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THE EIGENVALUE GAP FOR ONE-DIMENSIONAL CONVEX POTENTIALS

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ABSTRACT. For Schrödinger operators on an interval with convex potentials, the gap between the two lowest eigenvalues is minimized when the potential is constant.

1. INTRODUCTION

The Schrödinger operator $-\Delta + V(x)$ on a compact domain $\Omega \subset \mathbb{R}^n$ with Dirichlet or Neumann boundary conditions has discrete spectrum $E_1 < E_2 \leq E_3 \leq \cdots$, for bounded V. The gap $\Gamma = E_2 - E_1$ has attracted some interest. In [6], improving the result of [5], it was shown that if V and Ω are convex, $\Gamma \geq \pi^2/d^2$, where d is the diameter of Ω. In the one-dimensional case $\Omega = [-a, a]$, Ashbaugh and Benguria [2, 3] showed that if V is a symmetric single well potential, i.e., $V(x) = V(-x)$ and V is nondecreasing on $[0, a]$, then

$$\Gamma \geq \frac{3}{4}\left(\frac{\pi}{a}\right)^2, \tag{1.1}$$

and this is just the gap for V = const. They point out that nonsymmetric single wells can have smaller gaps but make the conjecture that among convex potentials on a convex domain the constant potentials minimize the gap. The above results are all for Dirichlet boundary conditions. Here we verify the one-dimensional conjecture for Dirichlet and Neumann boundary conditions.

One reason for our interest in this question is that the gap can be used to estimate the difference between a normalized solution u of the differential equation $-u'' + Vu = Eu$ and a multiple of the normalized ground state solution u_1, for E close to E_1. If H is the Schrödinger operator on $L^2([0, a])$ with Neumann boundary conditions, then u is in the domain of $(H - E_1)^{\frac{1}{2}}$, so, by spectral

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theory,

$$\begin{aligned}
\|u-\langle u, u_1\rangle u_1\|^2 &\le (E_2-E_1)^{-1}\,\|(H-E_1)^{\frac12}u\|^2\\
&=(E_2-E_1)^{-1}\int_0^a(|u'|^2+(V-E_1)|u|^2)\,dx\\
&=(E_2-E_1)^{-1}\left\{\int_0^a(-u''+(V-E_1)u)\bar u\,dx+u'(a)\overline{u(a)}-u'(0)\overline{u(0)}\right\}\\
&=\frac{E-E_1+u'(a)\overline{u(a)}-u'(0)\overline{u(0)}}{E_2-E_1}.
\end{aligned}$$

If the lowest Dirichlet and Neumann eigenvalues are close compared to E_2-E_1, then this result implies that the eigenfunctions are close, so the above result implies a similar one for the Dirichlet case. (The Dirichlet and Neumann eigenvalues will be close if the boundary values of V are large compared to its minimum.)

2. Preliminaries

Suppose that V is continuous on $[0, R]$, and let H be the selfadjoint operator on $L^2([0, R])$ given by $-d^2/dx^2+V(x)$ with Dirichlet or Neumann boundary conditions. H has spectrum $\{E_1<E_2<\cdots\}$ with corresponding normalized eigenfunctions $u_1, u_2, \ldots$. Basic to our work is the observation [1, 2] that if u_1 and u_2 are chosen positive near 0 so that $u_1>0$ on $(0, R)$ and, for some $x_0\in(0, R)$, $u_2>0$ on $(0, x_0)$ and $u_2<0$ on (x_0, R), then u_2/u_1 is decreasing on $(0, R)$. In fact

$$\begin{aligned}
\left(\frac{u_2(x)}{u_1(x)}\right)' &= u_1(x)^{-2}[u_2'(x)u_1(x)-u_2(x)u_1'(x)]\\
&=\frac{1}{u_1(x)^2}\int_0^x(E_1-E_2)u_1(s)u_2(s)\,ds<0
\end{aligned}$$

for $0<x<x_0$, and similarly

$$\left(\frac{u_2(x)}{u_1(x)}\right)' = -\frac{1}{u_1(x)^2}\int_x^R(E_1-E_2)u_1(s)u_2(s)\,ds<0$$

for $x_0<x<R$. Thus we have points $x_\pm$ with

$$0\le x_-<x_0<x_+\le R$$

and

$$u_2^2>u_1^2 \quad \text{on } (0, x_-)\cup(x_+, R), \qquad u_2^2<u_1^2 \quad \text{on } (x_-, x_+).$$

Neither of these sets is empty, since u_1 and u_2 are normalized.

We shall also need the standard formula for the derivative of E_j when V is changed. If $V(\tau, \cdot)$ is a one-parameter family of continuous potentials, differentiable in sup norm topology, and $E_j(\tau)$ is the jth eigenvalue of the corresponding Schrödinger operator,

$$\frac{dE_j(\tau)}{d\tau}=\int_0^R\frac{\partial V}{\partial\tau}(\tau, x)u_j(x)^2\,dx.$$

Then, if $\Gamma(\tau) = E_2(\tau) - E_1(\tau)$,

$$\frac{d}{d\tau}\Gamma(\tau) = \int_0^R \frac{\partial V}{\partial \tau}(\tau, x)(u_2(x)^2 - u_1(x)^2)\,dx. \tag{2.1}$$

The fact, proved in [1, 2], that among symmetric single well potentials the gap is minimized at constant V follows easily: If V is such a potential and $V(\tau, x) = \tau V(x)$, we have

$$\begin{aligned}\frac{d\Gamma(\tau)}{d\tau} &= \int_{(0, x_-)\cup(x_+, R)} V(x)(u_2(x)^2 - u_1(x)^2)\,dx \\ &\quad + \int_{x_-}^{x_+} V(x)(u_2(x)^2 - u_1(x)^2)\,dx \\ &\geq 0,\end{aligned}$$

because $V(x) \geq V(x_+) = V(x_-)$ and $u_2^2 - u_1^2 > 0$ in the first integral and $V(x) \leq V(x_+)$ and $u_2^2 - u_1^2 < 0$ in the second. Equality holds only if V is constant.

3. Convex potentials

If V is convex on $[0, R]$, then it is continuous on $(0, R)$ and the continuous extension to $[0, R]$ defines the same Schrödinger operator, so we may take V continuous.

Theorem 3.1. *Let V be convex on $[0, R]$, and let E_1 and E_2 be the first two eigenvalues for the Dirichlet [Neumann] Schrödinger operator $-d^2/dx^2 + V$ on $[0, R]$. Then $E_2 - E_1 \geq \Gamma_0$ where Γ_0 is the gap for constant V for the Dirichlet [Neumann] operator with equality only if V is constant.*

Thus, for the Dirichlet operator,

$$E_2 - E_1 \geq \frac{3\pi^2}{R^2}, \tag{3.1}$$

while, for the Neumann,

$$E_2 - E_1 \geq \frac{\pi^2}{R^2}. \tag{3.2}$$

We first reduce to the linear case and then handle this case.

Lemma 3.2. *If V is convex but not linear, there is a linear potential with a smaller gap.*

Proof. If W is convex and not linear, the corresponding Dirichlet or Neumann Schrödinger operator has points $x_\pm$, as in the previous section. If L_W is the linear function satisfying

$$L_W(x_\pm) = W(x_\pm),$$

then

$$\int_0^R (W(x) - L_W(x))(u_2(x)^2 - u_1(x)^2)\,dx > 0, \tag{3.3}$$

since both factors in the integrand are nonnegative on $(0, x_-) \cup (x_+, R)$ and both are nonpositive on (x_-, x_+) and at least one of these products is positive on some open set since W is not linear.

Define a one-parameter family of potentials

$$(3.4)\qquad \begin{aligned} &V(0, x) = V(x), \\ &\frac{\partial V}{\partial t}(t, x) = L_{V(t,\cdot)}(x) - V(t, x), \qquad 0 < x \le R. \end{aligned}$$

If $\Gamma(t)$ is the gap for $V(t, x)$, then $\Gamma'(t) < 0$ by (2.1) and (3.4). If

$$L_{V(t,\cdot)}(x) = a(t)x + b(t),$$

then

$$V(t, x) = e^{-t}V(x) + \int_0^t e^{s-t}(a(s)x + b(s))\, ds,$$

so $V(t, \cdot)$ differs from a linear function by at most $\exp(-t)\|V\|_\infty$, and the eigenvalues of $V(t, \cdot)$ are correspondingly close to those of the linear potential. □

So it is enough to show that for linear potentials the gap is minimized by the constant potential. First we note that the gap goes to infinity with the slope of the potential. We need only consider the case $a > 0$. If

$$-u''(x) + ax\, u(x) = \lambda u(x), \qquad 0 < x < R,$$

then $u_\alpha(x) = u(x/\alpha)$ satisfies

$$-u_\alpha''(x) + \alpha^{-3}ax\, u_\alpha(x) = \alpha^{-2}\lambda u_\alpha(x), \qquad 0 < x < \alpha R,$$

so $\alpha^{-2}\lambda$ is an eigenvalue for the potential $\alpha^{-3}ax$ on $[0, R\alpha]$ if and only if λ is an eigenvalue for ax on $[0, R]$. Thus, writing $\Gamma(V, R)$ for the gap for potential V on $[0, R]$, we find, taking $\alpha = a^{1/3}$, that

$$\Gamma(ax, R) = a^{2/3}\Gamma(x, a^{1/3}R).$$

As $a \to \infty$, $\Gamma(x, a^{1/3}R) \to \Gamma(x, \infty) > 0$. (The eigenvalues for $[0, a^{1/3}R]$ are bounded below by those of $[0, \infty)$. On the other hand, because of the rapid decay of eigenfunctions under the infinite barrier, they can be modified to get good trial functions for the $[0, a^{1/3}R]$ problem.) It follows that $\Gamma(ax, R) \to \infty$ as $a \to \infty$.

From this we see that there must be a gap minimizing potential V_0 in the class of linear ones. We may assume that $V_0(x) = ax$ for $a \ge 0$. A linear perturbation cannot decrease the gap, so by (2.1)

$$(3.5)\qquad \int_0^R x(u_2(x)^2 - u_1(x)^2)\, dx = 0$$

if u_1 and u_2 are the first two eigenfunctions for V_0. (This appears unlikely if $a > 0$, since the expected value of potential energy should be higher for u_2 than for u_1, but a proof of this seems elusive.) To show $V_0 = 0$, we use the following results which are similar to those in [3].

Lemma 3.3. *If g is three times differentiable, $g(0) = 0$, and u is real and satisfies*

$$-u''(x) + V(x)u(x) = \lambda u(x), \qquad 0 \le x \le R,$$

with Dirichlet or Neumann boundary conditions at the endpoints, then

$$\begin{aligned}
g(R)&(u'(R)^2 + (\lambda - V(R))u(R)^2) - g(0)[u'(0)^2 + (\lambda - V(0))u(0)^2] \\
&+ \frac{1}{2}[g''(R)u(R)^2 - g''(0)u(0)^2] \\
&= \int_0^R \left[2g'(x)(\lambda - V(x)) - g(x)V'(x) + \frac{g'''(x)}{2}\right] u(x)^2\,dx\,.
\end{aligned}$$

Proof. We have

$$\begin{aligned}
g(R)&[u'(R)^2 + (\lambda - V(R))u(R)^2] - g(0)[u'(0)^2 + (\lambda - V(0))u(0)^2] \\
&= \int_0^R \frac{d}{dx}\{g(x)[u'(x)^2 + (\lambda - V(x))u(x)^2]\}\,dx \\
&= \int_0^R \{g'(x)[u'(x)^2 + (\lambda - V(x))u(x)^2] - g(x)V'(x)u(x)^2\}\,dx
\end{aligned}$$

and

$$\begin{aligned}
0 &= \int_0^R (g'(x)u'(x)u(x))'\,dx \\
&= \int_0^R \{g''(x)u'(x)u(x) + g'(x)[u'(x)^2 + (V(x) - \lambda)u(x)^2]\}\,dx \\
&= \int_0^R \left\{g'(x)[u'(x)^2 + (V(x) - \lambda)u(x)^2] - \frac{g'''(x)}{2}u(x)^2\right\}\,dx \\
&\quad + \frac{1}{2}[g''(R)u(R)^2 - g''(0)u(0)^2].
\end{aligned}$$

Combining these gives the result. □

Now, taking $g(x) = x$ and $V = V_0 = ax$, we get

$$R(u'(R)^2 + (\lambda - aR)u(R)^2) = \int_0^R (2\lambda - 3ax)u(x)^2\,dx \tag{3.6}$$

and, with $g(x) = x^2$,

$$R(u'(R)^2 + (\lambda - aR)u(R)^2) = \frac{1}{R}\int_0^R x(4\lambda - 5ax)u(x)^2\,dx\,. \tag{3.7}$$

So

$$2\lambda = \left(3a + \frac{4\lambda}{R}\right)\int_0^R xu(x)^2 - \frac{5a}{R}\int_0^R x^2u(x)^2\,dx + (u(0)^2 - u(R)^2)R^{-1}. \tag{3.8}$$

If we write

$$\langle x\rangle = \int_0^R xu_1^2(x)\,dx = \int_0^R xu_2^2(x)\,dx\ ,$$

we obtain

$$\begin{aligned}
2(E_2 - E_1)&\left(1 - \frac{2}{R}\langle x\rangle\right) - R^{-1}[u_2(0)^2 - u_2(R)^2 - u_1(0)^2 + u_1(R)^2] \\
&= -\frac{5a}{R}\int_0^R x^2(u_2(x)^2 - u_1(x)^2)\,dx \qquad (3.9)\\
&= -\frac{5a}{R}\int_0^R (x^2 - Ax - B)(u_2(x)^2 - u_1(x)^2)\,dx\,.
\end{aligned}$$

The right-hand side is negative if $a > 0$, by the argument for (3.3), choosing A and B, so the first factor vanishes at $x_\pm$.

In the Dirichlet case, this gives $\langle x \rangle < R/2$. The same is true in the Neumann case: Taking $g = 1$ in Lemma 3.3 gives

$$u_j(0)^2 - u_j(R)^2 = aE_j^{-1}(1 - Ru_j(R)^2).$$

By the differential equation and Neumann boundary condition, it is easy to see that u_1 is decreasing, so the right side of this equation is positive for $j = 1$. Now (3.5) implies $u_1(R)^2 \le u_2(R)^2$, so subtraction shows that the boundary term in (3.9) is positive.

We get a contradiction when $a > 0$ from the following:

Lemma 3.4. *If $u_\tau > 0$ is the normalized ground state for the operator $-d^2/dx^2 + \tau x$ on $L^2([0, R])$ with Dirichlet or Neumann boundary condition, then, if $\tau > 0$,*

$$\int_0^R x u_\tau(x)^2 \, dx < \frac{R}{2}.$$

Proof. For $\tau = 0$ we have

$$\int_0^R x u_0(x)^2 \, dx = \frac{R}{2}.$$

But, writing $E_j(\tau)$ for the jth eigenvalue of the operator in question and u_j for the jth normalized eigenfunction $(j > 1)$,

$$\begin{aligned} \frac{d}{d\tau} \int_0^R x|u_\tau(x)|^2 \, dx &= \frac{d^2}{d\tau^2} E_1(\tau) \\ &= -\sum_{j \ne 1} (E_j(\tau) - E_1(\tau))^{-1} |\langle u_\tau , \tau x u_j \rangle|^2 < 0 , \end{aligned}$$

using the standard formula for the second derivative of an eigenvalue [4]. □

Remarks. 1. It would be more satisfying to have an estimate of the gap that takes convexity into account in a quantitative way. A scaling argument similar to the one given above for linear potentials shows that $\Gamma(\kappa^2 x^2, R) \sim 4\kappa$ as $\kappa \to \infty$.

2. The class of convex potentials does not include all of the symmetric single well potentials treated in [1, 2]. It would be interesting to find a general class of potentials for which constant potentials minimize the gap.

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