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Universal monotonicity of eigenvalue moments and sharp Lieb–Thirring inequalities

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Abstract. We show that phase space bounds on the eigenvalues of Schrödinger operators can be derived from universal bounds recently obtained by E. M. Harrell and the author via a monotonicity property with respect to coupling constants. In particular, we provide a new proof of sharp Lieb–Thirring inequalities.

Keywords. Universal bounds for eigenvalues, spectral gap, phase space bounds, Lieb–Thirring inequalities, Schrödinger operators

1. Introduction

We consider the eigenvalues $E_j(\alpha)$ of a one-parameter family of Schrödinger operators

$$H(\alpha) = -\alpha\Delta + V(x) \quad (1.1)$$

on \mathbb{R}^d for constants $\alpha > 0$. For simplicity we suppose that $V(x)$ is a continuous function of compact support and we denote its negative part by $V_-(x)$. It is a well-known fact (see e.g. [3, 9] and references therein) that for all $\sigma \geq 0$,

$$\lim_{\alpha \rightarrow 0^+} \alpha^{d/2} \sum_{E_j(\alpha) < 0} (-E_j(\alpha))^\sigma = L_{\sigma,d}^{\text{cl}} \int_{\mathbb{R}^d} V_-(x)^{\sigma+d/2} dx \quad (1.2)$$

with $L_{\sigma,d}^{\text{cl}}$, called the classical constant, given by

$$L_{\sigma,d}^{\text{cl}} = (4\pi)^{-d/2} \frac{\Gamma(\sigma + 1)}{\Gamma(\sigma + d/2 + 1)}. \quad (1.3)$$

Lieb–Thirring inequalities are inequalities of the form

$$\alpha^{d/2} \sum_{E_j(\alpha) < 0} (-E_j(\alpha))^\sigma \leq L_{\sigma,d} \int_{\mathbb{R}^d} V_-(x)^{\sigma+d/2} dx \quad (1.4)$$

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for some constant $L_{\sigma,d} \geq L_{\sigma,d}^{\text{cl}}$ and are widely discussed in the literature (see e.g. [3, 9, 11]). A longstanding question is when (1.4) holds with $L_{\sigma,d} = L_{\sigma,d}^{\text{cl}}$. The most general result is due to Laptev and Weidl [10] who proved that $L_{\sigma,d} = L_{\sigma,d}^{\text{cl}}$ for all $\sigma \geq 3/2$ and $d \geq 1$. Their proof is based on a dimensional reduction of Schrödinger operators with operator valued potentials, which allows them to make use of the bound for $\sigma = 3/2$, $d = 1$ which has been first proven by Lieb and Thirring [12]. For a simplified proof see also [2]. On the other hand, by analyzing the spectra of harmonic oscillators Helffer and Robert [8] have shown that $L_{\sigma,d} > L_{\sigma,d}^{\text{cl}}$ for $\sigma < 1$ while de la Bretèche showed that these spectra are in agreement with the conjecture $L_{\sigma,d} = L_{\sigma,d}^{\text{cl}}$ for $\sigma \geq 1$ [4].

Recently, Harrell and the author have established universal trace inequalities for abstract self-adjoint operators H modelled on Schrödinger operators [7]. If G is another self-adjoint operator, then under suitable domain conditions (see Corollary 2.3 of [7])

$$\begin{aligned} \sum_{E_j \in J} ((z - E_j)^2 \langle [G, [H, G]]\phi_j, \phi_j \rangle - 2(z - E_j) \langle [H, G]\phi_j, [H, G]\phi_j \rangle) \\ = 2 \sum_{E_j \in J} \int_{\kappa \in J^c} (z - E_j)(z - \kappa)(\kappa - E_j) dG_{j\kappa}^2 \end{aligned} \quad (1.5)$$

where J denotes a subset of the discrete spectrum of H and J^c its complement and the measure $dG_{j\kappa}^2$ corresponds to the matrix elements of the operator G with respect to the spectral projections onto J and J^c (see [7] for the details). Exploiting this identity we prove the following

Theorem 1.1. *Let $V(x)$ be a continuous function of compact support. Then the mapping*

$$\alpha \mapsto \alpha^{d/2} \sum_{E_j(\alpha) < 0} (-E_j(\alpha))^2 \quad (1.6)$$

is non-increasing for all $\alpha > 0$. Consequently,

$$\alpha^{d/2} \sum_{E_j(\alpha) < 0} (-E_j(\alpha))^2 \leq L_{2,d}^{\text{cl}} \int_{\mathbb{R}^d} V_-(x)^{2+d/2} dx \quad (1.7)$$

for all $\alpha > 0$.

The link between universal inequalities and semiclassical estimates has been first made in [6] where it has been shown for the Dirichlet Laplacian $-\Delta_D$ on a bounded domain $D \subset \mathbb{R}^d$ that the mapping

$$t \mapsto t^{d/2} \text{tr}(e^{-t\Delta_D}) \quad (1.8)$$

is always decreasing and therefore bounded by its semiclassical limit, that is,

$$\text{tr}(e^{-t\Delta_D}) \leq (4\pi t)^{-d/2} |D|. \quad (1.9)$$

Harrell and Hermi have extended this technique to Riesz means of the Dirichlet Laplacian [5]. In [7] it has been pointed out that the monotonicity of mappings like (1.8) is a

universal property of a large family of “trace-controllable” functions (as precisely defined in [7]) of Schrödinger operators and we shall derive in the present paper a corresponding universal property of one-parameter families of Schrödinger operators. Our second result extends this property to Schrödinger operators of the form (1.1) with confining potentials $V(x)$ such that

$$\int_{\mathbb{R}^d} e^{-tV(x)} dx < \infty \tag{1.10}$$

for all $t > 0$. We provide a monotonicity result implying the Golden–Thompson inequality (see e.g. [13]) for Schrödinger operators (1.1):

Theorem 1.2. *If (1.10) holds, then for all $t > 0$ the mapping*

$$\alpha \mapsto \alpha^{d/2} \operatorname{tr}(e^{-tH(\alpha)}) \tag{1.11}$$

is non-increasing for all $\alpha > 0$. Consequently, for all $\alpha > 0$,

$$\operatorname{tr}(e^{-tH(\alpha)}) \leq (4\pi\alpha t)^{-d/2} \int_{\mathbb{R}^d} e^{-tV(x)} dx < \infty. \tag{1.12}$$

2. Proof of main results

The key for proving our main results is the trace formula for self-adjoint operators proved in [7]. For convenience we reformulate this result for the operator $H(\alpha)$ in a slightly different and, as we believe, more transparent way. To make the present paper self-contained we give an elementary proof of the trace formula. For simplicity, we consider only the case of purely discrete spectra (more relevant for Theorem 1.2). In the presence of continuous spectrum one uses the spectral integral as in [7].

Theorem 2.1 (Trace formula for $H(\alpha)$). *Suppose that $H(\alpha)$ given in (1.1) has a spectrum consisting of eigenvalues $E_k = E_k(\alpha)$ with associated eigenfunctions ϕ_k forming an orthonormal basis of the underlying Hilbert space $L^2(\mathbb{R}^d)$. Then for any function $f : \mathbb{R} \rightarrow \mathbb{R}$,*

$$d \sum_{E_j} f(E_j) + 2\alpha \sum_{E_j \neq E_k} \sum_{T_{jk}} \frac{f(E_k) - f(E_j)}{E_k - E_j} = 0 \tag{2.1}$$

provided all sums are finite where

$$T_{jk} = T_{kj} = \left| \int_{\mathbb{R}^d} \phi_j \nabla \phi_k dx \right|^2 \tag{2.2}$$

denote the kinetic energy matrix elements.

Proof. Let $x_a, a = 1, \dots, d$, denote cartesian coordinates in \mathbb{R}^d and $D_a = \partial/\partial x_a$. The first identity we derive in the following is due to canonical commutation (or integration by parts) and the completeness of eigenfunctions. Indeed, for all j ,

$$1 = -2 \int_{\mathbb{R}^d} x_a \phi_j D_a \phi_j dx = -2 \sum_k \int_{\mathbb{R}^d} x_a \phi_j \phi_k dx \int_{\mathbb{R}^d} \phi_k D_a \phi_j dx. \quad (2.3)$$

Taking the scalar product of $H(\alpha)\phi_j = E_j\phi_j$ with ϕ_k and vice versa we derive, after subtracting both expressions, the gap formula

$$(E_k - E_j) \int_{\mathbb{R}^d} x_a \phi_j \phi_k dx = -2\alpha \int_{\mathbb{R}^d} (D_a \phi_j) \phi_k dx. \quad (2.4)$$

We note that the r.h.s. is zero for degenerate eigenvalues. Therefore after summing over all coordinates in (2.3) we get the sum rule

$$d = 4\alpha \sum_{E_k \neq E_j} \frac{T_{jk}}{E_k - E_j}. \quad (2.5)$$

Multiplying (2.5) by $f(E_j)$, summing over j and symmetrizing the double sum we finally obtain (2.1). \square

Applying Theorem 2.1 to $f(E) = (z - E)^2$ for $E < z$ and $f(E) = 0$ otherwise we recover (1.5) with G being the multiplication operator x_a after summing over all coordinates as shown in [6, 7]:

$$\sum_{E_j < z} (d(z - E_j)^2 - 4\alpha(z - E_j)T_j) = 4\alpha \sum_{E_j < z} \sum_{E_k \geq z} T_{jk} \frac{(z - E_j)(z - E_k)}{E_k - E_j} \quad (2.6)$$

with

$$T_j = \sum_{E_k} T_{jk} = \int_{\mathbb{R}^d} |\nabla \phi_j|^2 dx.$$

Remark 2.2. Formula (2.5) can also be easily derived from second order perturbation theory. Indeed, for a fixed vector $v \in \mathbb{R}^d$ consider the operator $H = (-i\sqrt{\alpha}\nabla + \gamma v)^2 + V(x)$. Obviously, the addition of a constant vector potential does not change the eigenvalues, and second order perturbation (i.e. first order in $\gamma^2 v^2$ and second order in $-2i\sqrt{\alpha}\gamma v\nabla$) yields (2.5) when choosing v to be the canonical unit vectors e_a and then summing over all $a = 1, \dots, d$. The author thanks R. Seiringer for indicating this proof.

Choosing f appropriately in Theorem 2.1 we may now prove our main results.

Proof of Theorem 1.1. We note that for any $\alpha > 0$ the operator $H(\alpha)$ has at most a finite number of negative eigenvalues. Obviously, the r.h.s. in (2.6) is negative. Making the dependence on the parameter α explicit we have therefore for all $z \leq 0$ the inequality

$$\alpha \sum_{E_j(\alpha) < 0} (z - E_j(\alpha))^2 - \frac{4}{d}\alpha^2 \sum_{E_j(\alpha) < 0} (z - E_j(\alpha))T_j(\alpha) \leq 0. \quad (2.7)$$

The functions $E_j(\alpha)$ are non-positive, continuous and increasing. Furthermore, let $\infty \geq \alpha_1 \geq \alpha_2 \geq \dots > 0$ denote the values at which $E_j(\alpha)$ appears. $E_j(\alpha)$ is continuously

differentiable for $\alpha \neq \alpha_k$ and by the Feynman–Hellmann theorem

$$\frac{d}{d\alpha} E_j(\alpha) = T_j(\alpha). \tag{2.8}$$

Taking $z = 0$, inequality (2.7) then reads

$$\alpha \sum_{E_j(\alpha) < 0} (-E_j(\alpha))^2 + \frac{2}{d} \alpha^2 \frac{d}{d\alpha} \sum_{E_j(\alpha) < 0} (-E_j(\alpha))^2 \leq 0.$$

For any $\alpha \in]\alpha_{N+1}, \alpha_N[$ the number of eigenvalues is constant and therefore

$$\frac{d}{d\alpha} \left(\alpha^{d/2} \sum_{E_j(\alpha) < 0} (-E_j(\alpha))^2 \right) \leq 0,$$

proving the theorem. □

Remark 2.3. Strictly speaking, the Feynman–Hellmann theorem only holds for non-degenerate eigenvalues. In the case of degenerate eigenvalues one has to take the right basis in the corresponding eigenspace and to change the numbering if necessary (see e.g. [14]).

Proof of Theorem 1.2. Choose $f(E) = e^{-tE}$ and $t > 0$. Since $f'(E) = -tf(E)$ is concave it follows that

$$f'(sE_j + (1-s)E_k) \geq sf'(E_j) + (1-s)f'(E_k).$$

Using the symmetry of T_{jk} we get

$$d \sum_{E_j(\alpha)} f(E_j(\alpha)) + 2\alpha \sum_{E_j(\alpha)} f'(E_j(\alpha))T_j(\alpha) \leq 0$$

and we conclude as in the proof of Theorem 1.1. □

3. Extensions and discussion

It has already been shown in [6, 5, 7] that one can obtain trace inequalities for the functions $f(E) = (z - E)^\sigma$ with $\sigma \geq 2$. In fact we have the following result:

Corollary 3.1. *Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be a C^1 function with support on the negative half axis such that f' is concave. Under the conditions of Theorem 1.1 the mapping*

$$\alpha \mapsto \alpha^{d/2} \sum_{E_j(\alpha) < 0} f(E_j(\alpha)) \tag{3.1}$$

is non-increasing for $\alpha > 0$. In particular, for all $\sigma \geq 2$,

$$\alpha \mapsto \alpha^{d/2} \sum_{E_j(\alpha) < 0} (-E_j(\alpha))^\sigma \tag{3.2}$$

is non-increasing for $\alpha > 0$. Consequently,

$$\alpha^{d/2} \sum_{E_j(\alpha) < 0} (-E_j(\alpha))^\sigma \leq L_{\sigma,d}^{cl} \int_{\mathbb{R}^d} V_-(x)^{\sigma+d/2} dx. \tag{3.3}$$

Proof. Since f is of class C^1 we may rewrite the trace formula (2.1) as follows (note that $T_{jj} = 0$):

$$d \sum_{E_j} f(E_j) + 2\alpha \sum_{E_j} \sum_{E_k} T_{jk} \int_0^1 f'(sE_j + (1-s)E_k) ds = 0.$$

The concavity of f' implies that

$$\int_0^1 f'(sE_j + (1-s)E_k) ds \geq \frac{1}{2} f'(E_j) + \frac{1}{2} f'(E_k).$$

Using the symmetry of T_{jk} and $f'(E) = 0$ for $E \geq 0$ we get

$$d \sum_{E_j(\alpha) < 0} f(E_j(\alpha)) + 2\alpha \sum_{E_j(\alpha) < 0} f'(E_j(\alpha)) T_j(\alpha) \leq 0.$$

As in the proof of Theorem 1.1 we use the Feynman–Hellmann theorem to prove (3.1). □

Remark 3.2. The sharp Lieb–Thirring inequality (3.3) follows also from (1.7) of Theorem 1.1 via the Aizenman–Lieb monotonicity principle [1]. However, the monotonicity of the mapping (3.2) is a stronger and new result.

Remark 3.3. Theorems 1.1 and 1.2 are also valid in the presence of magnetic fields, i.e. $H(\alpha) = -\alpha(-i\nabla + A(x))^2 + V(x)$, and in the case of matrix valued potentials, since all commutation relations remain unchanged and the trace formula (2.1) still holds [6, 7].

Remark 3.4. We cannot expect that the monotonicity holds for moments with $\sigma < 2$. For example, consider the d -dimensional harmonic oscillator with eigenvalues $E_j(\alpha) = \sqrt{\alpha} (2j_1 + \dots + 2j_d + d)$ for natural numbers j_1, \dots, j_d . We want to study the behaviour of the eigenvalue moments

$$S_\sigma(\alpha) = \sum_{E_j(\alpha) < 1} (1 - E_j(\alpha))^\sigma.$$

Then for all $\alpha \in [(d + 2)^{-2}, d^{-2}]$ we have

$$\alpha^{d/2} S_\sigma(\alpha) = \alpha^{d/2} (1 - d\sqrt{\alpha})^\sigma.$$

It is easy to see that the derivative of the above expression (with respect to α) is strictly positive at $\alpha = (d + 2)^{-2}$ for all $0 \leq \sigma < 2$. This behaviour persists also for the sum of the first two eigenvalues. Indeed, for all $\alpha \in [(d + 4)^{-2}, (d + 2)^{-2}]$ we have (taking into account the multiplicity of the second eigenvalue)

$$S_\sigma(\alpha) = (1 - d\sqrt{\alpha})^\sigma + d(1 - (d + 2)\sqrt{\alpha})^\sigma.$$

Then the function $p_\sigma(\alpha) := \alpha^{d/2} S_\sigma(\alpha)$ has a strictly positive derivative at $\alpha = (d + 4)^{-2}$ for all $0 \leq \sigma < 2$. Obviously, for $\sigma = 2$ the derivatives at these points vanish.

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