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 $\mathbb{R}^{d+1}$. 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 g is a real parameter and

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

with $\{\kappa_j\}$, $j = 1, \dots, d$ denoting the principal curvatures of M. For instance, by Theorem 2.1 and Corollary 3.4, 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,

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

reflect the analytic and geometric details of H. The connection between the size of the gap and H is often shown by calculations involving commutators of H with other operators, as in [1, 2, 10, 13, 14, 17], which are among the inspirations for this article. In contrast to most of those articles H is defined here on a curved hypersurface M, and commutators will be used to connect eigenvalue gaps and certain other functions defined on the spectrum $\sigma(H)$ to the mean curvature of M, which is found to pose tight constraints on the spectrum, including sharp bounds on Γ.

Certain bounds will be proved for Laplace and general Schrödinger operators, yet they take on their simplest form when the potential energy is proportional to the square of the mean curvature. Schrödinger operators depending explicitly on the principal curvatures $\kappa := \{\kappa_j\}$, $j = 1, \ldots, d$,

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

defined on a d-dimensional submanifold of $\mathbb{R}^\nu$, arise in the mathematics of nanophysics and thin structures, and connections between certain q and the shape of the structure have previously been studied in [8, 4, 6, 11, 12, 9], in some cases with sharp control of individual low–lying eigenvalues, $\lambda_1 < \lambda_2 \leq \cdots$, but as yet there has not been a focus on the eigenvalue gaps in this context.

Section 2 will be devoted to the fundamental eigenvalue gap, while in Section 3 an alternative algebraic approach is used to extend these results to all eigenvalue gaps. The results of Section 2 are largely subsumed by the Section 3, but as alternative, simpler methods are available for the simpler situation, it is felt useful to present multiple points of view.

Notation

- $\langle f, g\rangle$ denotes the standard inner product on $L^2(M)$. The measure is taken as that derived from the Euclidean metric on the ambient $\mathbb{R}^\nu$.

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

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 $\mathbf{t}_j$, while $h := \sum_{j=1}^{d} \kappa_j$.

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.

Assume for now only that H and G are a pair of 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 between commutators and eigenvalue gaps is the elementary 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 $[H, G]$ but also higher-order commutators such as $[G, [H, G]]$ are related to eigenvalue gaps. 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,

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

In particular,

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

Lemma 1.1 *Let H be a positive self-adjoint operator with discrete eigenvalues λ_1 and λ_2. Let P denote the orthogonal projector onto u_1, and suppose that 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*

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

Remark This is actually a special case of Theorem 2.1 of [13]. 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

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

which follows from the spectral functional calculus (e.g., see [5, 7, 19]), since for $\mu \in \sigma(H)$, $(\mu - \lambda_1)\,(\lambda_2 - \lambda_1) \le (\mu - \lambda_1)^2$. 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 [3]).

It is argued in Section 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 Bounds on the fundamental eigenvalue gap of Schrödinger operators on hypersurfaces

In this section M is a compact d-dimensional manifold smoothly immersed in $\mathbb{R}^{d+1}$.

Theorem 2.1 *Let H be a Schrödinger operator on M with a bounded potential, i.e.,*

$$H = -\Delta + V, \tag{2.1}$$

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

$$\begin{aligned}\Gamma(H) &\le \frac{1}{d}\int_M \left(4\left|\nabla_{||} u_1\right|^2 + h^2 u_1^2\right) dVol \\ &= \frac{4}{d}\left\langle u_1, \left(-\Delta + \frac{h^2}{4}\right) u_1 \right\rangle. \end{aligned} \tag{2.2}$$

Remark If V is simply a function of the position on M, rather than defined in terms of curvature, then H is an intrinsic object, whereas the extrinsic quantity h appears on the right side of the inequality (2.2). An interpretation of Theorem 2.1 in this situation is that if M is given as an abstract manifold, and if $\Gamma(H)$ and u_1 are found, then any immersion of M in $\mathbb{R}^{d+1}$ requires a mean curvature satisfying (2.2).

Proof. Let $\{x_m, m = 0, \dots, d\}$ 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

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

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 $-\Delta$:

$$(\lambda_2-\lambda_1)\sum_{m=0}^{d}\langle u_1,[X_m,[-\Delta,X_m]]\,u_1\rangle \le 2\sum_{m=0}^{d}\|[-\Delta,X_m]\,u_1\|^2. \qquad (2.3)$$

It will now be shown that the left side of (2.3) is $2d\Gamma$. The first step is to realize that $\sum_{m=0}^{d}[X_m,[-\Delta,X_m]]$ 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 (2.3) 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 (2.3) is therefore $2(\lambda_2-\lambda_1)\,d=2\Gamma d$.

To facilitate the calculation of the right side of (2.3), define an operator $\mathbf{P}$ mapping the domain of H to the space $\mathbb{R}^{d+1}\otimes L^2(M)$ 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 (2.3) is

$$8\,\|\mathbf{P}u_1\|^2_{\mathbb{R}^{d+1}\otimes L^2(M)}\,.$$

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 $p\in M$, $\Delta=\sum_{j=1}^{d}\frac{\partial^2}{\partial s_j^2}$, where $\{s_j\}$ measure arc length along the lines of curvature passing through p. Thus, at p,

$$[-\Delta,X_m]=\sum_{j=1}^{d}\left(-2\frac{\partial X_m}{\partial s_j}\frac{\partial}{\partial s_j}-\frac{\partial^2 X_m}{\partial s_j^2}\right), \qquad (2.4)$$

so

$$
\begin{aligned}
\mathbf{P}u_1 &= \sum_{j=1}^{d} \left(\frac{\partial \mathbf{X}}{\partial s_j} \frac{\partial u_1}{\partial s_j} + \frac{1}{2} \frac{\partial^2 \mathbf{X}}{\partial s_j^2} u_1 \right) \\
&= \sum_{j=1}^{d} \left(\mathbf{t}_j \frac{\partial u_1}{\partial s_j} \pm \frac{1}{2} \kappa_j \mathbf{n} u_1 \right). \qquad (2.5)
\end{aligned}
$$

The second line of (2.5) 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. I.e., $\{\mathbf{t}_j\}$ 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 normal 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,

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

This formula is equal to the coordinate-independent expression

$$
\left|\nabla_{||} u_1\right|^2 + \frac{h^2}{4} u_1^2, \qquad (2.6)
$$

which can now be integrated over M. When (2.6) is used in the right side of (2.3), which is then divided by $2d$, the result is

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

This is equivalent to (2.2). q.e.d.

An immediate consequence of Theorem 2.1 by partial integration is:

Corollary 2.2 *Let H be as in* (2.1) *and define* $\delta := \sup_M \left(\frac{h^2}{4} - V \right)$. *Then*

$$
\Gamma(H) \le \frac{4}{d} (\lambda_1 + \delta).
$$

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

Corollary 2.3 *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*

$$\lambda_2 - \lambda_1 \leq \frac{4\sigma\lambda_1}{d}\,, \tag{2.7}$$

with

$$\sigma := \max\left(1, \frac{1}{4g}\right). \tag{2.8}$$

For the ratio, these bounds read

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

and

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

The ratio bound (2.8) *is sharp for* $0 < g \leq \frac{1}{4}$.

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 (2.2): 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 (2.7).

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,

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

[18]. Thus

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

q.e.d.

3 Sum rules for eigenvalues

In 1925, Heisenberg [15] showed that the *Thomas–Reiche–Kuhn sum rules* of atomic physics could be derived with calculations supposing, for the first time, that observables do not commute. In [14] related sum rules for Laplacians and Schrödinger operators were obtained by commutator calculations, and in this section appropriately modified sum rules will be obtained for operators of the type (2.1). The derivation will follow [14] 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 (2.1) the calculations leading to (2.5) and (2.6) established the operator identities

$$\mathbf{P} = \sum_{j=1}^{d} \left(\mathbf{t}_j \frac{\partial}{\partial s_j} \pm \frac{1}{2} \kappa_j \mathbf{n} \right) \tag{3.1}$$

and, for a dense set of functions φ,

$$\|\mathbf{P}\varphi\|^2 = \left\langle \varphi, H_{1/4} \varphi \right\rangle . \tag{3.2}$$

The operator $\mathbf{P}$ 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,

$$\mathbf{1} = \frac{1}{d} \left[\mathbf{P}; \mathbf{X} \right] . \tag{3.3}$$

This is a coordinate-independent formula.

A sum rule for H, analogous to that of [14] reads as follows:

Proposition 3.1 *Let H be as in* (2.1)*, with eigenvalues $\{\lambda_k\}$ and normalized eigenfunctions $\{u_k\}$. Then for each fixed j,*

$$1 = \frac{4}{d} \sum_{\substack{k \\ \lambda_k \neq \lambda_j}} \frac{\left| \langle u_k, \mathbf{P} u_j \rangle \right|^2}{\lambda_k - \lambda_j} . \tag{3.4}$$

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

$$\sum_{j}^{\infty} f(\lambda_j) = -\frac{2}{d} \sum_{\substack{j,k \\ \lambda_k \neq \lambda_j}} \left| \langle u_k, \mathbf{P} u_j \rangle \right|^2 \frac{f(\lambda_j) - f(\lambda_k)}{\lambda_j - \lambda_k} . \tag{3.5}$$

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 $\lambda_j \neq \lambda_k$,

$$\langle u_j, \mathbf{X}u_k\rangle = -2\frac{\langle u_j, \mathbf{P}u_k\rangle}{\lambda_j - \lambda_k}. \tag{3.6}$$

Meanwhile, from (3.3) and the completeness of the orthonormal set of real-valued eigenfunctions $\{u_k\}$, it follows that

$$1 = \langle u_j, u_j\rangle = \frac{1}{d}\left\langle u_j, \left[\mathbf{P}; \mathbf{X}\right] u_j\right\rangle.$$

Since $\mathbf{P}$ is skew–symmetric,

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

Substitution from (3.6) yields (3.4). Observe that there is no sum on j in (3.4); it is true for all j. To derive the identity (3.5) from (3.4), 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 (3.4) and (3.5) are identical in form to the sum rules derived in [14], 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 [14] is $\sigma = \max\left(1, \frac{1}{4g}\right)$ as in (2.8). Corollary 3 of [14] is a kind of Hile-Protter inequality [16]. Its analogue is as follows:

Corollary 3.2 *Let H be as in* (2.1) *and $\delta := \sup_M\left(\frac{h^2}{4} - V\right)$ as in* Corollary 2.2. *Then for each $n = 1, 2, \ldots,$ such that $\lambda_{n+1} \neq \lambda_n$,*

$$1 \leq \frac{4}{dn}\sum_{j=1}^{n}\frac{\lambda_j + \delta}{\lambda_{n+1} - \lambda_j}. \tag{3.7}$$

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*

$$1 \leq \frac{4\sigma}{dn} \sum_{j=1}^{n} \frac{\lambda_j}{\lambda_{n+1} - \lambda_j}. \tag{3.8}$$

Proof. Sum (3.4) 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

$$1 \leq \frac{4}{nd} \sum_{j=1}^{n} \frac{1}{\lambda_{n+1} - \lambda_j} \sum_{k=0}^{\infty} |\langle u_k, \mathbf{P} u_j \rangle|^2 = \frac{4}{nd} \sum_{j=1}^{n} \frac{\|\mathbf{P} u_j\|^2}{\lambda_{n+1} - \lambda_j}.$$

Inequality (3.7) follows by substituting from (3.2) and using the elementary fact that

$$H_{1/4} = H + \frac{h^2}{4} - V \leq H + \delta \tag{3.9}$$

in the sense of quadratic forms.

For the universal inequality (3.8), 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 [14] is a "Yang-type" inequality [21, 1], which in the context of this article reads:

Corollary 3.3 *Let* H *be as in* (2.1), *with* M *a compact, smooth hypersurface. For* z *such that* $\lambda_n < z \leq \lambda_{n+1}$,

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

Proof. This results from multiplying (3.4) 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

$$\sum_{j=1}^{n}(z-\lambda_j)^2 \leq \frac{4}{d}\sum_{j=1}^{n}(z-\lambda_j)\sum_{k=n+1}^{\infty}|\langle u_k, \mathbf{P}u_j\rangle|^2$$
$$\leq \frac{4}{d}\sum_{j=1}^{n}(z-\lambda_j)\|\mathbf{P}u_j\|^2$$

by Bessel's inequality. The final inequality follows with (3.9) q.e.d.

Since Corollary 3.3 states that a certain quadratic function of z is negative when $\lambda_n < z \leq \lambda_{n+1}$, 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 3.4 a) *Let H be as* (2.1)*, with M a compact, smooth hypersurface. 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 hypersurface 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, *viz.*,

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

and to substitute from (3.2). (Cf. [14], 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 [18]: 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 [14]):

$$Z(t) \le \left(\frac{2t}{d}\right)\sum_j (\exp(-t\lambda_j)))\|\mathbf{P}u_j\|^2, \tag{3.10}$$

which implies the following bounds:

Corollary 3.5 a) *Let H be as in* (2.1)*, with M a compact, smooth hypersurface. 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 hypersurface M, $t^{\frac{d}{2\sigma}} Z(t)$ is a nonincreasing function.*

Proof. For general H, the right side of (3.10) 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 (3.10) with

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

q.e.d.

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