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TRACE IDENTITIES FOR COMMUTATORS, WITH APPLICATIONS TO THE DISTRIBUTION OF EIGENVALUES

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Abstract. We prove trace identities for commutators of operators, which are used to derive sum rules and sharp universal bounds for the eigenvalues of periodic Schrödinger operators and Schrödinger operators on immersed manifolds. In particular, we prove bounds on the eigenvalue λ_{N+1} in terms of the lower spectrum, bounds on ratios of means of eigenvalues, and universal monotonicity properties of eigenvalue moments, which imply sharp versions of Lieb-Thirring inequalities. In the case of a Schrödinger operator on an immersed manifold of dimension d, we derive a version of Reilly's inequality bounding the eigenvalue λ_{N+1} of the Laplace-Beltrami operator by a universal constant times $\|h\|_\infty^2 N^{2/d}$.

1. Introduction

In [13] the authors derived "sum rule" identities and sharp universal inequalities for certain self-adjoint operators H, including the Dirichlet Laplacian on bounded Euclidean domains and Schrödinger operators with discrete spectra. The essential idea was to exploit algebraic relations among the first and second commutators of H with an auxiliary self-adjoint operator G. (Notationally, the commutator is given by $[H, G] := HG - GH$, and by the first and second commutators we refer to $[H, G]$ and to $[G, [H, G]]$.) In the canonical case H was of the form $-\Delta + V(\mathbf{x})$, where $-\Delta$ designates the Dirichlet Laplacian on a bounded domain Ω, and G was chosen as a Euclidean coordinate function. Due to the Dirichlet condition, the product of G with the eigenfunctions of H remained in the domain of definition of H, allowing manipulation of products of operators without much needing to address technical questions of the domains of definition of partial differential operators. The trace identities of [13] were found to imply and unify several known inequalities for the spectra of Laplacians as well as new inequalities, which in many cases were shown to be optimal. Among the many more recent related articles are some establishing connections with "semiclassical" spectral analysis, for example by making connections with Lieb-Thirring inequalities and inequalities that are sharp in the Weyl limit [11, 12, 32].

The original intent of the present article was to use similar methods to study the spectrum of periodic Schrödinger operators, a case that has been much less

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considered from the point of view of universal spectral bounds. One reason for the lack of attention to periodic problems is that multiplication by a coordinate function does not preserve a core of the domain of self-adjointness of H, so the simple algebraic relations in the canonical case for $[H, G]$ and $[G, [H, G]]$ are not valid. We have therefore sought an alternative whereby H is commuted with a family of auxiliary operators G not assumed to be self-adjoint. Indeed the case of greatest interest will be when G is the unitary operator of multiplication by $\exp(-i\mathbf{q} \cdot \mathbf{x})$. The second section of this article contains an abstract trace formula of this sort (see Theorem 2.2), which exhibits useful simplifications when G is unitary.

The identity that forms the point of departure for the later parts of the article turned out to have the same algebraic form as one that applies to Schrödinger operators on embedded manifolds with bounded mean curvature [10], and it was consequently possible to derive spectral bounds in the two situations simultaneously. This is done in Sections 3 and 4 for the unperturbed Laplacian and for Schrödinger operators with bounded potentials. In particular we show that Riesz means still possess a monotonicity property similar to the one first discovered in [11] for Dirichlet Laplacians on bounded domains in $\mathbb{R}^d$ with, however, a constant shift in its argument depending on the geometry (see Theorem 4.1). In Section 5 we adapt the method of [32] to prove a universal monotonicity property of Riesz means for periodic Schrödinger operators and Schrödinger operators on manifolds of bounded mean curvature, which implies sharp Lieb-Thirring inequalities (see Theorem 5.1). Special cases include sharp Lieb-Thirring inequalities for Schrödinger operators on spheres $\mathbb{S}^d \subset \mathbb{R}^{d+1}$, which have been studied previously with applications to Navier-Stokes equations [18, 20]. In Section 6 we discuss applications of our abstract trace identity of Theorem 2.2 when commuting with unitary operators, which provides a new proof of the trace inequality of [10] on manifolds of bounded mean curvature. We then prove a new Reilly-type bound on eigenvalues optimal in the asymptotic behavior. Finally, in Section 7 we provide some simple explicit examples illustrating the optimality of our results, including some results on the distribution of lattice points.

2. Some trace identities and their consequences

On a Hilbert space $\mathcal{H}$ we consider a self-adjoint operator H with domain of definition $\mathcal{D}_H$, along with a second linear operator G subject to some conditions relating to $\mathcal{D}_H$. In many of the examples to be discussed in this article the spectrum of H consists entirely of eigenvalues λ_j, and the corresponding eigenfunctions ϕ_j are chosen to form an orthonormal basis of the underlying Hilbert space $\mathcal{H}$. (The extension needed if H has a continuous spectrum is not difficult and has been explicitly presented in the case where G is self-adjoint in [14].) Although this result is a special case of a more general trace identity based only on algebraic properties of operators, we first of all present a version assuming that H has a purely discrete spectrum:

Theorem 2.1. *Let H be a self-adjoint operator on $\mathcal{H}$ with a purely discrete spectrum. Let G be a linear operator with domain $\mathcal{D}_G$ and adjoint G^* defined on $\mathcal{D}_{G^*}$ such that $G(\mathcal{D}_H) \subseteq \mathcal{D}_H \subseteq \mathcal{D}_G$ and $G^*(\mathcal{D}_H) \subseteq \mathcal{D}_H \subseteq \mathcal{D}_{G^*}$, respectively. Fix a*

subset J of the spectrum of H. Then

$$\begin{aligned}(2.1)\qquad &\frac{1}{2}\sum_{\lambda_j\in J}(z-\lambda_j)^2\left(\langle[G^*,[H,G]]\phi_j,\phi_j\rangle+\langle[G,[H,G^*]]\phi_j,\phi_j\rangle\right)\\ &\qquad-\sum_{\lambda_j\in J}(z-\lambda_j)\left(\|[H,G]\phi_j\|^2+\|[H,G^*]\phi_j\|^2\right)\\ &=\sum_{\lambda_j\in J}\sum_{\lambda_k\notin J}(z-\lambda_j)(z-\lambda_k)(\lambda_k-\lambda_j)\big(|\langle G\phi_j,\phi_k\rangle|^2+|\langle G^*\phi_j,\phi_k\rangle|^2\big).\end{aligned}$$

If $G=G^*$, then (2.1) reduces to a key identity used in [13, 14] as a step towards the trace identities introduced there.

In preparation for the proof of Theorem 2.1 and the presentation of the general trace identity, we collect some straightforward algebraic identities. Let P be a spectral projector of the self-adjoint operator H and define the pair of operators A and B by

$$(2.2)\qquad A=(1-P)GP,\quad B=PG(1-P).$$

We recall the standard inclusions $\mathrm{Ran}\,(A^*A)\subseteq\mathrm{Ran}\,(P)$, $\mathrm{Ran}\,(AA^*)\subseteq\mathrm{Ran}\,(1-P)$, $\mathrm{Ran}\,(B^*B)\subseteq\mathrm{Ran}\,(1-P)$ and $\mathrm{Ran}\,(BB^*)\subseteq\mathrm{Ran}\,(P)$.

Theorem 2.2. *Let H be a self-adjoint operator on $\mathcal{H}$ and P be a spectral projector of H. Let G be a linear operator with domain $\mathcal{D}_G$ and adjoint G^* defined on $\mathcal{D}_{G^*}$ such that $G(\mathcal{D}_H)\subseteq\mathcal{D}_H\subseteq\mathcal{D}_G$ and $G^*(\mathcal{D}_H)\subseteq\mathcal{D}_H\subseteq\mathcal{D}_{G^*}$, respectively. Then*

$$\begin{aligned}(2.3)\quad &tr\left(H^2(G^*[H,G]+G[H,G^*])P\right)-tr\left(H([H,G^*][H,G]+[H,G][H,G^*])P\right)\\ &\quad=tr\left(HA^*H^2A-HAH^2A^*\right)+tr\left(HBH^2B^*-HB^*H^2B\right).\end{aligned}$$

Proof. Using the projectors P and $1-P$ we write

$$tr\left(H^2(G^*[H,G]+G[H,G^*])P\right)$$

in the form

$$tr\left(H^2(G^*P[H,G]+GP[H,G^*])P\right)+tr\left(H^2(G^*(1-P)[H,G]+G(1-P)[H,G^*])P\right),$$

the first term of which can be computed as

$$\begin{aligned}&tr\left(H^2(G^*P[H,G]+GP[H,G^*])P\right)\\ &\quad=tr\left(H^2G^*P(HG-GH)P+H^2GP(HG^*-G^*H)P\right)\\ &\quad=tr\left(H(HG^*-G^*H)P(HG-GH)P+H(HG-GH)P(HG^*-G^*H)P\right)\\ &\qquad+tr\left(HG^*HP(HG-GH)P+HGHP(HG^*-G^*H)P\right).\end{aligned}$$

The final term in this expression vanishes thanks to the cyclic property of the trace (*viz.*, $tr(AB)=tr(BA)$), and therefore

$$tr\left(H^2(G^*P[H,G]+GP[H,G^*])P\right)=tr\left(H([H,G^*]P[H,G]+[H,G]P[H,G^*])P\right).$$

Adding and subtracting the expression

$$tr\left(H([H,G^*](1-P)[H,G]+[H,G](1-P)[H,G^*])P\right),$$

we see that the left side of (2.3) equals

$$\begin{aligned}
&tr\left(H^2(G^*(1-P)[H,G]+G(1-P)[H,G^*])P\right)\\
&\quad - tr\left(H([H,G^*](1-P)[H,G]+[H,G](1-P)[H,G^*])P\right)\\
&\qquad = tr\left(HG^*H(1-P)[H,G]P+HGH(1-P)[H,G^*]P\right)\\
&\qquad = tr\left(HPG^*(1-P)H(1-P)[H,G]P+HPG(1-P)H(1-P)[H,G^*]P\right)\\
&\qquad = tr\left(HA^*H[H,A]+HBH[H,B^*]\right). \qquad \square
\end{aligned}$$

Since commutators are not affected by replacing H by $H-z$, we have an immediate corollary:

Corollary 2.3. *Under the assumptions of Theorem* 2.2*, for all* $z\in\mathbb{R}$*:*

$$\begin{aligned}
tr\left((z-H)^2(G^*[H,G]+G[H,G^*])P\right)&\\
+ tr\left((z-H)([H,G^*][H,G]+[H,G][H,G^*])P\right)&\\
= tr\left((z-H)A(z-H)^2A^*-(z-H)A^*(z-H)^2A\right)&\\
+ tr\left((z-H)B^*(z-H)^2B-(z-H)B(z-H)^2B^*\right).&
\end{aligned} \tag{2.4}$$

Proof of Theorem 2.1. We may write the first trace in Corollary 2.3 in terms of second commutators by applying the following algebraic identity, which is a direct computation:

$$G^*[H,G]+G[H,G^*]=\frac{1}{2}[G^*,[H,G]]+\frac{1}{2}[G,[H,G^*]]+\frac{1}{2}[H,GG^*+G^*G]. \tag{2.5}$$

When (2.5) is multiplied by P and the trace is taken, the last term vanishes, and for the left side of (2.3) we obtain

$$tr\left(H^2(G^*[H,G]+G[H,G^*])P\right)=\frac{1}{2}tr\left(H^2([G^*,[H,G]]+[G,[H,G^*]])P\right). \tag{2.6}$$

If the spectrum of H consists only of eigenvalues λ_j, with an orthonormal basis of eigenfunctions $\{\phi_j\}$, then the trace identity (2.6) and Corollary 2.3 imply

$$\begin{aligned}
&\frac{1}{2}\sum_{\lambda_j\in J}(z-\lambda_j)^2\left(\langle[G^*,[H,G]]\phi_j,\phi_j\rangle+\langle[G,[H,G^*]]\phi_j,\phi_j\rangle\right)\\
&\qquad -\sum_{\lambda_j\in J}(z-\lambda_j)\left(\langle[H,G]\phi_j,[H,G]\phi_j\rangle+\langle[H,G^*]\phi_j,[H,G^*]\phi_j\rangle\right)\\
&\quad =\sum_{\lambda_j\in J}\sum_{\lambda_k\notin J}(z-\lambda_j)(z-\lambda_k)(\lambda_k-\lambda_j)\left(|\langle G\phi_j,\phi_k\rangle|^2+|\langle G^*\phi_j,\phi_k\rangle|^2\right),
\end{aligned}$$

establishing (2.1). $\square$

If H has a gap in its spectrum, then we consider the spectral projector P that separates the two parts of the spectrum.

Theorem 2.4. *Let G, H satisfy the assumptions of Theorem 2.2. Suppose there exist constants $\lambda < \Lambda$ such that*

$$HP \leq \lambda < \Lambda \leq H(1-P). \tag{2.7}$$

Then for all $z \in [\lambda, \Lambda]$,

$$\begin{aligned} tr\left((z-H)^2(G^*[H,G]+G[H,G^*])P\right) \\ + tr\left((z-H)([H,G^*][H,G]+[H,G][H,G^*])P\right) \\ \leq tr\left((G^*[H,G]+G[H,G^*])P\right)(z-\lambda)(z-\Lambda). \end{aligned} \tag{2.8}$$

Remark 2.5. While this formula only makes sense if the spectrum of HP is discrete, it is not necessary for the whole spectrum of H to be discrete.

Proof of Theorem 2.4. We bound each term of the right side of (2.4). Since $z \in [\lambda, \Lambda]$ and $\mathrm{Ran}\,(A^*A) \subseteq \mathrm{Ran}\,(P)$, with the cyclic property of traces we get

$$\begin{aligned} tr\left((z-H)A(z-H)^2A^*\right) &\leq (z-\Lambda)\ tr\left(A(z-H)^2A^*\right) \\ &= (z-\Lambda)(z-\lambda)\ tr\left((z-H)^2A^*A\right) \\ &\leq (z-\Lambda)(z-\lambda)\ tr\left((z-H)A^*A\right). \end{aligned}$$

Since $\mathrm{Ran}\,(AA^*) \subseteq \mathrm{Ran}\,(1-P)$, we obtain similarly

$$-tr\left((z-H)A^*(z-H)^2A\right) \leq (z-\Lambda)(z-\lambda)\ tr\left((z-H)AA^*\right),$$

and therefore

$$tr\left((z-H)A(z-H)^2A^* - (z-H)A^*(z-H)^2A\right) \leq (z-\Lambda)(z-\lambda)\ tr\left((z-H)[A^*,A]\right).$$

In the same manner, we estimate the second trace in (2.4), obtaining

$$\begin{aligned} tr\left((z-H)A(z-H)^2A^* - (z-H)A^*(z-H)^2A\right) \\ + tr\left((z-H)B^*(z-H)^2B - (z-H)B(z-H)^2B^*\right) \\ \leq (z-\Lambda)(z-\lambda)\ tr\left((z-H)[A^*,A] + (z-H)[B,B^*]\right). \end{aligned}$$

Comparing the coefficients of z^2 in Corollary 2.3, we see that

$$tr\left((G^*[H,G]+G[H,G^*])P\right) = tr\ \left((z-H)[A^*,A] + (z-H)[B,B^*]\right),$$

which proves the theorem. □

If we take $P = P_{H<z}$, the spectral projector onto the spectrum below z, then we can rewrite (2.8) as follows:

$$\begin{aligned} tr\left((z-H)_+^2(G^*[H,G]+G[H,G^*])\right) \\ + tr\left((z-H)_+([H,G^*][H,G]+[H,G][H,G^*])\right) \leq 0, \end{aligned} \tag{2.9}$$

where $(z-H)_+ := (z-H)P_{H<z}$. We extend this inequality to the class of trace-controllable functions f of [14]: Let f be a C^3 function such that $f(0) = f'(0) = f''(0) = 0$ and $f'''(t) \geq 0$ for $t \geq 0$. From the identity

$$f(z-\lambda) = \frac{1}{2}\int_0^\infty (z-\lambda-t)_+^2 f'''(t)\ dt \tag{2.10}$$

we deduce the following inequality.

Theorem 2.6. *Let G, H satisfy the assumptions of Theorem 2.2 and let f be as above. Then*

$$tr\left(f((z-H)_+)(G^*[H,G]+G[H,G^*])\right) + \frac{1}{2}tr\left(f'((z-H)_+)([H,G^*][H,G]+[H,G][H,G^*])\right) \leq 0. \tag{2.11}$$

3. On the eigenvalues of periodic Schrödinger operators

In this section we suppose that H is of the form

$$H = -\Delta + V(\mathbf{x}) \tag{3.1}$$

and is defined as a self-adjoint operator on $L^2(\Omega)$, where $\Omega \subset \mathbb{R}^d$ is a bounded domain and the boundary conditions are such that the multiplication operator $G = \exp(-i\mathbf{q}\cdot\mathbf{x})$ satisfies the domain-mapping conditions of Theorem 2.1. This situation arises in the Floquet decomposition of H when $V(\mathbf{x})$ is a real, periodic, bounded measurable function [22, 26, 27, 31], where Ω is a fundamental domain of periodicity and $\mathbf{q}$ is a vector of the reciprocal lattice. It also covers the case of the Dirichlet Laplacian, with the same G, the vector $\mathbf{q}$ being arbitrary. Commutators with $\exp(-i\mathbf{q})$ are at the heart of the "Bethe sum rule" of quantum mechanics [2] and have appeared in some other analyses of the distribution of eigenvalues in [16, 23, 25, 30], although the specific consequences for universal bounds for eigenvalues of periodic operators have not, to our knowledge, been explored before.

In Section 5 we shall introduce a semiclassical parameter α proportional to the square of Planck's constant and study

$$H_\alpha = -\alpha\Delta + V(\mathbf{x}). \tag{3.2}$$

Although it is always possible to reset $\alpha > 0$ to 1 by a change of scale, we introduce H_α in order to study the semiclassical limit $\alpha \to 0$. A further possible extension would be to introduce a magnetic field through the systematic replacement of ∇ by $\nabla + i\mathbf{A}(\mathbf{x})$; this entails only minor changes, because in the key identities the magnetic vector potential $\mathbf{A}(\mathbf{x})$ occurs only in commutators that vanish. In the interest of clarity we leave this generalization as an exercise for the interested reader.

The commutators appearing in Theorem 2.1 are easily calculated:

$$[H,G] = \exp(-i\mathbf{q}\cdot\mathbf{x})\left(|\mathbf{q}|^2 + 2i\mathbf{q}\cdot\nabla\right) \tag{3.3}$$

and

$$[G^*,[H,G]] = [G,[H,G^*]] = 2|\mathbf{q}|^2. \tag{3.4}$$

With these facts in hand, Theorem 2.1 reads

$$\begin{aligned} &2|\mathbf{q}|^2 \sum_{\lambda_j\in J}(z-\lambda_j)^2 - \sum_{\lambda_j\in J}(z-\lambda_j)\left(2|\mathbf{q}|^4 + 8\|\mathbf{q}\cdot\nabla\phi_j\|^2\right) \\ &\quad = \sum_{\lambda_j\in J}\sum_{\lambda_k\notin J}(z-\lambda_j)(z-\lambda_k)(\lambda_k-\lambda_j)\left(|\langle G\phi_j,\phi_k\rangle|^2 + |\langle G^*\phi_j,\phi_k\rangle|^2\right) \end{aligned}$$

or

$$\begin{aligned} |\mathbf{q}|^2 \sum_{\lambda_j\in J}(z-\lambda_j)^2 - \sum_{\lambda_j\in J}(z-\lambda_j)\left(|\mathbf{q}|^4 + 4\|\mathbf{q}\cdot\nabla\phi_j\|^2\right) \\ = \sum_{\lambda_j\in J}\sum_{\lambda_k\notin J}(z-\lambda_j)(z-\lambda_k)(\lambda_k-\lambda_j)w_{jk\mathbf{q}}, \end{aligned} \tag{3.5}$$

where $w_{kj\mathbf{q}} := \frac{1}{2}\left(|\langle \exp(-i\mathbf{q}\cdot\mathbf{x})\phi_j, \phi_k\rangle|^2 + |\langle \exp(i\mathbf{q}\cdot\mathbf{x})\phi_j, \phi_k\rangle|^2\right)$. Here we collect some properties of $w_{kj\mathbf{q}}$ and associated "sum rules" for the eigenvalues:

Proposition 3.1. *The quantities $w_{kj\mathbf{q}}$ compose an infinite doubly stochastic matrix, i.e.,*

a) $$\textstyle\sum_k w_{kj\mathbf{q}} = \sum_j w_{kj\mathbf{q}} = 1,$$

with the symmetries

b) $$0 \le w_{kj\mathbf{q}} = w_{jk\mathbf{q}} \text{ and}$$

c) $$w_{kj-\mathbf{q}} = w_{kj\mathbf{q}}.$$

Moreover,

$$\sum_k (\lambda_k - \lambda_j) w_{kj\mathbf{q}} = |\mathbf{q}|^2, \tag{3.6}$$

and in particular, for each j,

$$\lambda_j = \sum_k \lambda_k w_{kj\mathbf{q}} - |\mathbf{q}|^2; \tag{3.7}$$

$$\sum_k (\lambda_k - \lambda_j)^2 w_{kj\mathbf{q}} = |\mathbf{q}|^4 + 4\|\mathbf{q}\cdot\nabla\phi_j\|^2. \tag{3.8}$$

Proof. Properties a)-c) are immediate from the definition of $w_{kj\mathbf{q}}$ and the completeness relation of the eigenfunctions.

Choosing $J = \{\lambda_j\}$, Identity (3.6) results from taking the second derivative of (3.5) with respect to z. Formula (3.7) is just a reformulation of (3.6). For (3.8), set $z = \lambda_k$, multiply (3.5) by $w_{kj\mathbf{q}}$, and then sum on k. □

In the spirit of [13, 11], we next exploit (3.5) to obtain control over eigenvalues and their means. For $J = \{\lambda_j\}$, we find

$$(z-\lambda_j)^2 - |\mathbf{q}|^2(z-\lambda_j) - 4(z-\lambda_j)T_{\mathbf{q}j} = H_{\mathbf{q}j},$$

where

$$T_{\mathbf{q}j} := \frac{\|\mathbf{q}\cdot\nabla\phi_j\|^2}{|\mathbf{q}|^2} \quad \text{and} \quad H_{\mathbf{q}j} := \sum_k (z-\lambda_i)(z-\lambda_k)(\lambda_k-\lambda_j)\frac{w_{kj\mathbf{q}}}{|\mathbf{q}|^2}.$$

For $J = \{\lambda_1, \dots, \lambda_N\}$, we sum in j, defining

$$\overline{\lambda_N} := \frac{1}{N}\sum_{j\le N}\lambda_j$$

and

$$\overline{\lambda_N^2} := \frac{1}{N}\sum_{j\le N}\lambda_j^2$$

to write (3.5) as

$$\begin{aligned}\sum_{j=1}^N (z-\lambda_j)^2 &= N(z^2 - 2\overline{\lambda_N}\,z + \overline{\lambda_N^2}) \\ &= |\mathbf{q}|^2\sum_{j=1}^N (z-\lambda_j) + 4\sum_{j=1}^N (z-\lambda_j)T_{\mathbf{q}j} + H,\end{aligned} \tag{3.9}$$

where

$$H := \sum_{j=1}^{N} \sum_{k=N+1}^{\infty} (z-\lambda_j)(z-\lambda_k)(\lambda_k-\lambda_j)\frac{w_{kj\mathbf{q}}}{|\mathbf{q}|^2} \leq 0$$

for $z \in [\lambda_N, \lambda_{N+1}]$. (The contribution to the sum for $k \leq N$ has dropped out by symmetry.)

Next we wish to let $\mathbf{q}$ range over the dual lattice and average; in order to concentrate on the most straightforward cases, we henceforth make two simplifying assumptions:

1. The fundamental domain of periodicity K of $V(\mathbf{x})$ is rectangular, with sides of length $2\pi/q_\ell$.
2. Periodic boundary conditions are imposed on functions in $L^2(K)$. This incidentally allows us to choose the eigenfunctions $\{\phi_j\}$ to be real-valued, with consequent simplifications for expressions such as $w_{kj\mathbf{q}}$.

(If one considers the problem of a general Floquet multiplier for a periodic problem with a fundamental cell that is not rectangular, then there are some complications of detail, but the results remain similar to the ones presented here.) With the simplifying assumptions, the basis of the dual lattice can be taken as consisting of multiples of the Cartesian basis, and in (3.5) we may set $\mathbf{q} = q_\ell \hat{e}_\ell$, $\ell = 1, \ldots, d$. With this choice $T_{\mathbf{q}j} = \|\frac{\partial \phi_j}{\partial x_\ell}\|^2$, and

$$\sum_{\ell=1}^{d} T_{\mathbf{q}j} = \|\nabla \phi_j\|^2 = \lambda_j - \langle \phi_j, V\phi_j \rangle =: \lambda_j - V_j =: T_j. \tag{3.10}$$

Let $g := \frac{1}{d}\sum_{\ell=1}^{d} q_\ell^2$, and define the "Riesz means"

$$R_\sigma(z) := \sum_j (z-\lambda_j)_+^\sigma.$$

Then (3.9) can be summed on ℓ, so that

$$R_2(z) \leq gR_1(z) + \frac{4}{d}\sum_j (z-\lambda_j)T_j. \tag{3.11}$$

(In the case of periodicity with respect to basis vectors $\{\mathbf{q}_\ell\}$ that are not orthogonal, the factor T_j may be replaced by CT_j for a constant $C \geq 1$ determined by the geometry of the set $\{\mathbf{q}_\ell\}$.) Because of (3.10), this inequality is equivalent to the statement that a certain quadratic polynomial, *viz.*,

$$z^2 - \left(\left(2+\frac{4}{d}\right)\overline{\lambda_N} + g - \frac{4}{d}\overline{V_N}\right)z + \left(1+\frac{4}{d}\right)\overline{\lambda_N^2} + g\overline{\lambda_N} - \frac{4}{d}\overline{\lambda V_N} \leq 0 \tag{3.12}$$

for all $z \in [\lambda_N, \lambda_{N+1}]$. Here, in keeping with the notation for the averages of eigenvalues and their squares, $\overline{V_N} := \frac{1}{N}\sum_{j\leq N} V_j$ and $\overline{\lambda V_N} := \frac{1}{N}\sum_{j\leq N}\lambda_j V_j$. Letting $z = \lambda_{N+1}$, we obtain a universal inequality on λ_{N+1} to be compared with a similar result for the Dirichlet Laplacian in [35]; cf. also Proposition 6 of [13]:

$$\lambda_{N+1} \leq \left(1+\frac{2}{d}\right)\overline{\lambda_N} + \frac{g-\overline{V_N}}{2} + \sqrt{\mathfrak{D}_N}, \tag{3.13}$$

where $\mathfrak{D}_N$, defined as the discriminant of the quadratic polynomial in (3.12), is guaranteed to be ≥ 0.

For the problem of Schrödinger operators on bounded domains with Dirichlet conditions we may let $g \to 0$, and if moreover $V = 0$, then (3.11) reduces to the inequality of Yang for the Dirichlet Laplacian [35, 13, 1].

4. Universal monotonicity of Riesz means for periodic Schrödinger operators and Schrödinger operators on manifolds of bounded mean curvature

Inequality (3.11) is identical in form to a bound that applies for a suitable value of g to Schrödinger operators on immersed manifolds of dimension d, according to Corollary 4.3 of [10], which was proved there with a different commutator argument. (In [10] refer to (1.10) and (4.2) to elucidate the notation, and note that the n's in the denominators in Corollary 4.3 are incorrect and should be deleted.) The inequality of [10] can be proved equally well with the methods of this article, as will be shown in Section 6. It is therefore possible to derive monotonicity properties and eigenvalue bounds simultaneously for these two categories of Schrödinger operators. In the earlier article, the additional term comes from the mean curvature of an immersed hypersurface and thus reflects the way in which the manifold can be immersed in Euclidean space. The periodic problem could be similarly regarded as being about a Schrödinger operator on a flat torus, but if instead of making arguments based on the fundamental domain, one embedded the torus in $\mathbb{R}^{d+1}$, then one would gain an additional term in the trace inequality from the associated mean curvature rather than from the basis of the dual lattice and would effectively convert the situation of Section 3 into that of [10]. We refer to [6] for extensions of [10] in various directions of geometric interest.

We shall refer to an operator $H = -\Delta + V(\mathbf{x})$ or $H_\alpha = -\alpha\Delta + V(\mathbf{x})$ as a *Schrödinger operator on a manifold M of bounded mean curvature* when $\Omega \subset M$ is a domain in a smooth closed manifold M immersed with finite mean curvature $h := \sum_{\ell=1}^{d} \kappa_\ell$ in $\mathbb{R}^{d+1}$, Dirichlet conditions being imposed on $\partial\Omega$ if it is nonempty, and the potential $V(\mathbf{x})$ is a real, periodic, bounded measurable function. Setting $\alpha = 1$, by Corollary 4.3 of [10] we get (3.11) with $g = \frac{\sup(h)^2}{d}$. (An independent proof of this is given below; cf. (6.8).)

As in [11], because $R_2'(z) = 2R_1(z)$, the difference inequality (3.11) for the periodic problem is equivalent to a differential inequality in the variable z:

$$\left(z + \frac{gd}{4}\right) R_2'(z) \geq \left(2 + \frac{d}{2}\right) R_2(z) + 2\sum_j (z - \lambda_j)_+ V_j. \tag{4.1}$$

Simplifying by replacing V_j by $\sup V$ and letting $\tau := gd/4 - \sup V$, we obtain the inequality

$$(z + \tau)\, R_2'(z) \geq \left(2 + \frac{d}{2}\right) R_2(z). \tag{4.2}$$

A Schrödinger operator H on a manifold of bounded mean curvature similarly satisfies (4.2) with $\tau := \frac{\sup(h)^2}{4} - \sup V$. The differential inequality (4.2) is easily solved, and we have thus proved:

Theorem 4.1. *Let $H = -\Delta + V(\mathbf{x})$ be a periodic Schrödinger operator with fundamental domain M or a Schrödinger operator on a bounded manifold M of bounded*

mean curvature and finite volume. Then the function

$$\frac{R_2(z)}{(z+\tau)^{2+d/2}},$$

with $\tau = \frac{gd}{4} - \sup V$ *or respectively* $\frac{\sup(h)^2}{4} - \sup V$*, is nondecreasing for all* z *real. Consequently,*

$$\frac{R_2(z)}{(z+\tau)^{2+d/2}} \leq L^{\mathrm{cl}}_{2,d}\mathrm{Vol}(M),$$

where $L^{cl}_{\sigma,d} = (4\pi)^{-\frac{d}{2}}\frac{\Gamma(3)}{\Gamma(3+\frac{d}{2})}$.

Corollary 4.2. *For* $k \geq j$*, the means of the eigenvalues of* H *satisfy*

$$\frac{d+2}{d}\left(\overline{\lambda_k}+\tau\right) \leq \left(\frac{k}{j}\right)^{\frac{2}{d}}\left(\frac{d+2}{d}\left(\overline{\lambda_j}+\tau\right)+\sqrt{D_j}\right), \tag{4.3}$$

where

$$D_j := \left(1+\frac{2}{d}\right)^2\left(\overline{\lambda_j}+\tau\right)^2 - \left(1+\frac{4}{d}\right)\left(\overline{\lambda_j}^2+2\overline{\lambda_j}\tau+\tau^2\right). \tag{4.4}$$

Consequently,

$$\frac{\overline{\lambda_k}+\tau}{\overline{\lambda_j}+\tau} \leq \frac{d+4}{d+2}\left(\frac{k}{j}\right)^{\frac{2}{d}}. \tag{4.5}$$

Remarks 4.3.

a) The more appealing bound (4.5) is strictly weaker than (4.3), which has the virtue of being sharp in the Weyl limit.
b) The corollary applies in particular to the Dirichlet Laplacian on a bounded domain, with $\tau = 0$. In this case it improves a recent inequality of [12] both in terms of the constant and in the range of j, k for which it is valid.
c) A similar monotonicity theorem can be proved for

$$\frac{R_\sigma(z)}{(z+\tau)^{\sigma+d/2}}$$

with $\sigma > 2$ as in [11].

Proof. It suffices to prove the corollary assuming that $\tau = 0$, as the effect on the eigenvalues of adding τ to z is equivalent to a systematic shift of τ in each eigenvalue. For any positive integer n we consider the function $P_{2,n} : [\lambda_n, \infty) \to \mathbb{R}_+$ defined by

$$P_{2,n}(z) := \sum_{j=1}^{n}(z-\lambda_j)\left(z-\left(1+\frac{4}{d}\right)\lambda_j\right). \tag{4.6}$$

From (3.13) we can see that $P_{2,n}(z) \leq 0$ for all $z \in (\lambda_n, \lambda_{n+1})$. As a consequence $P_{2,n}(z)$ has a largest zero $z_n^0 \geq \lambda_n$. Since for all $z \geq \lambda_n$,

$$R_2(z) \geq \sum_{j=1}^{n}(z-\lambda_j)^2,$$

as in [11] we conclude from (4.2) that for all $\zeta \geq z \geq \lambda_n$,

$$\zeta^{-2-\frac{d}{2}} R_2(\zeta) \geq z^{-2-\frac{d}{2}} \sum_{j=1}^{n} (z-\lambda_j)^2. \tag{4.7}$$

We want to optimize the right side of (4.7) with respect to z. Since

$$\frac{d}{dz}\, z^{-2-\frac{d}{2}} \sum_{j=1}^{n} (z-\lambda_j)^2 = -\frac{d}{2}\, P_{2,n}(z) z^{-2-\frac{d}{2}-1}, \tag{4.8}$$

an optimal choice is z_n^0, where

$$z_n^0 = \frac{d+2}{d}\overline{\lambda_n} + \sqrt{D_n} \leq \frac{d+4}{d}\overline{\lambda_n}, \tag{4.9}$$

in which D_n is the discriminant of the quadratic. (See [13] for further details.) Hence for all $\zeta \geq z_n^0$,

$$\zeta^{-2-\frac{d}{2}} R_2(\zeta) \geq (z_n^0)^{-2-\frac{d}{2}} \sum_{j=1}^{n} (z_n^0-\lambda_j)^2 = \frac{(z_n^0)^{1-2-\frac{d}{2}}}{1+\frac{d}{4}} \sum_{j=1}^{n} (z_n^0-\lambda_j).$$

Since $R_2'(\zeta) = 2R_1(\zeta)$, it follows from (4.2) that

$$R_2(\zeta) \leq \frac{\zeta}{1+\frac{d}{4}} R_1(\zeta).$$

Consequently, for all $\zeta \geq z_n^0$,

$$\zeta^{-1-\frac{d}{2}} R_1(\zeta) \geq (z_n^0)^{-1-\frac{d}{2}} \sum_{j=1}^{n} (z_n^0-\lambda_j). \tag{4.10}$$

Since $z_n^0 - \overline{\lambda_n} \geq \frac{2}{d+2} z_n^0$,

$$\zeta^{-1-\frac{d}{2}} R_1(\zeta) \geq \frac{n}{1+\frac{d}{2}}\, (z_n^0)^{-\frac{d}{2}}. \tag{4.11}$$

We note parenthetically that estimate (4.11) is asymptotically sharp since

$$\lim_{\zeta\to\infty} \zeta^{-1-\frac{d}{2}} R_1(\zeta) = \frac{|\Omega|}{1+\frac{d}{2}}\, C_d^{-\frac{d}{2}} = \lim_{n\to\infty} \frac{n}{1+\frac{d}{2}}\, (z_n^0)^{-\frac{d}{2}},$$

where C_d denotes the classical constant given by the Weyl limit,

$$C_d = \lim_{n\to\infty} \lambda_n (\frac{n}{|\Omega|})^{-\frac{2}{d}} = (2\pi)^2 \mathrm{Vol}(S^d)^- 2/d.$$

We now rewrite (4.11) as

$$R_1(\zeta) \geq \frac{n}{1+\frac{d}{2}}\, (z_n^0)^{-\frac{d}{2}} \zeta^{1+\frac{d}{2}}$$

and take the Legendre transformation on both sides, following standard calculations to be found, e.g., in [24, 11]. The result is that if w is restricted to values $\geq n$, then

$$(w-[w])\lambda_{[w]+1} + \sum_{k=1}^{[w]} \lambda_k \leq \frac{z_n^0}{(1+\frac{2}{d})n^{\frac{2}{d}}}\, w^{1+\frac{2}{d}}. \tag{4.12}$$

Hence for all $k \geq n$ (letting w approach k from below) we get

$$\frac{d+2}{d}\,\overline{\lambda_k} \leq \left(\frac{k}{n}\right)^{\frac{2}{d}} z_{2,n}^0 = \left(\frac{k}{n}\right)^{\frac{2}{d}} \left(\frac{d+2}{d}\,\overline{\lambda_n} + \sqrt{D_n}\right), \tag{4.13}$$

which proves the theorem. (The simplification (4.5) is achieved with the upper bound in (4.9).) □

5. Universal monotonicity of eigenvalue moments and sharp Lieb-Thirring inequalities for periodic Schrödinger operators and Schrödinger operators on manifolds of bounded mean curvature

We next turn our attention to the one-parameter family of operators H_α from (3.2) in order to derive inequalities of Lieb-Thirring type for periodic Schrödinger operators and for Schrödinger operators on domains of bounded mean curvature. Some inequalities of Lieb-Thirring type appear in [18, 19, 20] for Schrödinger operators on spheres after projection onto the set of functions of mean zero, and Sobolev type inequalities related to Lieb-Thirring may be found in [33]. We shall use the direct method introduced in [32] to derive an explicit form of a Lieb-Thirring inequality for eigenvalue moments of order $\sigma \geq 2$, without projection.

For the purposes of semiclassical analysis, we appeal to the Feynman-Hellman theorem to note that

$$T_j = \frac{\partial \lambda_j}{\partial \alpha} \tag{5.1}$$

(except at eigenvalue crossings; cf. [32]), and therefore, after scaling to incorporate α and introducing an integrating factor, (3.11) reads

$$\frac{\partial}{\partial \alpha}\left(\alpha^{d/2} R_2(z,\alpha)\right) \leq \frac{gd}{2}\alpha^{d/2} R_1(z,\alpha). \tag{5.2}$$

Recalling that $\partial R_2/\partial z = 2R_1$, we see that (5.2) can be regarded as a partial differential inequality. Letting $U(z,\alpha) := \alpha^{d/2} R_2(z,\alpha)$, the inequality has the form

$$\frac{\partial U}{\partial \alpha} \leq \frac{gd}{4}\frac{\partial U}{\partial z}, \tag{5.3}$$

which can be solved by changing to characteristic variables $\xi := \alpha - \frac{4}{gd}z$, $\eta := \alpha + \frac{4}{gd}z$, in terms of which

$$\frac{\partial U}{\partial \xi} \leq 0;$$

i.e., U decreases as ξ increases while η is fixed. In conclusion,

$$U(\alpha, z) \leq U\left(\alpha_s, z + \frac{gd}{4}(\alpha - \alpha_s)\right) \tag{5.4}$$

for $\alpha \geq \alpha_s$.

As $\alpha_s \to 0$, the right side of (5.4) tends to $L_{2,d}^{cl} \int \left|V(\mathbf{x}) - \left(z + \frac{gd}{4}\alpha\right)\right|_-^{2+d/2} d\mathbf{x}$. Since (see e.g. [3, 4, 17, 29] and the references therein) for all $\sigma \geq 0$,

$$\lim_{\alpha \to 0+} \alpha^{\frac{d}{2}} \sum_{E_j(\alpha) < z} (z - E_j(\alpha))^\sigma = L_{\sigma,d}^{cl} \int_M (V(\mathbf{x}) - z)_-^{\sigma + d/2}\, d\mathbf{x}, \tag{5.5}$$

with $L^{cl}_{\sigma,d}$, the *classical constant*, given by

$$L^{cl}_{\sigma,d} = (4\pi)^{-\frac{d}{2}} \frac{\Gamma(\sigma+1)}{\Gamma(\sigma+\frac{d}{2}+1)}, \tag{5.6}$$

we arrive at a sharp Lieb-Thirring inequality for R_2:

Theorem 5.1. *For all $\alpha > 0$ the mapping*

$$\alpha \mapsto \alpha^{\frac{d}{2}} R_2\left(z - \frac{\alpha g d}{4}\right) = \alpha^{\frac{d}{2}} \sum \left(z - \frac{\alpha g d}{4} - \lambda_j\right)_+^2 \tag{5.7}$$

is nonincreasing and therefore for all $z \in \mathbb{R}$ and all $\alpha > 0$ the following sharp Lieb-Thirring inequality holds:

$$R_2(z,\alpha) \le \alpha^{-d/2} L^{cl}_{2,d} \int_M \left(V(\mathbf{x}) - \left(z + \frac{gd}{4}\alpha\right)\right)_-^{2+d/2} d\mathbf{x}. \tag{5.8}$$

A similar monotonicity property can be proved for $R_\sigma(z,\alpha)$ with $\sigma > 2$ (see also [32]). Indeed:

Corollary 5.2. *For all $\alpha > 0$ the mapping*

$$\alpha \mapsto \alpha^{\frac{d}{2}} R_\sigma\left(z - \frac{\alpha g d}{4}\right) = \alpha^{\frac{d}{2}} \sum \left(z - \frac{\alpha g d}{4} - \lambda_j\right)_+^\sigma \tag{5.9}$$

is nonincreasing and therefore for all $z \in \mathbb{R}$ and all $\alpha > 0$ the following sharp Lieb-Thirring inequality holds:

$$R_\sigma(z,\alpha) \le \alpha^{-d/2} L^{cl}_{\sigma,d} \int_M \left(V(\mathbf{x}) - \left(z + \frac{gd}{4}\alpha\right)\right)_-^{\sigma+d/2} d\mathbf{x}. \tag{5.10}$$

The conclusion of Theorem 5.1 also holds in the presence of vector potentials. In particular, in the periodic case, the operator $\alpha(-i\nabla + \mathbf{k})^2 + V(\mathbf{x})$, with $\mathbf{k} \in \mathbb{R}^d$ (more precisely, $\mathbf{k}$ in the dual lattice) being a constant vector, satisfies the Lieb-Thirring inequality (5.8). Therefore, taking the average over a band, which we define by

$$\langle \lambda_j \rangle := \frac{1}{\mathrm{Vol}(M)} \int \lambda_j(\mathbf{k})\, d\mathbf{k},$$

and using the convexity of the function $\lambda \mapsto (z-\lambda)_+^\sigma$ we get the estimate

$$\sum (z - \langle \lambda_j \rangle)_+^\sigma \le \alpha^{-d/2} L^{cl}_{\sigma,d} \int_M \left(V(\mathbf{x}) - \left(z + \frac{gd}{4}\alpha\right)\right)_-^{\sigma+d/2} d\mathbf{x}. \tag{5.11}$$

6. Remarks on the commutation of self-adjoint and unitary operators

In Section 3 the operator G that was chosen to commute with the self-adjoint operator H was unitary, and it is reasonable to think that this property alone accounts for some of the simplifications that were achieved in comparison with the general trace inequalities of Section 2. In this section we choose $G = U$ as a unitary operator and explore some consequences and additional applications.

We define

$$H_U := U^*[H,U] = U^*HU - H. \tag{6.1}$$

Then $H_{U^*} = U[H, U^*]$, and we may rewrite the trace formula (2.4) as follows:

$$\begin{aligned} tr\left((z-H)^2(H_U+H_{U^*})P\right) - tr\left((z-H)(H_U^2+HUH_{U^*}^2)P\right) \\ = tr\left((z-H)A(z-H)^2A^* - (z-H)A^*(z-H)^2A\right) \\ + tr\left((z-H)B^*(z-H)^2B - (z-H)B(z-H)^2B^*\right). \end{aligned} \tag{6.2}$$

As before, if the spectrum of H consists only of eigenvalues λ_j and the corresponding eigenfunctions ϕ_j are chosen to form an orthonormal basis of the underlying Hilbert space $\mathcal{H}$, then (6.2) reads as follows:

$$\begin{aligned} \sum_{\lambda_j\in J}(z-\lambda_j)^2\left\langle (H_U+H_{U^*})\phi_j,\phi_j\right\rangle \\ - \sum_{\lambda_j\in J}(z-\lambda_j)\left(\langle H_U\phi_j, H_U\phi_j\rangle + \langle H_{U^*}\phi_j, H_{U^*}\phi_j\rangle\right) \\ = \sum_{\lambda_j\in J}\sum_{\lambda_k\notin J}(z-\lambda_j)(z-\lambda_k)(\lambda_k-\lambda_j)\left(|\langle U\phi_j,\phi_k\rangle|^2 + |\langle U^*\phi_j,\phi_k\rangle|^2\right). \end{aligned} \tag{6.3}$$

Equivalently, this may be written as

$$\begin{aligned} \sum_{\lambda_j\in J}\|(z-H)\phi_j\|^2\left\langle (2z-UHU^*-U^*HU)\phi_j,\phi_j\right\rangle \\ - \sum_{\lambda_j\in J}\left\langle (z-H)\phi_j,\phi_j\right\rangle\left(\|(z-UHU^*)\phi_j\|^2 + \|(z-U^*HU)\phi_j\|^2\right) \\ = \sum_{\lambda_j\in J}\sum_{\lambda_k\notin J}(z-\lambda_j)(z-\lambda_k)(\lambda_k-\lambda_j)\left(|\langle U\phi_j,\phi_k\rangle|^2 + |\langle U^*\phi_j,\phi_k\rangle|^2\right). \end{aligned} \tag{6.4}$$

In Section 3 we used the auxiliary unitary operator $U = e^{-i\mathbf{q}\cdot\mathbf{x}}$ to derive identities for periodic Schrödinger operators. As another illustration we turn to the case of Schrödinger operators on manifolds immersed in $\mathbb{R}^{d+1}$, which was studied by commutation with self-adjoint operators based on coordinate functions in [10, 6].

Consider a Schrödinger operator $H = -\Delta + V(\mathbf{x})$, where $-\Delta$ denotes the Laplace-Beltrami operator, on a domain Ω in a smooth, orientable, d-dimensional manifold $\mathcal{M}$ isometrically immersed in $\mathbb{R}^{d+1}$. (Higher codimensions could also be dealt with as in [6], but for simplicity we treat only the case of codimension 1.) If Ω has a boundary, Dirichlet conditions are imposed. It is assumed that the potential $V \in L^1_{\text{loc}}$, and other conditions are tacitly placed on V and Ω so that H is self-adjoint by closure of $C_c^\infty(\mathcal{M})$ with at least some discrete, finitely degenerate eigenvalues $\{\lambda_j\}$ at the bottom of the spectrum. In order to apply a trace identity we choose U as the multiplicative operator obtained by restricting $e^{-i\mathbf{q}\cdot\mathbf{x}}$ to values of $\mathbf{x} \in \mathcal{M} \subset \mathbb{R}^{d+1}$. We then calculate:

$$H_U = -2i\mathbf{q}_\parallel\cdot\nabla_\parallel - i\mathbf{q}\cdot\mathbf{h} + |\mathbf{q}_\parallel|^2. \tag{6.5}$$

Here, $\mathbf{q}_\parallel$ and $\nabla_\parallel$ are the tangential parts of $\mathbf{q}$ and the gradient, while the mean-curvature vector $\mathbf{h} = \left(\sum_\beta \kappa_\beta\right)\mathbf{n}$ is parallel to the unit normal $\mathbf{n}$. Using (6.3), the

analogue of (3.5) is

$$|\mathbf{q}_\parallel|^2 \sum_{\lambda_j\in J}(z-\lambda_j)^2 - \sum_{\lambda_j\in J}(z-\lambda_j)\left(|\mathbf{q}_\parallel|^4 + 4\|\mathbf{q}_\parallel\cdot\nabla_\parallel\phi_j\|^2 + \|\mathbf{q}\cdot\mathbf{h}\,\phi_j\|^2\right) = \sum_{\lambda_j\in J}\sum_{\lambda_k\notin J}(-\lambda_j)(z-\lambda_k)(\lambda_k-\lambda_j)w_{jk\mathbf{q}} \tag{6.6}$$

for some positive quantities $w_{jk\mathbf{q}}$ whose formal expression is identical to the ones in (3.5). To simplify this expression, one can sum as before for $\mathbf{q}$ taken from a frame of the form $\{q\,\mathbf{e}_\beta\}$, $\beta = 1,\dots,d+1$. (The same conclusion could alternatively be attained by fixing $|\mathbf{q}|$ and averaging over all directions.) The result, after a bit of calculation, is

$$\sum_{\lambda_j\in J}(z-\lambda_j)^2 - q^2\sum_{\lambda_j\in J}(z-\lambda_j) - \frac{4}{d}\sum_{\lambda_j\in J}(z-\lambda_j)\left(\left\langle\phi_j,\left(-\Delta+\frac{h^2}{4}\right)\phi_j\right\rangle\right) = \sum_{\lambda_j\in J}\sum_{\lambda_k\notin J}(z-\lambda_j)(z-\lambda_k)(\lambda_k-\lambda_j)\frac{\mathrm{Ave}_{\mathbf{q}}\,(w_{jk\mathbf{q}})}{q^2 d}. \tag{6.7}$$

In this identity it was convenient to assume a purely discrete spectrum, although in fact only J needs to be a discrete set if the sum over J^c is replaced by the appropriate spectral integral.

The situation of greatest interest occurs when $J = \{\lambda_1,\dots,\lambda_n\} < \inf J^c$, in which case the term on the right is nonpositive, and we may let $q\to 0$, yielding

$$R_2(z) \le \frac{4}{d}\sum_{\lambda_j\in J}(z-\lambda_j)\left(\left\langle\phi_j,\left(-\Delta+\frac{h^2}{4}\right)\phi_j\right\rangle\right) \tag{6.8}$$

for all z, or, in the case where the spectrum is not purely discrete, $z\le\inf\sigma_{\mathrm{ess}}$. As remarked in Section 4, this implies Inequality (4.1) and thereby Theorem 4.1, again in the case of a purely discrete spectrum. We observe that for the monotonicity part of Theorem 4.1 it is not necessary for the manifold M to be bounded or of finite volume, as long as the bottom part of the spectrum is discrete and z lies below that.

A basic question about the spectral geometry of immersed manifolds has to do with extensions of the Reilly inequality [28, 7, 8, 9, 6], whereby the eigenvalues of the Laplace-Beltrami operator are bounded from above in terms of mean curvature. The classic Reilly inequality says that the first nontrivial eigenvalue, which in our notation is λ_2, is bounded by $\frac{\|h\|_\infty^2}{d}$. In [6], Corollary 2.3, it was shown that every eigenvalue λ_N of the Laplace-Beltrami operator on closed immersed manifolds satisfies an upper bound of the form $C_R(d,N)\|h\|_\infty^2$, but unfortunately the constant $C_R(d,N)$ produced there grows exponentially with N.

For $N>1$ the Reilly bound on λ_{N+1} can be improved in a form that grows as $N^{2/d}$, the power expected from the Weyl law:

Theorem 6.1. *Let a smooth, compact, d-dimensional manifold $\mathcal{M}$, of finite volume and without boundary, be immersed in $\mathbb{R}^{d+1}$. Let $0=\lambda_1<\lambda_2\le\cdots$ denote the eigenvalues of the Laplace-Beltrami operator on $\mathcal{M}$. Then for each N,*

$$\lambda_{N+1} \le \left(\frac{(d+4)^2}{d(d+2)}N^{2/d} - \frac{4}{d}\right)\frac{\|h\|_\infty^2}{d}. \tag{6.9}$$

Proof. We start with (3.12) as adapted to this situation, *viz.*,

$$z^2 - \left(\left(2+\frac{4}{d}\right)\overline{\lambda_N} + \tau\right) z + \left(1+\frac{4}{d}\right)\overline{\lambda_N^2} + \tau\overline{\lambda_N} \le 0, \tag{6.10}$$

where $\tau = \frac{\|h\|_\infty^2}{d}$ and $z \in (\lambda_k, \lambda_{k+1}]$, and the corresponding specialization of the upper bound (3.13). In a standard fashion we use Cauchy-Schwarz to replace $\overline{\lambda_k^2} \ge \overline{\lambda_k}^2$ and weaken (3.13) to

$$\lambda_{N+1} \le \left(1+\frac{4}{d}\right)\overline{\lambda_N} + \tau. \tag{6.11}$$

As was already noted in [6], the case $N = 1$ reproduces the classic Reilly inequality. In order to bound higher eigenvalues, we now combine (6.11) with (4.5), choosing $k = N$ and $j = 1$. Recalling that $\lambda_1 = 0$,

$$\overline{\lambda_N} \le \left(\frac{d+4}{d+2} N^{\frac{2}{d}} - 1\right)\tau. \tag{6.12}$$

When this is substituted into (6.11), we obtain (6.9). □

As a final application of commutation with unitaries, consider the integral operator H defined on $L^2(\mathbb{R}^d)$ by

$$(Hf)(p) = T(p)f(p) + \int_{\mathbb{R}^d} V(p-p')f(p')\,dp', \tag{6.13}$$

and let U be the translation operator $(Uf)(p) = f(p-k)$ for some $k \in \mathbb{R}^d$. This is in a sense dual to the situation given above, as the unitary operator of multiplication by $e^{-i\mathbf{q}\cdot\mathbf{x}}$ corresponds to translation in the momenta by $\mathbf{q}$. Then

$$(H_U f)(p) = (T(p+k) - T(p))f(p).$$

For simplicity we assume that the spectrum of H consists only of eigenvalues. Applying the trace formula (6.4) we get

$$\begin{aligned} &\sum_{\lambda_j \in J} (z-\lambda_j)^2 \int_{\mathbb{R}^d} \big(T(p+k) + T(p-k) - 2T(p)\big)|\phi_j(p)|^2\,dp \\ &\quad - \sum_{\lambda_j \in J} (z-\lambda_j) \int_{\mathbb{R}^d} \big((T(p+k)-T(p))^2 + (T(p-k)-T(p))^2\big)|\phi_j(p)|^2\,dp \\ &\quad = \sum_{\lambda_j \in J} \sum_{\lambda_k \notin J} (z-\lambda_j)(z-\lambda_k)(\lambda_k - \lambda_j) \\ &\qquad \times \left(\left|\int_{\mathbb{R}^d} \phi_j(p-k)\phi_k^*(p)\,dp\right|^2 + \left|\int_{\mathbb{R}^d} \phi_j(p+k)\phi_k^*(p)\,dp\right|^2\right). \end{aligned} \tag{6.14}$$

One possibility to exploit this identity is to do a Taylor expansion about $k = 0$. We obtain the corresponding trace formula for a self adjoint operator G with G being the generator of the unitary group of translations in momentum space. Indeed, for C^2 functions $T(p)$ we have

$$T(p+k) + T(p-k) - 2T(p) = k(D^{(2)}T)(p)k + O(|k|^3)$$

and

$$(T(p+k)-T(p))^2 + (T(p-k)-T(p))^2 = 2\big(\nabla T(p)k\big)^2 + O(|k|^3),$$

and therefore, after division by $|k|^2$,

$$\begin{aligned}(6.15)\qquad &\sum_{\lambda_j\in J}(z-\lambda_j)^2\int_{\mathbb{R}^d}k^T(D^{(2)}T)(p)k|\phi_j(p)|^2\,dp\\ &\quad-2(z-\lambda_j)\int_{\mathbb{R}^d}\big((\nabla T(p))k\big)^2|\phi_j(p)|^2\,dp\\ &\qquad=2\sum_{\lambda_j\in J}\sum_{\lambda_k\notin J}(z-\lambda_j)(z-\lambda_k)(\lambda_k-\lambda_j)\left|\int_{\mathbb{R}^d}\phi_k^*(p)\nabla\phi_j(p)\,dp\right|^2.\end{aligned}$$

If $T(p)=\alpha p^2$, then

$$T(p+k)+T(p-k)-2T(p)=2\alpha k^2,$$

and

$$(T(p+k)-T(p))^2+(T(p-k)-T(p))^2=8\alpha^2(pk)^2+2\alpha^2k^4.$$

If $T(p)=\sqrt{p^2+m^2}-m$, then $T(p)^2=p^2-2mT(p)$, and

$$T(p+k)+T(p-k)-2T(p)=\frac{m^2k^2+p^2k^2-(kp)^2}{\sqrt{p^2+m^2}^3}+O(|k|^3)$$

and

$$(T(p+k)-T(p))^2+(T(p-k)-T(p))^2=\frac{2(pk)^2}{p^2+m^2}+O(|k|^3).$$

For related work on this relativistic kinetic energy operator we refer to [15].

7. Examples

The study of the distribution of positive quadratic forms on vectors of integers is sometimes referred to as the geometry of numbers (e.g., [31]). The values of any such quadratic form compose the spectrum of the Laplacian on a certain flat torus, the dimensions of which determine the coefficients of the quadratic form, or conversely. Therefore the inequalities of the preceding section have direct implications for the geometry of numbers. We begin this section by presenting those.

We note that $\sum_{\alpha=1}^d T_{\hat{\mathbf{e}}_\alpha j}=2d+8\|\nabla\phi_j\|^2=2d+8T_j$. In the case of the Laplacian, $T_j=\lambda_j$ and $\lambda_j=4\pi^2\sum_{\alpha=1}^d n_{\alpha j}^2$. Exploiting the abstract gap formula of Theorem 2.7, after some simplification we find the following inequality:

$$(7.1)\qquad P_{2,N}(z):=\sum_{j=1}^N(z-\lambda_j)\left(z-\frac{d+4}{d}\lambda_j-g\right)\le N(z-\lambda_N)(z-\lambda_{N+1})$$

for all $z\in[\lambda_N,\lambda_{N+1}]$. We recall that $g:=\frac{1}{d}\sum_{\alpha=1}^d q_\alpha^2$.

Analyzing the foregoing inequality following [13], we get

$$\left(\frac{\lambda_{N+1}-\lambda_N}{2}\right)^2\le D_N:=\left(\frac{d+2}{d}\overline{\lambda_N}+\frac{g}{2}\right)^2-\frac{d+4}{d}\overline{\lambda_N^2}-g\overline{\lambda_N}$$

and

$$\frac{d+2}{d}\overline{\lambda_N}+\frac{g}{2}-\sqrt{D_N}\le\lambda_N\le\lambda_{N+1}\le\frac{d+2}{d}\overline{\lambda_N}+\frac{g}{2}+\sqrt{D_N}.$$

As a first illustration we consider the case $d=1$. Obviously, we want to choose g as small as possible and the best choice is the first nontrivial eigenvalue of the periodic Laplacian, i.e. $g=4\pi^2$. Let n be a natural number and set $N:=2n+1$.

Then $\lambda_N = n^2$ and $\lambda_{N+1} = (n+1)^2$, which means that there is a gap. We easily verify that in this case,

$$D_N = \left(\frac{\lambda_{N+1} - \lambda_N}{2}\right)^2 = \pi^2 N^2.$$

Consequently, the quadratic polynomials (in z) on the right and left sides of (7.1) coincide for these values of N. Since (see also (4.8))

$$\frac{d}{dz}\,(z+\pi^2)^{-2-\frac{1}{2}} \sum_{j=1}^{N} (z-\lambda_j)^2 = -\frac{1}{2}\,\sum_{j=1}^{N} (z-\lambda_j)(z-5\lambda_j-4\pi^2)(z+\pi^2)^{-3-\frac{1}{2}},$$

we conclude that the nondecreasing function

$$z \mapsto (z+\pi^2)^{-2-\frac{1}{2}} R_2(z)$$

has critical points at the eigenvalues λ_j. Therefore the positive shift $gd/4 = \pi^2$ in z cannot be replaced by any smaller shift without losing the monotonicity property.

Next consider the two-dimensional Laplacian with periodic boundary conditions on the square $Q = [0, 2\pi] \times [0, 2\pi]$. Its eigenvalues are $m^2 + n^2$, $m, n \in \mathbb{Z}$ with corresponding eigenfunctions $\phi_{m,n}(x) = (2\pi)^{-1} \exp(imx + iny)$. The counting function $N = N(x)$ counts the number of lattice points inside the disc D_x of radius $\sqrt{x}$ centered at the origin, a sharp estimate of which is known in the literature on lattice points as the *Gauss circle problem* (see e.g. [21]). Here we only consider the bounds obtained from Theorem 4.1 and the general inequality (7.1), respectively. We follow [21], where, in place of $N(x)$ the common notation is

$$R(x) := \#\{(m,n) \in \mathbb{Z} \times \mathbb{Z} : m^2 + n^2 \le x\},$$

which counts the lattice points inside the disk D_x of radius x centered at the origin. Since

$$\sum_{m^2+n^2 \le x} f(m^2+n^2) = R(x)f(x) - \int_0^x f'(t)R(t)\,dt,$$

it follows that

$$R_2(x) = 2\int_0^x (x-t)R(t)\,dt.$$

The bound of Theorem 4.1 reads as follows:

$$R_2(x) \le \frac{\pi}{3}\left(x + \frac{1}{2}\right)^3.$$

Defining, as in [21], the fluctuation about the Weyl asymptotics by

$$R_2(x) - \frac{\pi}{3}x^3 = 2\Delta_2(x),$$

we find that

$$\Delta_2(x) \le \frac{\pi}{48}(12x^2 + 6x + 1),$$

which has to be compared with the standard asymptotic estimate [21]

$$\frac{|\Delta_2(x)|}{x^{\frac{5}{4}}} \le C$$

for some positive constant C. Our estimate is only one-sided and too crude for large x.

Finally, we test the sharpness of our Lieb-Thirring inequalities for periodic Schrödinger operators. Consider the case of $H(\alpha) = -\alpha\Delta - \gamma$ on $[0, 2\pi]$ with periodic boundary conditions, where γ is some positive constant. Its eigenvalues are $\lambda_j = \alpha j^2 - \gamma$ with $j \in \mathbb{Z}$. By Theorem 5.1, the function

$$\alpha \mapsto \sqrt{\alpha} \sum \left(z - \frac{\alpha}{4} - \lambda_j\right)_+^2$$

is nondecreasing and therefore by (5.8) the following Lieb-Thirring inequality holds:

$$\sqrt{\alpha} \sum (z - \alpha j^2 + \gamma)_+^2 \leq \frac{16}{15} \left(-\gamma - \frac{\alpha}{4} - z\right)_-^{\frac{5}{2}}.$$

In particular, taking $z = 0$ we have

$$\sum \left(\frac{\gamma}{\alpha} - j^2\right)_+^2 \leq \frac{16}{15} \left(\frac{\gamma}{\alpha} + \frac{1}{4}\right)^{\frac{5}{2}}.$$

As in our first example we see that the shift $\alpha/4$ in z cannot be replaced by any smaller shift without losing the monotonicity property (choose $\gamma/\alpha = m^2$ for an integer m). The presence of the shift is due to the zero eigenvalue. Indeed, if $\gamma/\alpha < 1$ we have

$$\left(\frac{\gamma}{\alpha}\right)^2 \leq \frac{16}{15} \left(\frac{\gamma}{\alpha} + \frac{1}{4}\right)^{\frac{5}{2}}$$

and without a shift this inequality clearly cannot be true.

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