Commutator Bounds for Eigenvalues of Some Differential Operators

EVANS M. HARRELL II[1]
PATRICIA L. MICHEL[2 3]

School of Mathematics, Georgia Institute of Technology
School of Mathematics, Georgia Institute of Technology

1 INTRODUCTION

Consider the evolution due to the linear diffusion equation

$$u_t = \kappa \Delta u$$

or to similar equations with popular additional complications, such as

$$u_t(x,t) = \mathrm{div}\,(P(x)\mathrm{grad}\; u(x,t)) + V(x)u(x,t)\,,$$

the heat equation with inhomogeneities and endothermic reactions, or

$$i\hbar u_t(x,t) = (\mathbf{p} - \mathbf{A}(x))^2 u(x,t) + V(x)u(x,t),$$

where

$$\mathbf{p} := -i\hbar\nabla,$$

the Schrödinger equation with a magnetic field. Here *div* and *grad* may be tensorially defined.

[1]Partially supported by the US NSF through grant DMS-9211624.
[2]Part of this research was conducted during the US-Sweden Workshop on Spectral Methods sponsored by the NSF under grant INT-9217529.
[3]Work related to Doctoral thesis in preparation at Georgia Institute of Technology.

Typically the generator of the semigroup $\exp(-tH)$, where H is the linear operator on the right side, has two important positivity properties, i.e., H is semibounded and $\exp(-tH)$ is positivity improving, which is essentially equivalent to having a positive integral kernel. In addition, often at least the lower portion of the spectrum is discrete, especially if the equation is defined on a bounded domain or manifold $\mathbf{\Omega}$.

The positivity properties of the evolution imply in a standard way that the lowest eigenvalue is nondegenerate and has a positive eigenfunction. Well-known arguments establish that estimates of gaps between eigenvalues correspond to exponential rates of convergence of the system to equilibrium: If the initial condition is $u(x,0)$, then, for example for the heat equation with Neumann boundary conditions:

$$u(x,t) - \langle u, u_0\rangle u_0 = \sum_{n=1}^{\infty} \exp(-\mu_n t)\langle u, u_n\rangle u_n = \mathbf{O}(\exp(-\mu_1 t)),$$

where $\langle\cdot,\cdot\rangle$ denotes the inner product on $L^2(\mathbf{\Omega})$ and the eigenfunctions are denoted u_n, and in this case $\lambda_0 = 0$, with $u_0 = 1/\sqrt{|\mathbf{\Omega}|}$. Analogous things occur for other problems. Estimates of this kind have been familiar at least since [14].

The work discussed here concerns upper bounds on eigenvalue gaps (and, implicitly, on rates of convergence of evolution equations), using a theorem we recently proved [9]. This in turn is closely related to earlier work of Hook [13], Harrell [7], and Davies and Harrell (appendix to [8]).

The essential reason for the association between eigenvalue gaps and commutators is elementary. Let H be a self-adjoint operator such that $Hu_k = \lambda_k u_k$, and suppose G is an auxiliary operator. Then a formal calculation (ignoring domain questions) shows that

$$\langle u_k, [H,G]u_j\rangle = (\lambda_k - \lambda_j)\langle u_k, Gu_j\rangle.$$

A great many of the good estimates known for eigenvalue gaps can be derived from this formula. As with all variational techniques, the test function – in this case G – must be chosen cleverly in order to get a good estimate. For further discussion of these points, see [8]. A novel feature of the bounds we discuss in this article is that they involve the interplay between first and second commutators. As was shown in [7], when particularized to $H =$ the Laplace-Beltrami operator on a Riemannian manifold, similar bounds show how the spectral gaps are controlled by the curvature. One application we make below is to sharpen some of the estimates of that paper. Other applications are made to bounds for Neumann boundary conditions and for bi-Laplacians.

The operator under study is a self-adjoint operator H, and there are two families of symmetric "test operators," which we call G_j and Π_j. (The Π_j's are often analogues of the momentum operator of quantum mechanics, accounting for our notation. Hook [13] earlier had a similar theorem, and a rough correlation with his notation is that our G's correspond to his B's and our Π's correspond to his T's times i.)

THEOREM 1.1 *Let H be self-adjoint on a Hilbert space $\mathcal{H}$, and suppose that the lower portion of its spectrum consists of discrete eigenvalues $\lambda_1 \le \lambda_2 \le \ldots \le \lambda_n < \lambda_{n+1} \le \ldots$ Let P be the spectral projection for $\lambda_1, \lambda_2, \ldots, \lambda_n$, and let $\{G_j\}$ and $\{\Pi_j\}$ be two families of symmetric operators such that all products of the form $\Pi_j G_j$, $G_j \Pi_j$, $G_j^2 H$, HG_j^2, and*

G_jHG_j are well defined. Then

$$\sum_{j=1}^{m} Tr\Big((\lambda_{n+1}I - H)^{-1}P\Pi_j^2\Big) \geq \frac{\Big|\sum_{j=1}^{m} Tr\Big(P[\Pi_j, G_j]\Big)\Big|^2}{2\sum_{j=1}^{m} Tr\Big(P[G_j,[H,G_j]]\Big)}, \tag{1.1}$$

assuming that these three traces are finite and nonzero.

REMARKS: Note that because of the hypothesis $\lambda_{n+1} > \lambda_n$, the operator $\lambda_{n+1}I - H$ is uniquely invertible from the range of P to itself.

The natural setting for this theorem is that of C^*-algebras, in which the assumption on products of operators is unnecessary. Here, however, we are interested in unbounded operators, so domain questions must be considered carefully. While there is a certain amount of freedom in the choice of the auxiliary operators Π_j and G_j, it is important that the G_j's are chosen in such a way that HG_j is defined on the given domain, i.e. for $u \in \mathcal{D}(H)$ we must have $G_j u \in \mathcal{D}(H)$. Similarly for $G_j^2 u$.

An upper bound for $\lambda_{n+1} - \lambda_n$ is obtained if the left hand side is increased to $(\lambda_{n+1} - \lambda_n)^{-1} \sum_{j=1}^{m} Tr(P\Pi_j^2)$ and then one solves for the gap $\lambda_{n+1} - \lambda_n$. The resulting bounds are analogous to the classic Payne-Pólya-Weinberger bounds [16] (see [1] for a discussion of this bound) and those derived in [7]. In most applications, m will be taken to be ν, the dimension of the underlying space, but other choices are possible and will in some cases give better results.

2 EXAMPLES

In this section we list a few applications of our technique, some of which are to a certain extent already known in some form, but which we feel we obtain more efficiently. Theorem 1.1 is an abstract version of the Hile–Protter inequality [10]. Hook's earlier abstract Hile–Protter bound in [13] contains a free parameter, which he needs to optimize in order to get some of the applications which we obtain directly below.

As in [9] we define two universal constants C_{PPW} and C_{HP} as follows

$$C_{PPW}(\mathcal{M}) := \sup_{n, \mathbf{\Omega} \subset \mathcal{M}} \frac{\lambda_{n+1} - \lambda_n}{\langle \lambda_\ell \rangle_{\ell \leq n}}$$

and

$$C_{HP}(\mathcal{M}) := \sup_{n, \mathbf{\Omega} \subset \mathcal{M}} \left\langle \frac{\lambda_\ell}{\lambda_{n+1} - \lambda_\ell} \right\rangle_{\ell \leq n}^{-1}$$

where $\langle f_\ell \rangle_{\ell \leq n}$ denotes the average of an expression involving eigenvalues over all $\ell \leq n$. Thus, for example $\langle \lambda_\ell \rangle_{\ell \leq n} = \frac{1}{n} \sum_{\ell \leq n} \lambda_\ell$. Or, as will occur later, if the sum starts at $\ell = 0$ then we divide by $n+1$. According to these definitions we always have $C_{HP} \geq C_{PPW}$.

Example 1: Operators with continuous spectra

We begin with a remark about operators with continuous spectra, which immediately follows from the original estimates of Payne, Pólya, and Weinberger [16] and of Hile and Protter [10], but which does not appear to have been appreciated. Under wide circumstances it is known that continuous spectra of Schrödinger operators, Sturm–Liouville operators, Jacobi matrices, etc. can be quantified by using a measure known as the density of states, defined by cut-off procedures (for example, see [4], [15], and [6]).

Let us call the density of states measure $dn(\lambda)$, and assume that it is well–defined (as a weak-$*$ limit and has bounded first moment) for the operator H, which is a local operator on $L^2(\mathbf{R}^\nu)$ or $L^2(\mathbf{Z}^\nu)$. Suppose that $\Gamma = (a, b)$ is a gap in the spectrum of H (i.e., an open interval of length $|\Gamma|$ in the resolvent set, the ends of which are in the spectrum), and, moreover, that when H is restricted to a bounded set with Dirichlet boundary conditions (vanishing conditions, in the discrete case), there is a finite C_{HP}. Then, when we restrict H to rectangles of side R and let $R \to \infty$, we get:

$$\frac{|\Gamma| \int_{-\infty}^{a} dn\,(\lambda)}{\int_{-\infty}^{a} \lambda dn\,(\lambda)} \;\leq C_{PPW} \;\leq C_{HP}.$$

For example, if H is a Schrödinger operator in ν dimensions with a smooth, periodic, non-negative potential, then

$$|\Gamma| \leq \frac{4 \int_{-\infty}^{a} \lambda dn\,(\lambda)}{\nu \int_{-\infty}^{a} dn\,(\lambda)} \;\leq \frac{4a}{\nu}.$$

In particular cases, where estimates can be made of the density of states, much sharper bounds than $4a/\nu$ are possible.

Example 2: Algebraic formulation of quantum mechanics

In quantum mechanics it is not strictly necessary to represent the algebra of observables with differential operators; for many purposes an abstract algebra is quite sufficient (cf. [17]).

In this setting, the fundamental phenomena of quantum mechanics have their origin in the quantum canonical commutation relations, which state that if H is a Hamiltonian operator, then canonically conjugate classical variables satisfy the Heisenberg uncertainty principle. In the Heisenberg picture, the operators X, Π are a canonically conjugate pair when

$$\dot{X} \;=\; \frac{\Pi}{m} \;=\; \frac{i}{\hbar}\,[H, X]\,,$$

where m is the mass of the particle and $\hbar$ is Planck's constant divided by 2π. In this case, the commutation relations state that $[X, \Pi] \;=\; i\hbar$.

If we identify X with G, and assume that $\Pi^2 \leq \beta H$, then the bound on C_{HP} in this case becomes:

$$C_{HP} \;\leq\; \frac{2\beta n}{mTr\,(P)} \;=\frac{2\beta}{m}\;.$$

If there are M canonical momenta, such that

$$\sum_{j=1}^{M} \Pi_j^2 \le \beta H \ ,$$

then, similarly,

$$C_{HP} \ \le \frac{2\beta n}{mMTr\,(P)} \ = \frac{2\beta}{mM} \ . \tag{2.1}$$

With the usual Euclidean momenta, $\beta = 2m$, and a Hile–Protter type bound results. In the language of quantum mechanics, inequality (2.1) states that the ratio of the gap excitation energy to the average of the energy below an energy gap is bounded by $2\beta/mM$ divided by the trace of the density matrix for the unexcited states.

Example 3: Schrödinger operators with magnetic fields and Dirichlet boundary conditions

Compare with [13] p. 628. Consider the case when $H = (\mathbf{p} - \mathbf{A}(\mathbf{x}))^2 + V(\mathbf{x})$ on $\mathbf{L}^2(\mathbf{\Omega})$ for $\mathbf{\Omega}$ a bounded domain in $\mathbf{R}^\nu$. And where $\mathbf{p} = -i\nabla$ and $\mathbf{A}(\mathbf{x}) = (A_1(\mathbf{x}), A_2(\mathbf{x}), \ldots, A_\nu(\mathbf{x}))$ is a magnetic vector potential for the magnetic field $\mathbf{B}(\mathbf{x})$. Suppose $Hu_i = \lambda_i u_i$. The operator H has some discrete eigenvalues under very wide circumstances (see [4]).

Assume that $V(\mathbf{x}) \ge -M$. The special choices to be made for the auxiliary operators whose indices will run from $1, \ldots, \nu + 1$ are

$$\begin{aligned}
\Pi_j &= -i\frac{\partial}{\partial x_j} - A_j(\mathbf{x}) \ , \qquad j = 1, \ldots, \nu \\
\Pi_{\nu+1} &= (V(\mathbf{x}) + M)^{\frac{1}{2}} \\
G_j &= x_j \ , \qquad j = 1, \ldots, \nu \\
G_{\nu+1} &= 1.
\end{aligned}$$

It is easy to see that $\sum_{j=1}^{\nu+1} \Pi_j^2 = H + M$. So we see that the left hand side of inequality (1.1) is,

$$\sum_{i=1}^{n} (\lambda_{n+1} - \lambda_i)^{-1} \langle u_i, (H + M)u_i \rangle = \sum_{i=1}^{n} (\lambda_{n+1} - \lambda_i)^{-1} (\lambda_i + M).$$

For the right hand side we must compute the commutators

$$\begin{aligned}
[\Pi_j, G_j] = [-i\frac{\partial}{\partial x_j}, x_j] &= -i \ , \qquad j = 1, \ldots, \nu \\
[\Pi_{\nu+1}, G_{\nu+1}] &= 0 \ .
\end{aligned}$$

And the double commutators,

$$
\begin{aligned}
\Big[G_j,[H,G_j]\Big] &= \Big[x_j,[-\Delta + i\nabla\cdot\mathbf{A} + i\mathbf{A}\cdot\nabla, x_j]\Big] \\
&= \Big[x_j,(-2\frac{\partial}{\partial x_j} + 2iA_j)\Big] \\
&= 2\,, \qquad j = 1,\ldots,\nu
\end{aligned}
$$

$$
\Big[G_{\nu+1},[H,G_{\nu+1}]\Big] = 0\,.
$$

Thus, the right hand side of inequality (1.1) is

$$
\frac{\left|\sum_{j=1}^{\nu} Tr(P)\right|^2}{2\,\sum_{j=1}^{\nu} Tr\Big(P\cdot 2\Big)} = \frac{\nu n}{4}
$$

and by the theorem,

$$
\sum_{i=1}^{n} \frac{\lambda_i + M}{\lambda_{n+1} - \lambda_i} \geq \frac{\nu n}{4}. \quad \Box
$$

Example 4: The bi-Laplacian

The operator $H = \Delta^2$ on $L^2(\mathbf{\Omega})$ where $\mathbf{\Omega} \subset \mathbf{R}^\nu$ is a bounded domain with smooth boundary has applications in the theory of elasticity. Compare with [3] and [13] p. 633. In particular, the problem

$$
\begin{aligned}
\Delta^2 u_i &= \mu_i u_i \quad \text{in } \mathbf{\Omega} \\
u_i = \frac{\partial u_i}{\partial n} &= 0 \quad \text{on } \partial\mathbf{\Omega}
\end{aligned}
$$

is related to the modes of vibration of a clamped plate. This problem was studied by Payne, Pólya, and Weinberger in [16] where they obtained the bound

$$
\mu_{n+1} - \mu_n \leq \frac{8(\nu+2)}{\nu^2 n} \sum_{i=1}^{n} \mu_i \tag{2.2}
$$

and later by Hile and Yeh in [11] where the result was improved to

$$
\sum_{i=1}^{n} \frac{\sqrt{\mu_i}}{\mu_{n+1} - \mu_i} \geq \frac{\nu^2 n^{\frac{3}{2}}}{8(\nu+2)} \left(\sum_{i=1}^{n} \mu_i\right)^{-\frac{1}{2}}. \tag{2.3}
$$

We now recover the result of [11] by applying Theorem 1.1. Assume that the eigenvalues are enumerated in the usual way. The choice for the auxiliary operators for this case is

$$
\begin{aligned}
\Pi_j &= -i\frac{\partial}{\partial x_j} \\
G_j &= x_j
\end{aligned}
$$

where $j = 1, \dots, \nu$.

The left hand side of equation (1.1) is then

$$\sum_{i=1}^{n}(\mu_{n+1}-\mu_i)^{-1}\langle u_i, -\Delta u_i\rangle \le \sum_{i=1}^{n}(\mu_{n+1}-\mu_i)^{-1}\langle u_i, u_i\rangle^{\frac{1}{2}}\langle u_i, \Delta^2 u_i\rangle^{\frac{1}{2}}$$

$$= \sum_{i=1}^{n}(\mu_{n+1}-\mu_i)^{-1}\mu_i^{\frac{1}{2}}$$

where the Schwarz inequality and the boundary conditions were used to obtain the inequality.

For the right hand side we again have $[\Pi_j, G_j] = -i$. And now the double commutators are

$$\Big[G_j, [H, G_j]\Big] = \Big[x_j, [\Delta^2, x_j]\Big] = \Big[x_j, 4\partial_j\Delta\Big] = -4(\Delta + 2\partial_j^2)$$

so that

$$\sum_{j=1}^{\nu}\Big[G_j, [H, G_j]\Big] = 4(\nu+2)(-\Delta).$$

Then, again applying the Schwarz inequality and the boundary conditions we have

$$\sum_{i=1}^{n}\langle u_i, -\Delta u_i\rangle \le \left(\sum_{i=1}^{n}\langle u_i, u_i\rangle\right)^{\frac{1}{2}}\left(\sum_{i=1}^{n}\langle u_i, \Delta^2 u_i\rangle\right)^{\frac{1}{2}}.$$

So for the right hand side of equation (1.1) we have

$$\frac{(\nu n)^2}{8(\nu+2)n^{\frac{1}{2}}}\left(\sum_{i=1}^{n}\mu_i\right)^{-\frac{1}{2}}$$

and so by the theorem we have

$$\sum_{i=1}^{n}\frac{\mu_i^{\frac{1}{2}}}{\mu_{n+1}-\mu_i} \ge \frac{\nu^2 n^{\frac{3}{2}}}{8(\nu+2)}\left(\sum_{i=1}^{n}\mu_i\right)^{-\frac{1}{2}}$$

as in [11]. $\square$

3 NEUMANN BOUNDS

As a final use of our techniques, we obtain an entirely new bound for the spectral geometry of the Laplacian with Neumann boundary conditions. We shall show that gaps in the spectrum of the Laplacian are controlled, inversely, by the inradius, which by definition is the radius of the largest inscribed ball. The inradius is known to control the ground state of the Dirichlet Laplacian, and thus to play an important role in the spectral geometry for that operator (cf. [2] and [5]). On the other hand, we believe that the constant we obtain is far from optimal.

Since the Neumann Laplacian has a zero eigenvalue, and in our technique we need it to dominate another expression, we let $H_M := -\Delta + M$, where M is a positive constant to be specified below. The addition of the constant M obviously does not affect any commutators with H. Let $\tilde{u}$ be the first nonconstant radial Neumann L^2 – normalized eigenfunction for the unit ball and let $\widetilde{\lambda}$ be the corresponding eigenvalue.

PROPOSITION 3.1 *Let* $\mathbf{\Omega}$ *be a domain in* R^ν *with piecewise smooth boundary and inradius* r*, and let* λ_k *be the eigenvalues of the Neumann Laplacian for* $\mathbf{\Omega}$*. Then*

$$\left\langle \frac{\lambda_\ell + M}{\lambda_{n+1} - \lambda_\ell} \right\rangle_{\ell \le n} \ge \frac{K}{n+1},$$

where:

$$M := \frac{\widetilde{\lambda}^2 \|\tilde{u}\|_\infty^2}{4r^2 \|\nabla \tilde{u}\|_\infty^2}$$

and

$$K := \frac{r^\nu \widetilde{\lambda}}{8\,|\mathbf{\Omega}|\,\|\nabla \tilde{u}\|_\infty^2}.$$

REMARK: This complicated expression implies a somewhat simpler bound of the form

$$\lambda_{n+1} - \lambda_n \le (n+1)\left(A\,\langle \lambda_\ell \rangle_{\ell \le n} + B\right),$$

where A and B depend only on the inradius r and $\mathbf{\Omega}$.

PROOF: The special choices are $G := \tilde{u}$, centered at the center of the inscribed ball and with variable $|x|/r$ in the ball and extended as a constant outside the ball, and $\Pi := i\,[H, G] \; = i\,(-\Delta G - 2\nabla G \cdot \nabla)$.

According to our usual calculation,

$$\left\langle \frac{\lambda_\ell + M}{\lambda_{n+1} - \lambda_\ell} \right\rangle_{\ell \le n} \ge \frac{|Tr\,(P[G,[H,G]])|^2}{2(n+1)\beta Tr\,(P[G,[H,G]])} = \frac{Tr\left(P\,|\nabla G|^2\right)}{(n+1)\beta}, \tag{3.1}$$

where β is any constant such that

$$\|\,(\Delta G)\,\zeta + 2\nabla G \cdot \nabla \zeta\|^2 \;\le \beta\left(\|\nabla \zeta\|^2 + M\|\zeta\|^2\right)$$

for all ζ in the quadratic form domain of the Neumann Laplacian.

Since the left side of this expression is

$$\left\| \frac{\widetilde{\lambda}}{r^2} \tilde{u}\left(\frac{x}{r}\right)\zeta + \frac{2}{r}\nabla \tilde{u}\left(\frac{x}{r}\right) \cdot \nabla \zeta \right\|^2 \le \frac{2\widetilde{\lambda}^2 \|\tilde{u}\|_\infty^2}{r^4}\|\zeta\|^2 \;+\; \frac{8}{r^2}\|\nabla \tilde{u}\|_\infty^2 \|\nabla \zeta\|^2$$

(the cross term has been estimated by $2ab \le a^2 + b^2$), we can take

$$\beta := \frac{8}{r^2}\|\nabla \tilde{u}\|_\infty^2 \;\text{ and }\; M := \frac{\widetilde{\lambda}^2 \|\tilde{u}\|_\infty^2}{4r^2 \|\nabla \tilde{u}\|_\infty^2}.$$

Since the ground state is $1/\sqrt{|\mathbf{\Omega}|}$, we estimate the numerator of equation (3.1) by

$$Tr(P\,|\nabla G|^2) \geq \int |\nabla G|^2 \frac{1}{|\mathbf{\Omega}|},$$

which

$$= \frac{r^\nu \widetilde{\lambda}}{r^2\,|\mathbf{\Omega}|},$$

and the claim follows. □

ACKNOWLEDGEMENTS

The first author is grateful to the Georgia Tech Foundation for support and to the Centre de Physique Théorique, Luminy, France, and the Université de Toulon, France, for hospitality while part of this work was performed.

The second author would like to thank the Mittag-Leffler Institute, Djursholm, Sweden, for their hospitality while some of this work was carried out.

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