Comm. Korean Math. Soc. **9** (1994), No. 1, pp. 79–87

THE EIGENVALUE GAP WITH SYMMETRIC SINGLE-WELL POTENTIALS FOR DIFFERENCE OPERATORS

INSUK KIM

1. Introduction

The difference Laplacian acting in $\ell^2(\mathbb{Z})$ may be regarded as a discrete version of $-\frac{d^2}{dx^2}$ in $L^2(\mathbb{R})$. Regarding $D : \varphi(n) \longmapsto \varphi(n+1) - \varphi(n)$ and $D^* : \varphi(n) \longmapsto \varphi(n-1) - \varphi(n)$ as operators in $\ell^2(\mathbb{Z})$ so that D^*D replaces $-\frac{d^2}{dx^2}$, the difference Laplacian D^*D is a self adjoint operator, and we have $D^*D\varphi(n) = -\varphi(n+1) + 2\varphi(n) - \varphi(n-1)$.

We will consider the perturbation H of D^*D, $H = D^*D + V$ on $\ell^2(\mathbb{Z}_N)$ with various boundary conditions, where $\mathbb{Z}_N = \{-N, \dots, N\}$, V multiplication by a real-valued function $V(n)$ on the integers with $\operatorname{supp} V \subset [-N, N]$.

For the difference operator on $\ell^2(\mathbb{Z}_N)$ with Dirichlet and Neumann boundary conditions, we would need the $(2N+1) \times (2N+1)$ matrix,

$$H_\gamma = \begin{pmatrix} V(-N)+2-\gamma & -1 & 0 & & & \cdots \\ -1 & V(-N+1)+2 & -1 & 0 & & \cdots \\ \vdots & & \ddots & & \vdots & \\ \cdots & & 0 & -1 & V(N-1)+2 & -1 \\ \cdots & & 0 & 0 & -1 & V(N)+2-\gamma \end{pmatrix}$$

with $\gamma = 0$ and $\gamma = 1$, respectively, analogous to the Schrödinger operator $-\frac{d^2}{dx^2} + V$ on $L^2(\mathbb{R})$ with Dirichlet and Neumann boundary conditions.

The difference operator $H = D^*D + V$ on $\ell^2(\mathbb{Z}_N)$ with Dirichlet or Neumann boundary conditions has discrete spectrum $E_1 < E_2 \le E_3 \le \cdots$, for bounded V. The gap $\Gamma = E_2 - E_1$ has attracted some interest.

Received May 18, 1993.
Supported by GARC.

Ashbaugh and Benguria [A-B-2] showed that if V is a symmetric single-well potential in $[-N, N]$, i.e. $V(n) = V(-n)$ and V is nondecreasing on $[0, N]$, then

$$\Gamma \geq 2\left[\cos\left(\frac{\pi}{2(N+1)}\right) - \cos\left(\frac{\pi}{N+1}\right)\right] \tag{1.1}$$

and this is just the gap for $V =$ constant. The above result is for Dirichlet boundary conditions. Here we verify the result with a different proof.

One reason for our interest in this question is that the gap can be used to estimate the difference between a solution φ of the difference equation $H_\gamma\varphi(n) = D^*D\varphi(n) + V(n)\varphi(n) = E\varphi(n)$ and a multiple of the normalized ground state solution φ_1, for E close to E_1. If H_1 is the difference operator on $\ell^2(\mathbb{Z}_N)$ with Neumann boundary conditions,

$$\begin{aligned}
||\varphi - <\varphi, \varphi_1> \varphi_1||^2 &\leq <\varphi, \frac{H_1 - E_1}{E_2 - E_1}\varphi> \\
&= \frac{1}{E_2 - E_1}\Big\{ \sum_{n=-N+1}^{N-1} \big[(D^*D + V(n) - E_1)\varphi(n)\big]\bar{\varphi}(n) \\
&\quad + \big(1 + V(N) - E_1\big)|\varphi(N)|^2 - \varphi(N-1)\bar{\varphi}(N) \\
&\quad + \big(1 + V(-N) - E_1\big)|\varphi(-N)|^2 - \varphi(-N+1)\bar{\varphi}(-N)\Big\} \\
&= \frac{\sum_{n=-N}^{N}(H_\gamma - E_1)|\varphi(n)|^2 + (\gamma - 1)(|\varphi(N)|^2 + |\varphi(-N)|^2)}{E_2 - E_1} \\
&= \frac{(E - E_1)||\varphi||^2 + (\gamma - 1)(|\varphi(N)|^2 + |\varphi(-N)|^2)}{E_2 - E_1}.
\end{aligned}$$

2. Preliminaries

The difference Laplacian on a graph was studied in [DOD]. In this article, two kinds of functions are defined:

Let K be an arbitrary graph, i.e., a connected simplicial complex of one dimension, and $V(K)$ be the set of vertices of K. For two vertices $x, y \in V(K)$, $x \sim y$ denotes a geometric edge (an edge without regard to its direction) connecting x and y. $[x, y]$ denotes a directed edge beginning at x and ending at y, and $E(K)$ denotes the set of all directed edges of K. Furthermore, we denote by $C^0(K)$ the space of all real-valued functions f on $V(K)$, and $C^1(K)$ the space of all functions F on $E(K)$, satisfying

$$F([x,y]) = -F([y,x]). \tag{2.1}$$

For every edge of K, we fix a direction. (Here, in our case $V(K) \subset \mathbb{Z}$ and $E(K) \subset \{[n, n+1] : n \in \mathbb{Z}\}$.)

For $f \in C^0(K)$, we define ∇ as a bounded mapping of $C^0(K)$ into $C^1(K)$ by

$$\nabla f([x,y]) = f(y) - f(x). \tag{2.2}$$

If $F \in C^1(K)$, define

$$\nabla \cdot F(x) = \sum_{y \sim x} F([x,y]), \tag{2.3}$$

as a mapping of $C^1(K)$ into $C^0(K)$. Furthermore, let us define products $fF \in C^1(K)$ for f and F as above by

$$fF([x,y]) = \frac{f(x) + f(y)}{2} F([x,y]), \tag{2.4}$$

and for F, $G \in C^1(K)$, products $F \cdot G \in C^0(K)$ by

$$(F \cdot G)(x) = \sum_{y \sim x} \frac{F([x,y])G([x,y])}{2}. \tag{2.5}$$

Note that these multiplications are commutative, but not associative, that is, $f(gF) \neq (fg)F$ and $(fF) \cdot G \neq f(F \cdot G)$.

We have

$$\begin{aligned}(\nabla \cdot fF)(x) &= \sum_{y \sim x} \frac{f(x) + f(y)}{2} F([x,y]) \qquad \text{by (2.3) and (2.4)} \\ &= \frac{1}{2} \sum_{y \sim x} (f(y) - f(x)) F([x,y]) + \sum_{y \sim x} F([x,y]) f(x) \\ &= (\nabla f \cdot F)(x) + (\nabla \cdot F) f(x).\end{aligned}$$

Moreover, notice that for $f,\, g \in C^0(K)$

$$\begin{aligned}\nabla(fg)([x,y]) &= f(y)g(y) - f(x)g(x) \qquad \text{by} \qquad (2.2)\\ &= \frac{f(x)+f(y)}{2}(g(y)-g(x)) + (f(y)-f(x))\frac{g(x)+g(y)}{2}\\ &= (f\nabla g + \nabla f g)([x,y]) \qquad \text{by} \quad (2.4) \quad \text{and} \quad (2.2).\end{aligned}$$

Hence we have formulas similar to those for ordinary functions so that

$$\nabla\cdot(f\nabla g) = \nabla f\cdot\nabla g + f\nabla\cdot\nabla g.$$

When $K \subset \mathbb{Z}$, $\nabla\cdot\nabla$ agrees with our definition of $-D^*D$, since

$$\begin{aligned}\nabla\cdot\nabla f(n) &= \sum_{n'\sim n}\nabla f([n,n']) \qquad \text{by} \qquad (2.3)\\ &= \nabla f([n,n+1]) + \nabla f([n,n-1])\\ &= f(n+1) - 2f(n) + f(n-1)\\ &= -D^*Df(n).\end{aligned}$$

We also have a version of the divergence theorem:

$$\begin{aligned}\sum_{x\in K}\nabla\cdot F(x) &= \sum_{x\in K}\Big(\sum_{y\sim x}F([x,y])\Big) \qquad \text{by} \quad (2.3)\\ &= \sum_{\substack{x,y\in K\\ y\sim x}}\big(F([x,y]) + F([y,x])\big) + \sum_{\substack{x\in K\ y\notin K\\ x\sim y}}F([x,y])\\ &= \sum_{\substack{x\in K\ y\notin K\\ x\sim y}}F([x,y]) \qquad \text{by} \quad (2.1),\end{aligned}$$

so for $f,\, \psi \in C^0(K)$

$$\sum_{x\in K}\nabla\cdot(f\nabla\psi)(x) = \sum_{\substack{x\in K\ y\notin K\\ x\sim y}}\frac{f(x)+f(y)}{2}(\psi(y)-\psi(x)). \tag{2.6}$$

3. Main Theorem.

THEOREM. *Consider $H_0 = D^* + D + V$ on $[-N, N]$ with Dirichlet boundary conditions. Suppose that V is a symmetric single-well potential so that $V(-n) = V(n)$ on $[-N, N]$ and $\nabla V([n, n+1]) \geq 0$ on $[0, N]$. If E_1 is the lowest eigenvalue and E_2, the next eigenvalue above E_1 for H_0, then*

$$E_2 - E_1 \geq 2\left[\cos\left(\frac{\pi}{2(N+1)}\right) - \cos\left(\frac{\pi}{N+1}\right)\right],$$

with equality if and only if V is constant.

Proof. For $i = 1, 2$, let

$$H_0\varphi_i = E_i\varphi_i$$

on $[-N, N]$ and define $\varphi_i(-N-1) = \varphi_i(N+1) = 0$. Notice that $(H_0 + C)^{-1}$ has positive entries and therefore φ_1 can be chosen positive ([G]) so that $\varphi_1(n) > 0$ is symmetric, $\varphi_1(-n) = \varphi_1(n)$ and $\varphi_2(-n) = -\varphi_2(n)$ for $-N \leq n \leq N$ and $\varphi_2(0) = 0$ (See Appendix). It may be assumed that $\varphi_2(n) \geq 0$ on $[-N, 0]$. Then we have that if $-N \leq n \leq 0$,

(3.1)
$$\begin{aligned}
\nabla\left(\frac{\varphi_2}{\varphi_1}\right)([n, n+1]) &= \frac{\varphi_2(n+1)}{\varphi_1(n+1)} - \frac{\varphi_2(n)}{\varphi_1(n)} \\
&= \frac{1}{\varphi_1(n+1)\varphi_1(n)}\left\{\left(\varphi_2(n+1) - \varphi_2(n)\right)\frac{\varphi_1(n+1) + \varphi_1(n)}{2}\right. \\
&\qquad \left. - \left(\varphi_1(n+1) - \varphi_1(n)\right)\frac{\varphi_2(n+1) + \varphi_2(n)}{2}\right\} \\
&= \frac{1}{\varphi_1(n+1)\varphi_1(n)}(\nabla\varphi_2\varphi_1 - \varphi_2\nabla\varphi_1)([n, n+1])
\end{aligned}$$

by noting (2.2) and (2.4). Then by using our version of the divergence theorem (2.6) and $\varphi_i(-N-1)=0$ $(i=0,1)$, the above (3.1) becomes

$$\begin{aligned}\nabla\Big(\frac{\varphi_2}{\varphi_1}\Big)([n,n+1]) &= \frac{1}{\varphi_1(n+1)\varphi_1(n)}\sum_{k=-N}^{n}\nabla\cdot(\nabla\varphi_2\varphi_1-\varphi_2\nabla\varphi_1)(k)\\ &= \frac{1}{\varphi_1(n+1)\varphi\cdot(n)}\sum_{k=-N}^{n}(-D^*D\varphi_2\varphi_1+D^*D\varphi_1\varphi_2)(k)\\ &= \frac{E_1-E_2}{\varphi_1(n+1)\varphi_1(n)}\sum_{k=-N}^{n}\varphi_1\varphi_2(k)\le 0.\end{aligned}$$

So $(\varphi_2/\varphi_1)(n)$ is decreasing as n goes from $-N$ to 0, and by symmetry $(\varphi_2/\varphi_1)(n)$ is also decreasing as n goes from 0 to N, which implies $(\varphi_2/\varphi_1)^2(n)$ is increasing as $|n|$ goes from 0 to N.

Choose the largest integer $a\in(0,N)$ so that $(\varphi_2^2/\varphi_1^2)(a)<1$. By symmetry we get $(\varphi_2^2/\varphi_1^2)(n)<1$ on $[-a,a]$ and $(\varphi_2^2/\varphi_1^2)(n)\ge 1$ on $[-N,-a-1]\cup[a+1,N]$. Since for unit eigenfuctions φ_2 and φ_1,

$$0=\Big(\sum_{n=-N}^{-a-1}+\sum_{n=-a}^{a}+\sum_{n=a+1}^{N}\Big)\Big(\frac{\varphi_2^2(n)}{\varphi_1^2(n)}-1\Big)\varphi_1^2(n),$$

if $W(n)$ is any symmetric function, increasing on $[0,N]$, we know

$$\begin{aligned}&\sum_{n=-N}^{N}\Big(\frac{\varphi_2^2(n)}{\varphi_1^2(n)}-1\Big)\varphi_1^2(n)W(n)\\ &=\sum_{n=-a}^{a}\Big(\frac{\varphi_2^2(n)}{\varphi_1^2(n)}-1\Big)\varphi_1^2(n)W(n)\\ &\qquad+\Big(\sum_{n=-N}^{-a-1}+\sum_{n=a+1}^{N}\Big)\Big(\frac{\varphi_2^2(n)}{\varphi_1^2(n)}-1\Big)\varphi_1^2(n)W(n)\\ &\ge W(a+1)\sum_{n=-N}^{N}\Big(\frac{\varphi_2^2(n)}{\varphi_1^2(n)}-1\Big)\varphi_1^2(n)=0,\end{aligned}$$

with equality if and only if W is constant. Thus it follows that

$$\sum_{n=-N}^{N} \varphi_2^2(n)W(n) \geq \sum_{n=-N}^{N} \varphi_1^2(n)W(n), \tag{3.2}$$

with equality if and only if W is constant.

Now let $H_0(\tau)$ be the operator H_0 with τV replacing V for $0 \leq \tau \leq 1$, where $V(-n) = V(n)$ and $\nabla V[n, n+1] \geq 0$ for $0 \leq n \leq N$. Let $E_j(\tau)$ be the jth eigenvalue for $H_0(\tau)$ with unit eigenvector $\varphi_j(\tau)$. Then we get

$$\begin{aligned}
&\left[E_j(\tau') - E_j(\tau)\right] \sum_{n=-N}^{N} \varphi_j(\tau)\varphi_j(\tau')(n) \\
&= \sum_{n=-N}^{N} \left(H_0(\tau')\varphi_j(\tau')\varphi_j(\tau) - H_0(\tau)\varphi_j(\tau)\varphi_j(\tau')\right)(n) \\
&= \sum_{n=-N}^{N} \left(\tau' V(n) - \tau V(n)\right)\varphi_j(\tau)\varphi_j(\tau')(n),
\end{aligned}$$

so

$$\frac{dE_j(\tau)}{d\tau} = \sum_{n=-N}^{N} V(n)\varphi_j^2(\tau)(n).$$

Thus

$$\frac{d}{d\tau}\left(E_2(\tau) - E_1(\tau)\right) = \sum_{n=-N}^{N} V(n)\left(\varphi_2^2(\tau) - \varphi_1^2(\tau)\right)(n) \geq 0,$$

by (3.2), with equality if and only if V is constant. Therefore the gap $E_2(\tau) - E_1(\tau)$ is nondecreasing with τ and we derive

$$E_2(1) - E_1(1) \geq E_2(0) - E_1(0) = 2\left[\cos\left(\frac{\pi}{2(N+1)}\right) - \cos\left(\frac{\pi}{N+1}\right)\right],$$

with equality if and only if V is constant.

References

[A] Agmon, S., *Lectures on exponential decay of solutions of second order elliptic equations*, Princeton University Press, Princeton, N.J., 1982.

[A-B-1] Ashbaugh, M. S., Benguria, R. D., *Optimal lower bound for the gap between the first two eigenvalues of one-dimensional Schrödinger operators with symmetric single-well potentials*, Proc. Amer. Math. Soc. **105** (1989), 419–424.

[A-B-2] ———, *Some eigenvalue inequalities for a class of Jacobi matrices*, Linear Algebra Appl. **136** (1990), 215–234.

[DOD] Dodziuk, J., *Difference equations, isoperimetric inequality and transience of certain random walks*, Trans. Amer. Math. Soc. **284** (1984), 787–794.

[F-L] Fernandez, C., Lavine, R., *Lower bounds for resonance widths in potential and obstacle scattering*, Comm. Math. Phys. **128** (1990), 263–284.

[G] Gantmacher, F. R., *Applications of the theory of matrices*, Interscience, New York, 1959.

[L] Lavine, R., *Spectral density and sojourn times. In: Nuttall, J.(ed.) Atomic scattering theory. London, Ontario* (1978), Univ. Western Ontario, 45–61.

[R-S] Reed, M., Simon, B., *Methods of modern mathematical physics*, vol. IV, Academic Press, New York, 1978.

Appendix

LEMMA. *Let $H_0 = D^*D + V$ on $[-N, N]$ with $V(-n) = V(n)$. For $i = 1, 2$, let $H_0\varphi_i(n) = E_i\varphi_i(n)$, where E_1 is the lowest eigenvalue and E_2, the next eigenvalue above E_1 for H_0. Then φ_2 is odd and changes sign only at 0, so we may choose φ_2 positive on $[-N, -1]$ and negative on $[1, N]$.*

Proof. We may choose $\varphi_1(n) > 0$ and $\varphi_1(-n) = \varphi_1(n)$ on $[-N, N]$. This implies φ_2 changes sign on $[-N, N]$ because $\varphi_2 \perp \varphi_1$. Furthermore, φ_2 is even or odd, because if $(J\varphi)(n) = \varphi(-n)$ we have $H_0J = JH_0$, so $H_0\varphi = \lambda\varphi$ implies $J\varphi$ is an eigenvector with same eigenvalue and so $J\varphi_2 = c\varphi_2$ and J has eigenvalue 1 or -1 with even or odd eigenvector, respectively.

If φ_2 is odd, then $\varphi_2(0) = 0$ and E_2 is an eigenvalue for $D^*D + V$ on $[-N, -1]$ with Dirichlet boundary conditions. Any other eigenvalue of this operator also is an eigenvalue of H_0 with odd eigenvector. Thus E_2 must be the lowest eigenvalue of H_0 on $[-N, -1]$ and φ_2 may be chosen positive on $[-N, -1]$ and Lemma is proved.

Suppose φ_2 is even. Then φ_2 must change sign somewhere between $-N$ and -1, say at k so that $\varphi_2(k)\varphi_2(k+1) \leq 0$.

Set

$$\varphi(j) = \begin{cases} \varphi_2(j) & \text{for} \quad j \leq k \\ 0 & \text{for} \quad j > k. \end{cases}$$

Then if E is the lowest eigenvalue with odd eigenvector, i.e., the lowest eigenvalue of the Dirichlet operator on $[-N, -1]$,

$$\begin{aligned}
E = &\inf_{\substack{\psi(0)=0 \\ \psi(-N-1)=0}} \left\{ \frac{\sum_{j=-N}^{-1}[-\psi(j+1)+(2+V(j))\psi(j)-\psi(j-1)]\psi(j)}{\sum_{j=-N}^{-1}\psi(j)^2} \right\} \\
&\leq \frac{\sum_{j=-N}^{-1}[-\varphi(j+1)+(2+V(j))\varphi(j)-\varphi(j-1)]\varphi(j)}{\sum_{j=-N}^{-1}\varphi(j)^2} \\
&= \left\{ (2+V(k))\varphi_2(k)^2 - \varphi_2(k-1)\varphi_2(k) + \sum_{j=-N}^{k-1}[-\varphi_2(j+1) \right. \\
&\qquad \left. + (2+V(j))\varphi_2(j) - \varphi_2(j-1)]\varphi_2(j) \right\} \Big/ \sum_{j=-N}^{k} \varphi_2(j)^2 \\
&\leq \left\{ \sum_{j=-N}^{k} [-\varphi_2(j+1) \right. \\
&\qquad \left. + (2+V(j))\varphi_2(j) - \varphi_2(j-1)]\varphi_2(j) \right\} \Big/ \sum_{j=-N}^{k} \varphi_2(j)^2 \\
&= E_2,
\end{aligned}$$

since $-\varphi_2(k)\varphi_2(k+1) \geq 0$. This is a contradiction, since E_2 is supposed to be the next eigenvalue above E_1 (E_2 cannot equal E since eigenvalues of H_0 are simple).

Global Analysis Research Center
Department of Mathematics
Seoul National University
Seoul 151–742, Korea