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A COMPARISON THEOREM OF THE EIGENVALUE GAP FOR ONE-DIMENSIONAL BARRIER POTENTIALS

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ABSTRACT. The fundamental gap between the lowest two Dirichlet eigenvalues for a Schrödinger operator $H_R = -\frac{d^2}{dx^2} + V(x)$ on $L^2([-R,R])$ is compared with the gap for a same operator H_S with a different domain $[-S,S]$ and the difference is exponentially small when the potential has a large barrier.

1. Introduction

It is well known that all eigenvalues of one dimensional Schrödinger operators and the lowest eigenvalue of higher dimensional Schrödinger operators are nondegenerate. Although general bounds on gap between any consecutive eigenvalues has been considered in the various situations[4, 6], the fundamental gap between the first two eigenvalues has particular attraction because it represents the first excitation energy as well as can be used to estimate the probability of quantum tunneling[5]. One can easily see an upper bound for the gap as $\lambda_1 - \lambda_0 \le 3\lambda_0$ but it is not easy to find a lower bound. For symmetric single well potentials or convex potentials, the gap satisfies

$$\lambda_1 - \lambda_0 \ge \frac{3}{4}\left(\frac{\pi}{S}\right)^2 \tag{1}$$

where domain is $[0,S]$ (see [1, 7]).

Since barrier potential on $[0,R]$ cut off onto $[0,S]$ at some suitable point S (usually the first peak) would be a single well, it is natural to

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guess that the gap for barrier potentials would not differ much from the one of a single well. So we show the difference is exponentially small. It would be interesting in calculating gap between two consecutive eigenvalues but we need more knowledge about eigenfunctions within the technique used here.

2. A Comparison Theorem

Consider a Schrödinger operator $H_R = -\frac{d^2}{dx^2} + V(x)$ on $L^2([-R, R])$ with Dirichlet boundary condition at the end points. Let $\lambda_i(R)$ be the two lowest eigenvalues for $H_R (i = 0, 1)$. Also we define $\lambda_i(S)$ the lowest two Dirichlet eigenvalues for $H_S = -\frac{d^2}{dx^2} + V(x)\chi_{[-S,S]}$ on $L^2([-S, S])$. Let $x_1(\lambda) = \inf\{x \in [0, S] \,|V(x) \geq \lambda\}$ and $x_2(\lambda) = \sup\{x \in [0, S] \,|V(x) \geq \lambda\}$ i.e., $[x_1(\lambda), x_2(\lambda)]$ is the least interval containing the classically forbidden region. The following proposition is a kind of WKB estimate of wave functions. Let

$$B(\lambda) = \exp\left(-2\int_{x_1(\lambda)}^{x_2(\lambda)} \sqrt{V(x) - \lambda}dx\right). \tag{2}$$

PROPOSITION 2.1. *Suppose that* $-\varphi''(x) + V(x)\varphi(x) = \lambda\varphi(x)$ *with* $\varphi(0) = 0$. *For any* $0 < \delta < x_2(\lambda) - x_1(\lambda)$, *if*

$$\varphi'(x_2(\lambda))\varphi(x_2(\lambda)) \leq 0 \tag{3}$$

then

$$\begin{aligned} &\int_{x_2(\lambda)-\delta}^{x_2(\lambda)} (V(x) - \lambda) |\varphi(x)|^2 dx \\ \leq\ &\exp\left(-2\int_{x_1(\lambda)}^{x_2(\lambda)-\delta} \sqrt{V(x) - \lambda}dx\right) \int_0^{x_1(\lambda)} (\lambda - V(x)) |\varphi(x)|^2 dx. \end{aligned}$$

Proof. For $F(x)$ differentiable and $F(x) \equiv 1$ on $[0, x_1(\lambda)]$, note that

$$
\begin{aligned}
& F(x)\varphi'(x)\varphi(x)\Big|_0^{x_2(\lambda)-\delta} \\
(4) \qquad & = \int_0^{x_2(\lambda)-\delta}\left[F'\frac{\varphi'\overline{\varphi}+\varphi\overline{\varphi}'}{2}+F\left((V-\lambda)\left|\varphi\right|^2+\left|\varphi'\right|^2\right)\right]dx \\
& \geq \int_{x_1(\lambda)}^{x_2(\lambda)-\delta}\left[(V-\lambda)\left|\varphi\right|^2+\left|\varphi'\right|^2\right]\left(F-\frac{|F'|}{2\sqrt{V-\lambda}}\right)dx \\
& \quad -\int_0^{x_1(\lambda)}(\lambda-V)\left|\varphi\right|^2 dx
\end{aligned}
$$

using the inequality $ab = (a\sqrt{c})\,(b/\sqrt{c}) \geq -\frac{a^2c^2+b^2}{2c}$ and choosing $c = \sqrt{V(x)-\lambda}$. Define $F(x)$ as follows:

$$
F(x) = \begin{cases} \exp\left(2\int_{x_1(\lambda)}^{x}\sqrt{V(t)-\lambda}dt\right) & \text{on} \quad x \geq x_1(\lambda) \\ 1 & \text{on} \quad 0 \leq x < x_1(\lambda). \end{cases}
$$

The choice of $F(x)$ makes the first integrals in (4) vanish and gives

$$
\begin{aligned}
& \varphi'(x_2(\lambda)-\delta)\varphi(x_2(\lambda)-\delta) \\
\leq \; & \exp\left(-2\int_{x_1(\lambda)}^{x_2(\lambda)-\delta}\sqrt{V(x)-\lambda}dx\right)\int_0^{x_1(\lambda)}(\lambda-V(x))\left|\varphi(x)\right|^2 dx.
\end{aligned}
$$

Similarly we have

$$
\varphi'(x)\varphi(x)\Big|_{x_2(\lambda)-\delta}^{x_2(\lambda)} = \int_{x_2(\lambda)-\delta}^{x_2(\lambda)}\left(\left|\varphi'(x)\right|^2+(V(x)-\lambda)\left|\varphi(x)\right|^2\right)dx
$$

so that by hypothesis

$$
\begin{aligned}
& \int_{x_2(\lambda)-\delta}^{x_2(\lambda)}(V(x)-\lambda)\left|\varphi(x)\right|^2 dx \\
\leq \; & \varphi'(x)\varphi(x)\Big|_{x_2(\lambda)-\delta}^{x_2(\lambda)} \\
\leq \; & \exp\left(-2\int_{x_1(\lambda)}^{x_2(\lambda)-\delta}\sqrt{V(x)-\lambda}dx\right)\int_0^{x_1(\lambda)}(\lambda-V(x))\left|\varphi(x)\right|^2 dx. \qquad \square
\end{aligned}
$$

As we see in [3], gap could be small when $V(x)$ is double well. So we need to rule out the case. If $V(x) \geq \lambda$ on $[x_1(\lambda), x_2(\lambda)]$, the following holds:

COROLLARY 2.2. *Assume that φ satisfies (3). If $V(x) \geq 0$ on $[0, S]$, $V(x) \geq \lambda$ on $[x_1(\lambda), x_2(\lambda)]$ and*

$$\int_{x_1(\lambda)}^{x_2(\lambda)} \sqrt{V(x) - \lambda}\,dx \geq 1,$$

then we have

$$\int_{x_2(\lambda)-\delta}^{x_2(\lambda)} (V(x) - \lambda) |\varphi(x)|^2 \, dx \leq e^2 \lambda B(\lambda) \int_0^{x_1(\lambda)} |\varphi(x)|^2 \, dx.$$

Proof. Since $V(x) \geq 0$ for $0 \leq x \leq S$,

$$\begin{aligned}
&\int_{x_2(\lambda)-\delta}^{x_2(\lambda)} \big(V(x) - \lambda\big) |\varphi(x)|^2 \, dx \\
\leq\ & \exp\Big(-2 \int_{x_1(\lambda)}^{x_2(\lambda)-\delta} \sqrt{V(x) - \lambda}\,dx \Big) \int_0^{x_1(\lambda)} (\lambda - V(x)) |\varphi(x)|^2 \, dx \\
\leq\ & e^2 \lambda B(\lambda) \int_0^{x_1(\lambda)} |\varphi(x)|^2 \, dx.
\end{aligned}$$

□

Corollary 2.2 implies that eigenvalues are insensitive to boundary conditions when barrier is high. The next Lemma holds for Neumann eigenvalues too.

LEMMA 2.3. *Suppose that $0 \leq V(x) \leq C([0, S])$ and for real β, E_β is the lowest eigenvalue of the operator $H_\beta = -\frac{d^2}{dx^2} + V(x)$ on $L^2([0, S])$ with the Dirichlet boundary condition at 0 and $\varphi'(S) = \beta\varphi(S)$. Let E_∞ be the one for $\varphi(S) = 0$. For each $\beta \leq 0$, if $V(x) \geq E_\beta$ on $[x_1(E_\beta), x_2(E_\beta)]$ and*

$$\int_{x_1(E_\beta)}^{x_2(E_\beta)} \sqrt{V(x) - E_\beta}\,dx \geq 1,$$

then

$$0 \leq E_\infty - E_\beta \leq e^2 E_\beta B(E_\beta).$$

Proof. For any $\varphi \in L^2([0,S])$ with $\varphi(0) = 0$ and $\varphi(S) = 0$,

$$\begin{aligned} E_\infty \int_0^S |\varphi(x)|^2 \, dx &= \inf_{\varphi \in \mathcal{D}(H_\beta)} (H_\beta \varphi, \varphi) \\ &\leq \int_0^S \left(|\varphi'(x)|^2 + V(x) |\varphi(x)|^2 \right) dx. \end{aligned}$$

Let ψ_β be a real normalized eigenfunction for E_β and suppose $\chi(x)$ is real, has a bounded derivative and $\chi(0) = 0$, $\chi(S) = 0$. Then

$$\begin{aligned} E_\infty \int_0^S |\chi\psi_\beta(x)|^2 \, dx &\leq \int_0^S \left(\left|(\chi\psi_\beta)'(x)\right|^2 + V(x) |\chi\psi_\beta(x)|^2 \right) dx \\ &= \int_0^S \left(|\chi'(x)\psi_\beta(x)|^2 + E_\beta |\chi\psi_\beta(x)|^2 \right) dx \end{aligned}$$

so that

$$E_\infty - E_\beta \leq \frac{\int_0^S |\chi'(x)\psi_\beta(x)|^2 \, dx}{\int_0^S |\chi\psi_\beta(x)|^2}.$$

Choose

$$\chi(x) = \begin{cases} 1 & 0 \leq x < x_2(E_\beta) - \delta_\beta \\ \int_x^{x_2(E_\beta)} \sqrt{V(t) - E_\beta} dt & x_2(E_\beta) - \delta_\beta \leq x \leq x_2(E_\beta) \\ 0 & x_2(E_\beta) \leq x \leq S \end{cases}$$

where δ_β is chosen so that

$$\int_{x_2(E_\beta)-\delta_\beta}^{x_2(E_\beta)} \sqrt{V(x) - E_\beta} dx = 1.$$

By Corollary 2.2 we have

$$\begin{aligned} \int_0^S |\chi'\psi_\beta(x)|^2 \, dx &\leq \int_{x_2(E_\beta)-\delta_\beta}^{x_2(E_\beta)} (V(x) - E_\beta) |\psi_\beta(x)|^2 \, dx \\ &\leq e^2 E_\beta B(E_\beta) \int_0^{x_1(E_\beta)} |\psi_\beta(x)|^2 \, dx \\ &\leq e^2 E_\beta B(E_\beta) \int_0^S |\chi\psi_\beta(x)|^2 \, dx \end{aligned}$$

since $x_1(E_\beta) \leq x_2(E_\beta) - \delta_\beta$ and $\chi \equiv 1$ on $[0, x_2(E_\beta) - \delta_\beta]$. □

As in [2], existence of eigenvalues of a BVP

$$(5)\qquad \begin{cases} \varphi''(x) + (\lambda - V(x))\,\varphi(x) = 0 & \text{for } x \in [a,b] \\ \varphi(a)\cos\alpha - \varphi'(a)\sin\alpha = 0 & \\ \varphi(b)\cos\beta - \varphi'(b)\sin\beta = 0 & \end{cases}$$

can be shown by Prüfer transform. One can choose an eigenfunction $\varphi(x)$ as $r(x)\sin\theta(x,\lambda)$ and its derivative $\varphi'(x)$ as $r(x)\cos\theta(x,\lambda)$ in (5) where $r(x) > 0$ so that the derivative $\varphi'(x)$ vanishes where $\theta(x,\lambda) = 1$.

THEOREM 2.4. *Suppose that $V(x)$ is continuous, positive, symmetric on $[-R,R]$. Let $\lambda_i(R)$ be the lowest two eigenvalues for the Dirichlet Schrödinger operator $H_R = -\frac{d^2}{dx^2}+V(x)$ on $L^2([-R,R])$ and $\lambda_i(S)$ for the Dirichlet Schrödinger operator $H_S = -\frac{d^2}{dx^2} + V(x)\chi_{[-S,S]}$ on $L^2([-S,S])$. Suppose $V(x) \geq \lambda_1(R)$ on $[x_1(\lambda_1(R)), x_2(\lambda_1(R))]$. If $\frac{R}{2} \leq S \leq R$, $x_2(\lambda_1(R)) = S$, and*

$$\int_{x_1(\lambda_1(R))}^{x_2(\lambda_1(R))} \sqrt{V(x) - \lambda_1(R)}\,dx \geq 1$$

then the gap satisfies

$$\lambda_1(R) - \lambda_0(R) \geq \lambda_1(S) - \lambda_0(S) - e^2\lambda_1(R)B(\lambda_1(R))$$

where $B(\lambda)$ is defined in (2).

REMARK 1. The interval $[x_1(\lambda_1(R)), x_2(\lambda_1(R))]$ satisfying the hypothesis in Theorem 2.4 could be empty for a certain class of potentials. However when a barrier is high like a radioactive model for a quantum particle, the classically forbidden region is not empty. For example consider a harmonic oscillator $\frac{d^2}{dx^2} + \frac{1}{2}kx^2$ on $L^2(\mathbf{R})$. Then it is known that the eigenvalue $E_n = \left(n + \frac{1}{2}\right)\sqrt{2k}$. The second lowest eigenvalue $E_1 = \frac{2}{3}\sqrt{2k}$ and the forbidden region corresponding to E_1 is the interval $\left(-\infty, -\frac{3\sqrt{2}}{\sqrt{k}}\right) \bigcup \left(\frac{3\sqrt{2}}{\sqrt{k}}, \infty\right)$. We would think of the barrier potential as a perturbation of a harmonic oscillator.

Proof. By Min-max principle, we know $\lambda_i(R) \leq \lambda_i(S)$ which gives

$$\begin{aligned} \lambda_1(R) - \lambda_0(R) &\geq \lambda_1(R) - \lambda_0(S) \\ &= \lambda_1(S) - \lambda_0(S) - (\lambda_1(S) - \lambda_1(R)). \end{aligned}$$

So it is enough to estimate $\lambda_1(S)-\lambda_1(R)$. Let $\psi_1(x)$ be a eigenfunction for $\lambda_1(S)$. Then it has only one zero on $(-S,S)$ and it should be 0 since $V(x)$ is symmetric. Hence $\psi_1(x)0$ is an eigenfunction for the lowest Dirichlet eigenvalue on $[0,S]$ since it has no zeros on the open interval $(0,S)$. As in notations in Lemma 2.3, $\lambda_1(S)=E_{\infty}$. The same argument works for $\lambda_1(R)=E_\beta$ by cutting the eigenfunction $\varphi_1(x)$ for $\lambda_1(R)$ onto $[-S,S]$ where $\beta=\frac{\varphi_1'(S)}{\varphi_1(S)}$. By Lemma 2.3 the estimate for $\lambda_1(S)-\lambda_1(R)$ can be obtained as long as $\beta\le 0$. The preceding remark of Lemma 2.3 says the derivative of $\varphi_1(x)$ vanishes where $\theta(x,\lambda)=1$. This occurs at $x=\frac{R}{2}$ since the domain is $[-R,R]$. Hence if $\frac{R}{2}\le S\le R$, then $\varphi_1'(x)\le 0$ as required. □

The theorem above can be applied to calculate a lower bound for eigenvalue gap approximately comparing the known result. Suppose that a symmetric high barrier potential $V(x)$ is increasing on $[0,S]$ and decreasing on $[S,R]$. If $\frac{R}{2}\le S\le R$, from (1) we know

$$\lambda_1(R)-\lambda_0(R)\ge\frac{3}{4}(\frac{\pi}{S})^2-e^2\lambda_1(R)B(\lambda_1(R)).$$

The assumption for symmetry of potential $V(x)$ can be omitted. Then the domain compared will be different like $[T,S]$ where T is the zero of $\psi_1(x)$ as in Theorem 2.4. Also positivity was adopted for a simple calculation since gap does not change by adding a constant.

References

[1] M. Ashbaugh and R. Benguria, *Optimal Lower Bound for the Gap Between the First Two Eigenvalues of One-dimensional Schrödinger Operators with Symmetric Single-well Potentials*, Proc. A. M. S. **105** (1989), 419-242.

[2] E. Coddington and N. Levinson, *Theory of Ordinary Differential Equations*, Mcgraw-Hill Book Company, Inc. 1955.

[3] E. Harrell II, *Double wells*, Comm. Math. Phys. **75** (1980), 239-261.

[4] ———, *General bounds for the eigenvalues of Schrödinger operators in Conference on Maximum principles and eigenvalue problems in partial differential equations*, University of Tennessee, Knoxville, 1987.

[5] J. Hyun, *Exponential Decay for Barrier Potentials*, J. Math. Anal. Appl. **221** (1998), 238-261.

[6] W. Kirsh and B. Simon, *Universal Lower Bounds on Eigenvalue Splitting for One-dimensional Schrödinger Operators*, Comm. Math. Phys. **97** (1985), 453-460.

[7] R. Lavine, *The Eigenvalue Gap for One-dimensional Convex Potential*, Proc. A. M. S. **121** (1994), 815-821.

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