COMMUTATORS, EIGENVALUE GAPS, AND MEAN CURVATURE IN THE THEORY OF SCHRÖDINGER OPERATORS

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Abstract

Commutator relations are used to investigate the spectra of Schrödinger Hamiltonians, $H = -\Delta + V(x)$, acting on functions of a smooth, compact d-dimensional manifold M immersed in $\mathbb{R}^\nu, \nu \geq d+1$. Here Δ denotes the Laplace-Beltrami operator, and the real-valued potential–energy function $V(x)$ acts by multiplication. The manifold M may be complete or it may have a boundary, in which case Dirichlet boundary conditions are imposed.

It is found that the mean curvature of a manifold poses tight constraints on the spectrum of H. Further, a special algebraic rôle is found to be played by a Schrödinger operator with potential proportional to the square of the mean curvature:

$$H_g := -\Delta + gh^2,$$

where $\nu = d+1$, g is a real parameter, and

$$h := \sum_{j=1}^{d} \kappa_j,$$

with $\{\kappa_j\}$, $j = 1, \ldots, d$ denoting the principal curvatures of M. For instance, by Theorem 3.1 and Corollary 4.4, each eigenvalue gap of an arbitrary Schrödinger operator is bounded above by an expression using $H_{1/4}$. The "isoperimetric" parts of these theorems state that these bounds are sharp for the fundamental eigenvalue gap and for infinitely many other eigenvalue gaps.

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1 Introduction

Eigenvalue gaps for Laplacians and Schrödinger Hamiltonians,

$$H = -\Delta + V(x),$$

especially the fundamental gap,

$$\Gamma := \lambda_2 - \lambda_1,$$

are connected to the analytic and geometric details of H in many familiar ways, yet the most elementary connections between eigenvalue gaps and operators are algebraic, through calculations of commutators. Commutators and their relation to eigenvalue gaps and inverse spectral problems have been studied in [1, 2, 12, 15, 16, 17, 19], which partly inspired this work. Here H will be defined on a hypersurface, and commutators will be used to connect eigenvalue gaps and certain other functions defined on the spectrum $\sigma(H)$ to the mean curvature of the manifold M, which is found to pose tight constraints on the spectrum.

Furthermore, Schrödinger operators of specific kinds depending explicitly on curvature,

$$-\nabla^2 + q(\kappa), \tag{1.1}$$

defined on a d-dimensional submanifold $\mathbb{R}^\nu$ having principal curvatures $\kappa := \{\kappa_j\}$, $j = 1, \ldots, d$, arise in the mathematics of nanophysics and thin structures. Coincidentally, simplifications are achieved when the potential energy is of this form. Low-lying eigenvalues, $\lambda_1 < \lambda_2 \leq \cdots$, of (1.1) have been studied, and sharp estimates have been discovered relating to the geometry of M in [10, 6, 8, 13, 14, 11]. For certain operators of the type (1.1) with quadratic functions q, the estimates of the gap Γ in this article will likewise be sharp.

Section 2 will be devoted to the fundamental eigenvalue gap in the one–dimensional situation, where M is a space curve. In Section 3, a similar analysis will be carried out when $d > 1$, while in Section 4 an alternative algebraic approach is used to extend these results to all eigenvalue gaps. The results of each section are both generalized and largely subsumed by the later sections, but as alternative, simpler methods are available for the simpler situations, it is felt useful to present multiple points of view.

Notation

$\langle f, g\rangle$ denotes the standard inner product on $L^2(M)$.

$[A, B] := AB - BA$ denotes the commutator of operators A and B

$\mathbf{t}, \mathbf{n}$, and $\mathbf{b}$ are the moving trihedron of unit vectors for a space curve in $\mathbb{R}^3$. The corresponding curvature and torsion are κ and τ.

When the dimension $d \geq 2$, M will denote a compact, smooth, connected manifold of dimension d immersed in $\mathbb{R}^{d+1}$, with principal curvatures $\{\kappa_j\}$, $j = 1, \ldots, d$. The corresponding normalized eigenvectors of the shape operator will be denoted $\mathbf{t}_j$, and $h := \sum_{j=1}^{d} \kappa_j$.

The notation u_k, λ_k, $k = 1, \ldots,$ will be used for the normalized eigenfunctions and associated eigenvalues, in increasing order, of H, an operator on a Hilbert space $\mathcal{H}$. When H is a Schrödinger Hamiltonian, it will be assumed without loss of generality that $\{u_k\}$ are real-valued, and that u_1 is nonnegative.

Eigenvalue gaps are connected with commutators at a rather general level. Assume for now only that H and G are symmetric operators on a Hilbert space, that $\sigma(H)$ contains discrete eigenvalues, and that certain products of operators are well-defined. (Assumptions are spelled out below in Lemma 1.1.) The most basic relationship of this kind is the elementary commutator gap formula,

$$\langle u_j, [H, G] u_k \rangle = (\lambda_j - \lambda_k) \langle u_j, G u_k \rangle . \tag{1.2}$$

It turns out that not only the $[H, G]$ but also higher-order commutators such as $[G, [H, G]]$ are related to eigenvalue gaps for second-order differential operators. The basis for that analysis can be recapitulated as follows.

For the first commutator of H with G, since $[H, G] u_k = (H - \lambda_k) G u_k$, it follows that

$$\| [H, G] u_k \|^2 = \left\langle G u_k, (H - \lambda_k)^2 G u_k \right\rangle , \tag{1.3}$$

and more generally

$$\langle [H, G] u_j, [H, G] u_k \rangle = \langle G u_j, (H - \lambda_j) (H - \lambda_k) G u_k \rangle . \tag{1.4}$$

For the second commutator, a similar short calculation shows that, formally,

$$\langle u_j \mid [G, [H, G]] \, u_k \rangle = \langle G u_j \mid (2H - \lambda_j - \lambda_k) \, G u_k \rangle . \tag{1.5}$$

In particular,

$$\langle u_j \mid [G, [H, G]] \, u_j \rangle = 2 \langle G u_j \mid (H - \lambda_j) \, G u_j \rangle . \tag{1.6}$$

Lemma 1.1 *Let H be a positive self-adjoint operator with discrete eigenvalues λ_1 and λ_2. Let P denote the orthogonal projection onto u_1, and suppose G is a self-adjoint operator such that the products GP, G^2P, HG^2P, H^2GP, and $GHGP$ are defined. Then the fundamental gap $\Gamma := \Gamma(H)$ satisfies*

$$\Gamma \langle u_1, [G, [H, G]]\, u_1 \rangle \leq 2\|[H, G]u_1\|^2. \tag{1.7}$$

Remark This is actually a special case of Theorem 2.1 of [15]. A simplified proof is presented here for convenience.

Proof. The assumptions on the products justify formulae (1.3)–(1.6). With $k = j = 1$, the inequality is thus equivalent to

$$\langle Gu_1 \mid (H - \lambda_1)\,(\lambda_2 - \lambda_1)\, Gu_1 \rangle \leq \left\langle Gu_1 \mid (H - \lambda_1)^2 Gu_1 \right\rangle,$$

which follows from the spectral functional calculus (e.g., see [7, 9, 21]), since for $\mu \in \sigma(H)$, $(\mu - \lambda_1))\,(\lambda_2 - \lambda_1)) \leq (\mu - \lambda_1))^2$. q.e.d.

Whereas identities (1.3)–(1.6) and Lemma 1.1 are general facts about operator algebra, if H is a differential operator, then its commutators satisfy further algebraic relations. For instance, if $H = -\Delta$ is a Laplace operator on a Euclidean set Ω, then with the choice $G = x_k$:

$$\sum_{k=1}^{\nu} [H, x_k]^* \,[H, x_k] = 4H, \tag{1.8}$$

and

$$[x_k, [H, x_k]] = 2, \tag{1.9}$$

which is a version of *canonical commutation.* These identities are fundamental for the subject of universal bounds on eigenvalues (for which see [5]).

It is argued in Sections 2 and 3 that from an algebraic point of view, the operator on a closed manifold most closely analogous to the flat Laplacian is not the Laplace-Beltrami operator, but rather

$$H_g := -\Delta + gh^2 \tag{1.10}$$

with the specific value $g = \frac{1}{4}$.

2 Upper bounds on the fundamental gap when M is a curve

In this section, suppose that M is a smooth plane or space curve of finite length. If s denotes the arc length, then Schrödinger operators have the form

$$H = -\frac{d^2}{ds^2} + V(s). \tag{2.1}$$

Assuming V is bounded and measurable, H is a self-adjoint operator defined using the Friedrichs extension from $C_c^\infty(M)$. The form domain is thereby $W_0^1(M)$, which for a closed curve coincides with $W^1(M)$; otherwise Dirichlet boundary conditions apply at the end points. (For standard technical facts about the domains of definition of Sturm-Liouville operators the reader is referred to [21, 23].)

Let $G = X_m$, the restriction to M of a Euclidean coordinate x_m in the ambient flat space, and calculate the first and second commutators with H, recalling the classical Serret-Frenet equations:

$$[H, X_m] = -\frac{d^2 X_m}{ds^2} - 2\,\frac{dX_m}{ds}\frac{d}{ds} = -\kappa n_m - 2t_m \frac{d}{ds}, \tag{2.2}$$

and

$$[X_m\,[H, X_m]] = 2t_m^2. \tag{2.3}$$

There follows:

Proposition 2.1 *Let M be a smooth curve in $\mathbb{R}^\nu, \nu = 2$ or 3. Then for H as in* (2.1) *and $\varphi \in W_0^1(M)$,*

$$\sum_{m=1}^{\nu} \|[H, X_m]\,\varphi\|^2 = 4\int_M \left(\left|\frac{d\varphi}{ds}\right|^2 + \frac{\kappa^2}{4}\,|\varphi|^2\right) ds. \tag{2.4}$$

Remark The assumptions on the curve can be relaxed, providing that the curvature and unit normal vector exist a.e. and are square-integrable. Likewise, potentials can be allowed to have certain singularities, as long as the domain of self-adjointness remains the same. (For conditions guaranteeing this, see [9, 22, 23].)

Proof. By closure it may be assumed that $\varphi \in C_c^\infty(M)$. Apply (2.2) to φ and square the result, to obtain

$$4\left(t_m^2\left(\frac{d\varphi}{ds}\right)^2 + \frac{1}{4}\,\kappa^2 n_m^2 \varphi^2 + \frac{1}{2}\,\kappa n_m t_m \varphi\,\frac{d\varphi}{ds}\right).$$

When the sum is taken on on m the last term drops out because $\mathbf{t}$ and $\mathbf{n}$ are orthogonal. Integration then produces Eq. (2.4). q.e.d.

For φ sufficiently regular, the right side of (2.4) equals the one-dimensional version of

$$4\langle \varphi, H_{1/4}\varphi \rangle.$$

Consequently, Proposition 2.1 implies universal spectral bounds for operators of the form H_g:

Corollary 2.2 *Let M be as in* Proposition 2.1 *and suppose that H is a Schrödinger Hamiltonian with $V(s)$ bounded and measurable. Then*

$$\Gamma \leq 4 \int_M \left(\left(\frac{du_1}{ds} \right)^2 + \frac{\kappa^2}{4} u_1^2 \right) ds. \tag{2.5}$$

Furthermore, if H is of the form

$$H_g := -\frac{d^2}{ds^2} + g\kappa^2,$$

then

$$\Gamma \leq \max\left(4, \frac{1}{g}\right) \lambda_1. \tag{2.6}$$

Equivalently, the universal ratio bound

$$\frac{\lambda_2}{\lambda_1} \leq \max\left(5, 1 + \frac{1}{g}\right)$$

holds. This bound is sharp for $0 < g \leq \frac{1}{4}$.

Remark In case $g < 0$, somewhat less simple-looking bounds on the gap in lieu of (2.6) follow easily from (2.5).

Proof. To establish (2.5), make the choice $G = X_m$ in Lemma 1.1, and use (2.3) to rewrite the left side of Lemma 1.1. With (2.4),

$$\Gamma \cdot 2 \sum_m \left\langle u_1, t_m^2 u_1 \right\rangle \leq 8 \int_M \left(\left(\frac{du_1}{ds} \right)^2 + \frac{\kappa^2}{4} {u_1}^2 \right) ds$$

Because $\sum_m t_m^2 = 1$, by dividing by 2 we arrive at (2.5). Since

$$\lambda_1 = \int_M \left(\left(\frac{du_1}{ds} \right)^2 + g\kappa^2 u_1^2 \right) ds,$$

simple algebra yields (2.6) and the equivalent ratio bound. To see that the latter bound is sharp for $g \leq \frac{1}{4}$, consider the case of the circle, for which the eigenvalues are explicitly known, and:

$$\frac{\lambda_2}{\lambda_1} = \frac{4\pi^2 (1+g)}{4\pi^2 g} = 1 + \frac{1}{g}.$$

q.e.d.

3 Bounds on the fundamental gap when M is a hypersurface

This section treats the case where M is a compact d-dimensional manifold smoothly immersed in $\mathbb{R}^{d+1}$. The results are precisely as in Section 2.

Theorem 3.1 *Let H be a Schrödinger operator on M with a bounded potential, i.e.,*

$$H = -\Delta + V, \tag{3.1}$$

where V is a bounded, measurable, real-valued function on M. If M has a boundary, Dirichlet conditions are imposed (in the weak sense that H is defined as the Friedrichs extension from $C_c^\infty(M)$). Then

$$\begin{aligned}\Gamma(H) &\leq \frac{1}{d} \int_M \left(4 \left|\nabla_{||} u_1\right|^2 + h^2 u_1^2\right) dVol \\ &= \frac{4}{d} \left\langle u_1, \left(-\Delta + \frac{h^2}{4}\right) u_1 \right\rangle. \end{aligned} \tag{3.2}$$

Remark The assumption of boundedness of V can be considerably relaxed, as long as the form domain of H remains the Sobolev space $W_0^1(M)$. Conditions for this can be found in [9, 22].

Proof. Let $\{x_m, m = 0, \ldots, d\}$ be a fixed Cartesian coordinate system for $\mathbb{R}^{d+1}$, and denote by $\mathbf{e}_m$ the corresponding unit vectors. Ambient coordinates are introduced because they will be convenient for some calculations. The notation $\{X_m\}$ will be used for the functions $M \to \mathbb{R}$ obtained by restricting x_m to M. Let $\nabla_{||}$ denote the tangential gradient, which can be written in terms of the ambient gradient by projecting away the component along $\mathbf{n}$:

$$\nabla_{||} = \nabla - \mathbf{n}\, \mathbf{n} \cdot \nabla.$$

Here, $\mathbf{n}$ denotes the outward normal to M. Note that the vector position on M, i.e., $\mathbf{X} := \sum_{m=0}^{d} X_m \mathbf{e}_m$ is independent of the ambient coordinate system, and that $\nabla_{||}$ is independent of the local coordinates on M. Also, in an ambient coordinate system the Laplace-Beltrami operator Δ can be identified with $\nabla_{||}^2$.

The commutator formula (1.7) using $G = X_m$ states

$$(\lambda_2 - \lambda_1) \langle u_1, [X_m, [H, X_m]] \, u_1 \rangle \leq 2 \| [H, X_m] \, u_1 \|^2.$$

A simplification can be achieved after summing on m, and noting that since the potential in H commutes with X_m, H may be replaced in the commutators by $-\Delta$:

$$(\lambda_2 - \lambda_1) \sum_{m=0}^{d} \langle u_1, [X_m, [-\Delta, X_m]] \, u_1 \rangle \leq 2 \sum_{m=0}^{d} \| [-\Delta, X_m] \, u_1 \|^2. \tag{3.3}$$

It will now be shown that the left side of (3.3) is $2d\Gamma$. The first step is to realize that $\sum\limits_{m=0}^{d} [X_m, [-\Delta, X_m]]$ is independent of the orientation of the ambient Cartesian system, because with the orthogonality of $\{\mathbf{e}_m\}$ a short calculation shows that it is equal to the invariant expression $\mathbf{X} \cdot [(-\Delta), \mathbf{X}] - [(-\Delta), \mathbf{X}] \cdot \mathbf{X}$.

This allows the left side of (3.3) to be calculated locally in a conveniently oriented ambient Cartesian system: At any point of M, choose the orientation so that $\mathbf{n} = \mathbf{e}_0$, in which case $\left[-\nabla_{||}^2, X_m\right] = -2\frac{\partial}{\partial x_m} + (\text{scalar function})$, $m = 1, \ldots, d$, while $\left[-\nabla_{||}^2, X_0\right]$ is a scalar function. Consequently,

$$\sum_{m=0}^{d} [X_m, [-\Delta, X_m]] = \sum_{m=0}^{d} \left[X_m, \left[-\nabla_{||}^2, X_m\right]\right] = 2d.$$

By integrating, the left side of (3.3) is therefore $2d\,(\lambda_2 - \lambda_1) = 2d\Gamma$.

To facilitate the calculation of the right side of (3.3), define an operator $\mathbf{P}$ mapping the domain of H to $\mathbb{R}^{d+1} \otimes L^2(M)$ via

$$\mathbf{P} f := -\frac{1}{2} \sum_{m=0}^{d} \mathbf{e}_m \, [-\Delta, X_m] \, f = \frac{1}{2} \, [\Delta, \mathbf{X}] \, f.$$

Observe now that due to the orthonormality of $\{\mathbf{e}_m\}$, the right side of (3.3) is

$$4 \, \| \mathbf{P} u_1 \|^2_{\mathbb{R}^{d+1} \otimes L^2(M)} .$$

The Laplace-Beltrami operator can be conveniently expressed in local Riemann normal coordinates on M, in which it is arranged that at a chosen point $p \in M$, $\Delta = \sum_{j=1}^{d} \frac{\partial^2}{\partial s_j}$, where $\{s_j\}$ measure arc length along the lines of curvature passing through p. Thus, at p,

$$[-\Delta, X_m] = \sum_{j=1}^{d} \left(-2 \frac{\partial X_m}{\partial s_j} \frac{\partial}{\partial s_j} - \frac{\partial^2 X_m}{\partial s_j^2} \right), \tag{3.4}$$

so

$$\begin{aligned} \mathbf{P} u_1 &= \sum_{j=1}^{d} \left(\frac{\partial \mathbf{X}}{\partial s_j} \frac{\partial u_1}{\partial s_j} + \frac{1}{2} \frac{\partial^2 \mathbf{X}}{\partial s_j^2} u_1 \right) \\ &= \sum_{j=1}^{d} \left(\mathbf{t}_j \frac{\partial u_1}{\partial s_j} \pm \frac{1}{2} \kappa_j \mathbf{n} u_1 \right). \end{aligned} \tag{3.5}$$

The second line of (3.5) uses the Serret-Frenet equations, according to which $\mathbf{t}_j$ is a unit tangent vector parallel to the line of curvature parametrized by s_j, and κ_j is the associated principal curvature. In other words, $\{\mathbf{t}_j\}$ are the normalized eigenvectors of the shape operator. The varying sign enters because here $\mathbf{n}$ is by convention outward, whereas the normal defined by the Serret-Frenet equations may be outward or inward. Where the latter is not defined, its coefficient is 0, and it drops out.

Since $\{\mathbf{n}, \mathbf{t}_j\}$ is an orthonormal system, at the point p,

$$\|\mathbf{P} u_1\|^2_{\mathbb{R}^{d+1}}(p) = \sum_{j=1}^{d} \frac{\partial u_1}{\partial s_j^2} + \frac{1}{4} \left(\sum_{j=1}^{d} \kappa_j u_1 \right)^2.$$

This formula is equal to the coordinate-independent expression

$$\left| \nabla_{||} u_1 \right|^2 + \frac{h^2}{4} u_1^2, \tag{3.6}$$

which can now be integrated over M. When (3.6) is used in the right side of (3.3), which is then divided by $2d$, the result is

$$(\lambda_2 - \lambda_1) \leq \frac{4}{d} \int_M \left(\left| \nabla_{||} u_1 \right|^2 + \frac{h^2}{4} u_1^2 \right) dVol.$$

This is equivalent to (3.2). q.e.d.

An immediate consequence of Theorem 3.1 by partial integration is:

Corollary 3.2 *Let H be as in* (3.1) *and define* $\delta := \sup_M \left(\frac{h^2}{4} - V\right)$. *Then*

$$\Gamma(H) \leq \frac{4}{d}\left(\lambda_1 + \delta\right).$$

A further corollary is an isoperimetric spectral theorem for operators of the form H_g from (1.10):

Corollary 3.3 *Let H_g be defined on M, a d-dimensional manifold smoothly immersed in $\mathbb{R}^{d+1}$. Then for $0 < g \leq \frac{1}{4}$, the eigenvalues satisfy*

$$\lambda_2 - \lambda_1 \leq \frac{4\sigma\lambda_1}{d}, \tag{3.7}$$

with

$$\sigma = \max\left(1, \frac{1}{4g}\right). \tag{3.8}$$

For the ratio, these bounds read

$$\frac{\lambda_2}{\lambda_1} \leq \frac{1+gd}{gd}, \quad \text{for } 0 < g \leq \frac{1}{4}$$

and

$$\frac{\lambda_2}{\lambda_1} \leq \frac{4+d}{d}, \quad \text{for } g \geq \frac{1}{4}.$$

The bounds (3.7) *are optimal for $g \leq \frac{1}{4}$.*

Proof. If $H = H_g$, then

$$\int_M \left(\left|\nabla_{||}u_1\right|^2 + gh^2u_1^2\right) dVol = (u_1, H_g u_1) = \lambda_1,$$

a multiple of which majorizes the right side of (3.2): When $g \leq \frac{1}{4}$, this is immediate. Otherwise first multiply $\left|\nabla_{||}u_1\right|^2$ by $\frac{1}{4g} > 1$. The result is (3.7).

Optimality is established for $g \leq \frac{1}{4}$ by the example of the sphere S^d, for which, after normalizing the scale so that S^d embeds in $\mathbb{R}^{d+1}$ as the unit sphere,

$$\lambda_1 = gd^2, \quad \lambda_2 = gd^2 + d$$

[20]. Thus

$$d = \lambda_2 - \lambda_1 \leq \left(\frac{gd^2}{gd}\right) = d.$$

q.e.d.

4 Sum rules for eigenvalues

In [16] universal estimates for Laplacians and Schrödinger operators were obtained by deriving *sum rules* with commutator relations, and appropriately modified versions of these apply to operators of the type (3.1). This section follows that article closely, but with the purpose of displaying the effect of mean curvature. The results will subsume those of Section 3 and give information about the spectrum above the first two eigenvalues.

For H as in (3.1) the calculations leading to (3.5) and (3.6) established the operator identities

$$\mathbf{P} = \sum_{j=1}^{d} \left(\mathbf{t}_j \frac{\partial}{\partial s_j} \pm \frac{1}{2} \kappa_j \mathbf{n} \right) \tag{4.1}$$

and for a dense set of functions φ,

$$\|\mathbf{P}\varphi\|^2 = \left\langle \varphi, H_{1/4}\varphi \right\rangle. \tag{4.2}$$

Thus $\mathbf{P}$ plays the rôle of a momentum operator, with which there is a version of canonical commutation (cf. (1.9)) as follows. Defining a variant commutator bracket for operators $L^2(M) \to \mathbb{R}^{d+1} \otimes L^2(M)$ by $[A; B] := A \cdot B - B \cdot A$, a calculation shows that $[\mathbf{P}; X_k \mathbf{e}_k] = \sum_{j=1}^{d} \mathbf{t}_j \cdot \frac{\partial X_k \mathbf{e}_k}{\partial s_j} = \mathbf{1}$ (identity operator), and by averaging on k,

$$\mathbf{1} = \frac{1}{d} \left[\mathbf{P}; \mathbf{X} \right]. \tag{4.3}$$

This is a coordinate-independent formula.

A sum rule for H, analogous to that of [16] reads as follows:

Proposition 4.1 *Let H be as in* (3.1)*, with eigenvalues $\{\lambda_k\}$ and normalized eigenfunctions $\{u_k\}$. Then*

$$1 = \frac{4}{d} \sum_{\substack{k \\ \lambda_k \neq \lambda_j}} \frac{|\langle u_k, \mathbf{P} u_j \rangle|^2}{\lambda_k - \lambda_j}. \tag{4.4}$$

Furthermore, if f is any function summable on the spectrum $\sigma(H)$, then

$$\sum_{j}^{\infty} f(\lambda_j) = -\frac{2}{d} \sum_{\substack{j,k \\ \lambda_k \neq \lambda_j}} |\langle u_k, \mathbf{P} u_j \rangle|^2 \frac{f(\lambda_j) - f(\lambda_k)}{\lambda_j - \lambda_k}. \tag{4.5}$$

Proof. From the commutator gap formula (1.2), with $G = \mathbf{X}$,

$$-2\left\langle u_j, \mathbf{P}u_k\right\rangle = \left(\lambda_j - \lambda_k\right)\left\langle u_j, \mathbf{X}u_k\right\rangle,$$

so for $\lambda_j \neq \lambda_k$,

$$\langle u_j, \mathbf{X}u_k\rangle = -2\frac{\langle u_j, \mathbf{P}u_k\rangle}{\lambda_j - \lambda_k}. \tag{4.6}$$

Meanwhile, from (4.3) and the completeness of the orthonormal set of real-valued eigenfunctions $\{u_k\}$, it follows that

$$\begin{aligned} 1 = \langle u_j, u_j\rangle &= \frac{1}{d}\left\langle u_j, [\mathbf{P};\mathbf{X}]\, u_j\right\rangle = \frac{2}{d}\left\langle u_j, \mathbf{P}\cdot\mathbf{X}u_j\right\rangle \\ &= \frac{2}{d}\sum_k \langle u_j, \mathbf{P}u_k\rangle \cdot \langle u_k, \mathbf{X}u_j\rangle. \end{aligned}$$

Substitution from (4.6) yields (4.4). Observe that there is no sum on j in (4.4); it is true for all j. To derive the identity (4.5) from (4.4), sum on j to obtain

$$\sum_j^{\infty} f\left(\lambda_j\right) = -\frac{4}{d}\sum_{\substack{j,k\\ \lambda_k\neq\lambda_j}} \left|\langle u_k, \mathbf{P}u_j\rangle\right|^2 \frac{f\left(\lambda_j\right)}{\lambda_j - \lambda_k},$$

and then symmetrize in the indices j and k. q.e.d.

Because (4.4) and (4.5) are identical in form to the sum rules derived in [16], the corollaries in that article can be carried over directly. Accordingly, the proofs of their analogues will be given in outline only. For operators H_g, the constant σ in Eq. (10) of [16] is $\sigma = \max\left(1, \frac{1}{4g}\right)$ as in (3.8). Corollary 3 of [16] is a kind of Hile-Protter inequality [18]. Its analogue is as follows:

Corollary 4.2 *Let H be as in* (3.1) *and $\delta := \sup_M\left(\frac{h^2}{4} - V\right)$ as in* Corollary 3.2*. Then for each $n = 1, 2, \ldots,$ such that $\lambda_{n+1} \neq \lambda_n$,*

$$1 \leq \frac{4}{dn}\sum_{j=1}^{n} \frac{\lambda_j + \delta}{\lambda_{n+1} - \lambda_j}. \tag{4.7}$$

Suppose that H_g is as in (1.10) *with M as in* Section 3 *and $g > 0$. If $\lambda_{n+1} \neq \lambda_n$, then*

$$1 \leq \frac{4\sigma}{dn}\sum_{j=1}^{n} \frac{\lambda_j}{\lambda_{n+1} - \lambda_j}. \tag{4.8}$$

Proof. Sum (4.4) on j from 1 to n. Since by symmetry,

$$\sum_{\substack{j,k\leq n\\ \lambda_k\neq\lambda_j}} \frac{|\langle u_k, \mathbf{P}u_j\rangle|^2}{\lambda_k-\lambda_j} = 0,$$

this produces

$$n = \frac{4}{d}\sum_{\substack{j\leq n\\ k\geq n+1}} \frac{|\langle u_k, \mathbf{P}u_j\rangle|^2}{\lambda_k-\lambda_j},$$

so

$$1 \leq \sum_{j=1}^{n} \frac{1}{\lambda_{n+1}-\lambda_j}\sum_{k=0}^{\infty}|\langle u_k, \mathbf{P}u_j\rangle|^2 = \sum_{j=1}^{n}\frac{\|\mathbf{P}u_j\|^2}{\lambda_{n+1}-\lambda_j}.$$

Inequality (4.7) follows by substituting from (4.2) and using the elementary fact that

$$H_{1/4} = H + \frac{h^2}{4} - V \leq H + \delta \tag{4.9}$$

in the sense of quadratic forms.

For the universal inequality (4.8), we instead use the fact that $g' \geq g$ implies $H_{g'} \geq H_g$ and, for $g < \frac{1}{4}$, that $H_{1/4} \leq \frac{1}{4g}H_g$, again in the sense of quadratic forms. q.e.d.

Theorem 5 of [16] is a "Yang-type" inequality [24], which in the context of this article reads:

Corollary 4.3 *Let H be as in* (3.1)*, with M a compact, smooth submanifold. For z such that $\lambda_n < z \leq \lambda_n + 1$,*

$$\sum_{j=1}^{n}(z-\lambda_j)^2 \leq \frac{4}{nd}\sum_{j=1}^{n}(z-\lambda_j)\|\mathbf{P}u_j\|^2$$
$$\leq \frac{4}{nd}\sum_{j=1}^{n}(z-\lambda_j)(\lambda_j+\delta).$$

Proof. This results from multiplying (4.4) by $(z-\lambda_j)^2$ and summing on j from 1 to n. The sum on k from 1 to n can be dropped because the summand is antisymmetric under exchange of j and k. For $\lambda_k \geq z$, $\frac{(z-\lambda_j)^2}{\lambda_k-\lambda_j} \leq (z-\lambda_j)$, whence

$$\begin{aligned}\sum_{j=1}^{n}(z-\lambda_j)^2 &\le \frac{4}{nd}\sum_{j=1}^{n}(z-\lambda_j)\sum_{k=n+1}^{\infty}|\langle u_k,\mathbf{P}u_j\rangle|^2\\ &\le \frac{4}{nd}\sum_{j=1}^{n}(z-\lambda_j)\|\mathbf{P}u_j\|^2\end{aligned}$$

by Bessel's inequality. The final inequality follows with (4.9) q.e.d.

Since Corollary 4.3 states that a certain quadratic function of z is negative when $\lambda_n < z \le \lambda_n+1$, it implies that each spectral gap can be bounded by an explicit expression in terms of the distribution of lower eigenvalues. Define

$$\overline{\lambda_n} := \frac{1}{n}\sum_{k=1}^{n}\lambda_k$$

and

$$\overline{\lambda_n^2} := \frac{1}{n}\sum_{k=1}^{n}\lambda_k^2.$$

Then each eigenvalue gap of a generic H is bounded by a complicated, explicit expression where the mean curvature enters through δ, whereas the eigenvalue gaps of operators of the form H_g are bounded by a simpler universal expression:

Corollary 4.4 a) *Let H be as* (3.1)*, with M a compact, smooth submanifold. Then*

$$[\lambda_n,\lambda_{n+1}] \subseteq \left[\left(1+\frac{2}{d}\right)\overline{\lambda_n} - \sqrt{D_n^\delta}, \left(1+\frac{2}{d}\right)\overline{\lambda_n} + \sqrt{D_n^\delta}\right],$$

with

$$D_n^\delta := \frac{4}{d^2}\left(\left(\frac{dn+2}{2}\right)^2\overline{\lambda_n}^2 + (dn-d+2)\,\delta\overline{\lambda_n} - d\left(\frac{dn+4}{4}\right)\overline{\lambda_n^2} + \delta^2\right).$$

b) *For H_g, $0 < g$, of the form* (1.10) *on a smooth, compact submanifold M,*

$$[\lambda_n,\lambda_{n+1}] \subseteq \left[\left(1+\frac{2\sigma}{d}\right)\overline{\lambda_n} - \sqrt{D_n}, \left(1+\frac{2\sigma}{d}\right)\overline{\lambda_n} + \sqrt{D_n}\right],$$

with

$$D_n := \left(\left(1+\frac{2\sigma}{d}\right)\overline{\lambda_n}\right)^2 - \left(1+\frac{4\sigma}{d}\right)\overline{\lambda_n^2} > 0.$$

This bound is sharp for every non–zero eigenvalue gap of $H_{\frac{1}{4}}$ *on the sphere.*

Proof. It is only necessary to calculate the roots of the quadratic expression from the preceding Corollary,

$$z \to \sum_{j=1}^{n}(z-\lambda_j)^2 - \frac{4}{nd}\sum_{j=1}^{n}(z-\lambda_j)\|\mathbf{P}u_j\|^2$$

and to substitute from (4.2). (Cf. [16], Proposition 6; the bound b) is in fact identical in form to the one in that article.)

An explicit calculation shows that the bound is sharp for the non-zero eigenvalue gaps of the sphere, for which all the eigenvalues are known and elementary [20]: For simplicity, assume that $d = 2, g = \frac{1}{4}$, and that M is the sphere of radius 1 embedded in $\mathbb{R}^3$. Then $h = 2, \sigma = 1$, and:

$$\lambda_1 = 1; \lambda_2 = \lambda_3 = \lambda_4 = 3; \ldots ; \lambda_{(m-1)^2+1} = \cdots = \lambda_{m^2} = m^2 - m + 1.$$

For $n = m^2$, the calculation shows that $\overline{\lambda_n} = \frac{n+1}{2}$, and $\overline{\lambda_n^2} = \frac{n^2+n+1}{3}$. Hence $D_n = n$, and b) informs us that

$$\begin{aligned} 2\overline{\lambda_{m^2}} - m = m^2 - m + 1 &\le \lambda_{m^2} = m^2 - m + 1 \\ \le \lambda_{m^2+1} = m^2 + m + 1 &\le 2\overline{\lambda_{m^2}} + m = m^2 + m + 1, \end{aligned}$$

and thus λ_{m^2} equals the lower bound $2\overline{\lambda_{m^2}} - m$ and λ_{m^2+1} equals the upper bound $2\overline{\lambda_{m^2}} + m$.

q.e.d.

Finally, consider the partition function for H,

$$Z(t) := \mathrm{tr}(\exp(-tH)),$$

If the function f of Proposition 4.1 is chosen as $f(x) := \exp(-tx)$, then (after a short calculation exactly as for Eq. (15) of [16]):

$$Z(t) \le \left(\frac{2t}{d}\right)\sum_j (\exp(-t\lambda_j)))\|\mathbf{P}u_j\|^2, \tag{4.10}$$

which implies the following bounds:

Corollary 4.5 a) *Let H be as in* (3.1)*, with M a compact, smooth submanifold. Then $t^{\frac{d}{2}} \exp(-\delta t)\, Z(t)$ is a nonincreasing function;*

b) *For H_g be of the form* (1.10) *on a smooth, compact submanifold M, $t^{\frac{d}{2\sigma}} Z(t)$ is a nonincreasing function.*

Proof. For general H, the right side of (4.10) is majorized by

$$\left(\frac{2t}{d}\right) \sum_j \lambda_j \exp(-t\lambda_j) + \left(\frac{2t\delta}{d}\right) Z(t).$$

Hence

$$\left(1 - \frac{2t\delta}{d}\right) Z(t) + \left(\frac{2t}{d}\right) Z'(t) \leq 0,$$

and when multiplied by the integrating factor $t^{\frac{d}{2}} \exp(-\delta t)$ the left side becomes a positive multiple of the derivative of $t^{\frac{d}{2}} \exp(-\delta t)\, Z(t)$.

Statement b) follows similarly, after majorizing the right side of (4.10) with

$$\left(\frac{2\sigma t}{d}\right) \sum_j (\exp(-t\lambda_j)))\lambda_j.$$

q.e.d.

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