathrm{d}x}\Big(|\lambda_1| G(x) - \frac{\gamma_1 \varphi_1'(x)^2 \Phi_1(x)^2 - \gamma_1^2 \varphi_1'(x)\varphi_1(x)^3 \Phi_1(x) + \frac{1}{3}\gamma_1^3 \varphi_1(x)^6}{\Phi_1(x)^3}\Big) \end{aligned}$$

holds, where $\Phi_1(x) = 1 + \gamma_1 \int_0^x |\varphi_1(t)|^2 \,\mathrm{d}t$. Here, all involved quantities are well defined even if φ_1 has zeros. This shows that the double commutation method does not require us to remove the eigenvalues in increasing order. Furthermore, in a more general setting, the double commutation method could be used to remove eigenvalues in gaps of the essential spectrum other than the lowest one.

The above remark shows that we can apply the double commutation method to the Schrödinger operator $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$ on $L^2(\mathbb{R}_+)$ with Dirichlet boundary condition at the origin. After the initial step, the operator $H_1 = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_1$ is characterised (see Remark 2.4) by the vanishing Wronskian $\psi(0)\varphi_1'(0) - \psi'(0)\varphi_1(0) = 0$ which reduces to $\psi(0) = 0$. Following the procedure above, we obtain the identity

$$\int_0^\infty V_1(x)^2 \,\mathrm{d}x = -\frac{16}{3}|\lambda_1|^{\frac{3}{2}} - 4\frac{|\varphi_1'(0)|^2}{\|\varphi_1\|^2} + \int_0^\infty V(x)^2 \,\mathrm{d}x.$$

From (5), we see that $\psi_1'(0) = \varphi_2'(0)$. We can then continue removing eigenvalues from the spectrum. Repeating the process for altogether N steps and using again that $\int_0^\infty V_N(x)^2 \,\mathrm{d}x \geq 0$ we obtain

$$\sum_{j=1}^N |\lambda_1|^{\frac{3}{2}} + \frac{3}{4}\sum_{j=1}^N \frac{|\varphi_j'(0)|^2}{\|\varphi_j\|^2} \leq \frac{3}{16}\int_0^\infty V(x)^2 \,\mathrm{d}x.$$

This finishes the proof if the operator has only finitely many eigenvalues. The general case follows from taking $N \to \infty$ and noting that all three terms are non-negative and non-decreasing in N.

4. Comparison and simplifications

4.1. Comparison to Theorem 1.5

Under the assumptions of Theorem 1.1 and if $V \leq 0$, the presented inequality is stronger than the result of Theorem 1.5. To this end, we note that, by definition,

$\sigma_j - \sigma_{j-1} \geq 0$ as well as $|\lambda_j| \leq |\lambda_1|$, and thus, for any $N \geq 1$,

$$\frac{3}{4}\sum_{j=1}^{N} |\lambda_j|(\sigma_j - \sigma_{j-1}) + \frac{1}{4}(\sigma_0^3 - \sigma_N^3) \leq \frac{3}{4}|\lambda_1|(\sigma_N - \sigma_0) + \frac{1}{4}(\sigma_0^3 - \sigma_N^3). \tag{6}$$

If $\sigma_0 \geq 0$, then also $\sigma_N \geq 0$ and by Young's inequality

$$\frac{3}{4}|\lambda_1|\sigma_N \leq \frac{1}{2}|\lambda_1|^{\frac{3}{2}} + \frac{1}{4}\sigma_N^3. \tag{7}$$

If $\sigma_0 < 0$, then the inequality still holds true. To this end, we note that by the min–max principle $|\lambda_1| \geq \sigma_0^2$ since $V \leq 0$ and since the operator without potential has a single negative eigenvalue $-\sigma_0^2$. Thus, $(2|\lambda_1|^{\frac{1}{2}} + \sigma_N) \geq 0$ and from the identity

$$\frac{3}{4}|\lambda_1|\sigma_N = \frac{1}{2}|\lambda_1|^{\frac{3}{2}} + \frac{1}{4}\sigma_N^3 - \frac{1}{4}(|\lambda_1|^{\frac{1}{2}} - \sigma_N)^2(2|\lambda_1|^{\frac{1}{2}} + \sigma_N) \tag{8}$$

we again obtain (7). Inserting (7) into (6) establishes that the inequality in Theorem 1.1 implies the inequality in Theorem 1.5 if $V \in L^1(\mathbb{R}_+) \cap L^2(\mathbb{R}_+)$, $V \leq 0$. The assumptions in the latter can then be relaxed to $V \in L^2(\mathbb{R}_+)$, $V \leq 0$ by the standard approximation arguments.

We will provide an explicit example where the former inequality becomes an equality, while the latter remains a strict inequality. To this end, we apply the double commutation method to insert a single eigenvalue into the spectrum of the free Schrödinger operator $-\frac{d^2}{dx^2}$ with Neumann boundary condition $\varphi'(0) = 0$. For fixed $\omega \in \mathbb{R}$, we consider $\varphi(x) = \cosh(\omega x)$, which satisfies $-\varphi'' = -\omega^2\varphi$ as well as $\varphi'(0) = 0$. Note that, in contrast to the assumptions in Theorem 2.3, the function φ is not an element of $L^2(\mathbb{R}_+)$. Furthermore, we choose $\gamma > 0$. From [14, Theorem 3.2], we can conclude that the operator $-\frac{d^2}{dx^2} + V$ with potential

$$V(x) = -2\frac{d}{dx}\Big(\frac{\gamma\cosh^2(\omega x)}{1 + \gamma\int_0^x \cosh^2(\omega t)\,dt}\Big)$$

and Robin boundary condition $\varphi'(0) + \gamma\varphi(0) = 0$ has a single negative eigenvalue $-\omega^2$. By construction (or by direct computation), the inequality of Theorem 1.1 is found to be an equality in this case. In particular,

$$\frac{3}{16}\int_0^\infty V(x)^2\,dx = \frac{1}{4}\gamma^3 - \frac{3}{4}\gamma\omega^2 + \omega^3.$$

The inequality of Theorem 1.5, on the other hand, reduces to $\frac{\omega^3}{2} \leq \omega^3$, which shows that for this example, the factor of $\frac{1}{2}$ in front of the lowest eigenvalue is not necessary.

Both inequalities are sharp for the free operator $-\frac{d^2}{dx^2}$ with boundary condition $\varphi'(0) - \sigma_0\varphi(0) = 0$, which for $\sigma_0 < 0$ has a single negative eigenvalue $-\sigma_0^2$ with normalised eigenfunction $\varphi_1(x) = \sqrt{-2\sigma_0}e^{\sigma_0 x}$. Under the assumptions of Theorem 1.1, the inequality of Theorem 1.5 cannot be an identity for potentials $V \in L^1(\mathbb{R}_+) \cap L^2(\mathbb{R}_+)$ with more than one eigenvalue, since the bound was proved by applying (1) to the Dirichlet problem obtained after the initial step of the single commutation method. By Theorem 1.3, this yields a strict inequality.

4.2. Some simplifications in special cases

In some cases, the bound in Theorem 1.1 can be simplified such that it does not depend on the (often unknown) quantities σ_j for $j \geq 1$.

If $\sigma_0 \geq 0$, then Young's inequality allows us to conclude that

$$\begin{aligned}\frac{3}{4}|\lambda_1|(\sigma_N - \sigma_0) + \frac{1}{4}(\sigma_0^3 - \sigma_N^3) &\leq \frac{1}{2}|\lambda_1|^{\frac{3}{2}} + \frac{1}{4}(\sigma_N - \sigma_0)^3 + \frac{1}{4}(\sigma_0^3 - \sigma_N^3)\\ &= \frac{1}{2}|\lambda_1|^{\frac{3}{2}} - \frac{3}{4}\sigma_0\sigma_N(\sigma_N - \sigma_0) \leq \frac{1}{2}|\lambda_1|^{\frac{3}{2}}.\end{aligned}$$

From (6), we thus obtain that Theorem 1.1 implies

$$\frac{1}{2}|\lambda_1|^{\frac{3}{2}} + \sum_{j\geq 2}|\lambda_j|^{\frac{3}{2}} \leq \frac{3}{16}\int_0^\infty V(x)^2\,dx.$$

While this result cannot be read off directly from the bound in Theorem 1.5, we note that it can be alternatively obtained by first applying the min-max principle and subsequently using Theorem 1.5 in the special case of a Neumann boundary condition $\sigma_0 = 0$.

More can be said if one can establish that $\sigma_0 \geq |\lambda_1|^{1/2}$. In this case,

$$(|\lambda_1|^{1/2} - \sigma_N)^2 \geq (|\lambda_1|^{1/2} - \sigma_0)^2,$$

and thus (8) shows

$$\begin{aligned}\frac{3}{4}|\lambda_1|\sigma_N &\leq \frac{1}{2}|\lambda_1|^{\frac{3}{2}} + \frac{1}{4}\sigma_N^3 - \frac{1}{4}(|\lambda_1|^{\frac{1}{2}} - \sigma_0)^2(2|\lambda_1|^{\frac{1}{2}} + \sigma_0)\\ &= \frac{3}{4}|\lambda_1|\sigma_0 - \frac{1}{4}\sigma_0^3 + \frac{1}{4}\sigma_N^3.\end{aligned}$$

As a consequence,

$$\frac{3}{4}|\lambda_1|(\sigma_N - \sigma_0) + \frac{1}{4}(\sigma_0^3 - \sigma_N^3) \leq 0$$

and thus, on account of (6), we obtain

$$\sum_{j \geq 1} |\lambda_j|^{\frac{3}{2}} \leq \frac{3}{16} \int_0^\infty V(x)^2 \, dx$$

from Theorem 1.1. We observe that, in this special case, the Lieb–Thirring bound holds without any additional terms. It is not possible to obtain this result from Theorem 1.5 as the additional term in the inequality has the opposite sign, i.e.,

$$\frac{1}{2}|\lambda_1|^{\frac{3}{2}} - \frac{3}{4}|\lambda_1|\sigma_0 + \frac{1}{4}\sigma_0^3 \geq 0$$

by Young's inequality.

Lastly, if $\sigma_0 \leq 0$ and $V \leq 0$ then Young's inequality implies

$$-\frac{3}{4}|\lambda_1|^{\frac{1}{2}}\sigma_0 \leq \frac{1}{2}|\lambda_1|^{\frac{3}{2}} - \frac{1}{4}\sigma_0^3$$

and together with (7) and (6) we conclude that Theorem 1.1 implies

$$\sum_{j \geq 2} |\lambda_j|^{\frac{3}{2}} \leq \frac{3}{16} \int_0^\infty V(x)^2 \, dx.$$

This result also follows from Theorem 1.5 by the same argument.

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References

[1] R. Benguria and M. Loss, A simple proof of a theorem of Laptev and Weidl. *Math. Res. Lett.* **7** (2000), no. 2-3, 195–203 Zbl 0963.34077 MR 1764316

[2] A. Boumenir and V. K. Tuan, A trace formula and Schmincke inequality on the half-line. *Proc. Amer. Math. Soc.* **137** (2009), no. 3, 1039–1049 Zbl 1173.34053 MR 2457445

[3] V. S. Buslaev and L. D. Faddeev, Formulas for traces for a singular Sturm-Liouville differential operator. *Dokl. Akad. Nauk SSSR* **132** (196), 13–16; English transl., *Soviet Math. Dokl.* **1** (1960), 451–454 Zbl 0129.06501 MR 0120417

[4] M. M. Crum, Associated Sturm–Liouville systems. *Quart. J. Math. Oxford Ser. (2)* **6** (1955), 121–127 Zbl 0065.31901 MR 72332

[5] M. Cwikel, Weak type estimates for singular values and the number of bound states of Schrödinger operators. *Ann. of Math. (2)* **106** (1977), no. 1, 93–100 Zbl 0362.47006 MR 473576

[6] M. Danish Zia and M. Usman, Sharp spectral inequalities for fourth order differential operators on semi-axis. *Math. Phys. Anal. Geom.* **22** (2019), no. 4, article no. 24 Zbl 1430.35177 MR 4039077

[7] G. Darboux, *Sur une proposition relative aux équations linéaires*. *C. R. Acad. Sci. Paris* **94** (1882), 1456–1459 (1882). JFM 14.0264.01

[8] P. Deift and R. Killip, On the absolutely continuous spectrum of one-dimensional Schrödinger operators with square summable potentials. *Comm. Math. Phys.* **203** (1999), no. 2, 341–347 Zbl 0934.34075 MR 1697600

[9] P. A. Deift, Applications of a commutation formula. *Duke Math. J.* **45** (1978), no. 2, 267–310 Zbl 0392.47013 MR 495676

[10] S. Demirel and M. Usman, Trace formulas for Schrödinger operators on the half-line. *Bull. Math. Sci.* **1** (2011), no. 2, 397–427 Zbl 1256.35041 MR 2901006

[11] P. Exner, A. Laptev, and M. Usman, On some sharp spectral inequalities for Schrödinger operators on semiaxis. *Comm. Math. Phys.* **326** (2014), no. 2, 531–541 Zbl 1297.35155 MR 3165466

[12] C. S. Gardner, J. M. Greene, M. D. Kruskal, and R. M. Miura, Korteweg-deVries equation and generalization. VI. Methods for exact solution. *Comm. Pure Appl. Math.* **27** (1974), 97–133 Zbl 0291.35012 MR 336122

[13] F. Gesztesy, A complete spectral characterization of the double commutation method. *J. Funct. Anal.* **117** (1993), no. 2, 401–446 Zbl 0813.34074 MR 1244942

[14] F. Gesztesy and G. Teschl, On the double commutation method. *Proc. Amer. Math. Soc.* **124** (1996), no. 6, 1831–1840 Zbl 0855.34028 MR 1322925

[15] J. Hoppe, A. Laptev, and J. Östensson, Solitons and the removal of eigenvalues for fourth-order differential operators. *Int. Math. Res. Not.* (2006), article no. 85050 Zbl 1123.34067 MR 2233712

[16] C. G. J. Jacobi, Zur Theorie der Variations-Rechnung und der Differential-Gleichungen. *J. Reine Angew. Math.* **17** (1837), 68–82 Zbl 017.0558cj MR 1578150

[17] A. Laptev and T. Weidl, Sharp Lieb–Thirring inequalities in high dimensions. *Acta Math.* **184** (2000), no. 1, 87–111 Zbl 1142.35531 MR 1756570

[18] B. M. Levitan, *Inverse Sturm-Liouville problems*. VSP, Zeist, 1987 Zbl 0749.34001 MR 933088

[19] E. H. Lieb, Bounds on the eigenvalues of the Laplace and Schroedinger operators. *Bull. Amer. Math. Soc.* **82** (1976), no. 5, 751–753 Zbl 0329.35018 MR 407909

[20] E. H. Lieb and W. E. Thirring, Bound for the kinetic energy of Fermions which proves the stability of matter. *Phys. Rev. Lett.* **35** (1975), 687–689; errata *ibid.* (1975), 1116

[21] E. H. Lieb and W. E. Thirring, Inequalities for the moments of the eigenvalues of the Schrödinger hamiltonian and their relation to Sobolev inequalities. *Studies in Mathematical Physics,* pp. 269–303, Princeton University Press, Princeton, NJ, 1976 Zbl 0342.35044

[22] M. A. Naimark, *Linear differential operators.* Part I: Elementary theory of linear differential operators. Frederick Ungar, New York, 1967 Zbl 0227.34020 MR 0216050

[23] G. V. Rozenblum, Distribution of the discrete spectrum of singular differential operators. *Izv. Vysš. Učebn. Zaved. Matematika* (1976), no. 1(164), 75–86 Zbl 0342.35045 MR 0430557

[24] L. Schimmer, Spectral inequalities for Jacobi operators and related sharp Lieb–Thirring inequalities on the continuum. *Comm. Math. Phys.* **334** (2015), no. 1, 473–505 Zbl 1317.35155 MR 3304283

[25] L. Schimmer, The state of the Lieb–Thirring conjecture. In *The physics and mathematics of Elliott Lieb.* Vol. II, pp. 253–275, EMS Press, Berlin, 2022 Zbl 1500.81037 MR 4531363

[26] U.-W. Schmincke, On Schrödinger's factorization method for Sturm–Liouville operators. *Proc. Roy. Soc. Edinburgh Sect. A* **80** (1978), no. 1–2, 67–84 Zbl 0395.47022 MR 529570

[27] T. Weidl, On the Lieb-Thirring constants $L_{\gamma,1}$ for $\gamma \geq 1/2$. *Comm. Math. Phys.* **178** (1996), no. 1, 135–146 Zbl 0858.34075 MR 1387945

[28] V. E. Zaharov and L. D. Faddeev, The Korteweg–de Vries equation is a fully integrable Hamiltonian system. *Funkcional. Anal. i Priložen.* **5** (1971), no. 4, 18–27; English transl., *Funct. Anal. Appl.* **5** (1972), 280–287 Zbl 0257.35074 MR 0303132

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