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Universal Lower Bounds on Eigenvalue Splittings for One Dimensional Schrödinger Operators

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Abstract. We provide lower bounds on the eigenvalue splitting for $-d^2/dx^2 + V(x)$ depending only on qualitative properties of V. For example, if V is C^∞ on $[a,b]$ and E_n, E_{n-1} are two successive eigenvalues of $-d^2/dx^2 + V$ with $u(a) = u(b) = 0$ boundary conditions, and if $\lambda = \max_{E\in(E_{n-1},E_n);x\in(a,b)} |E - V(x)|^{1/2}$, then

$$E_n - E_{n-1} \geqq \pi\lambda^2 \exp[-\lambda(b-a)].$$

The exponential factor in such bounds are saturated precisely in tunneling examples. Our results are *not* restricted to V's of compact support, but only require $E_n < \varliminf_{x\to\infty} V(x)$.

1. Introduction

There are two cases where it is well known that Schrödinger operators have non-degenerate eigenvalues: The lowest eigenvalue in general dimension and all one dimensional eigenvalues. One can ask about making this quantitative, i.e. obtain explicit lower bounds on the distance to the nearest eigenvalues. Obviously, one cannot hope to do this without any restriction on V, since, for example, if χ is the characteristic function of $(-1,1)$, one can show that, for ℓ large, $-d^2/dx^2 - \chi(x) - \chi(x-\ell)$ has at least two eigenvalues and $E_1 - E_0 \to 0$ as $\ell \to \infty$ (see e.g. Harrell [5]). Thus, we ask the following: Can one obtain lower bounds on eigenvalues splittings only in terms of geometric properties of the set where $V(x) < E$ (E at or near the eigenvalues in question) and the size of V on this set. We will do precisely this for the one dimensional case in this note, and we will prove results on the ground state in multi-dimensions in [8] (see also Wong, Yau and Yau [12]).

While these questions are of interest for their own value, we came upon them with specific applications in mind [7, 9].

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Let us state our basic results. (a,b) will denote an interval connected with V which, for simplicity, we take continuous. E_n and E_{n-1} will denote the $(n+1)^{\text{st}}$ and n^{th} eigenvalues of $-d^2/dx^2+V$, and we define

$$\lambda = \max_{E\in[E_{n-1},E_n],\,x\in(a,b)} |E-V(x)|^{1/2}. \tag{1.1}$$

Theorem 1. *Let $V\in C_0^\infty$ with $\operatorname{supp} V\subset[a,b]$. Let $0>E_n>E_{n-1}$ be eigenvalues of $-d^2/dx^2+V$, and let λ be given by (1.1). Then*

$$E_n-E_{n-1}\geqq\frac{\pi}{2}\left[\frac{1}{2\lambda^2}+\frac{\lambda}{2\sqrt{|E_n|}(\lambda^2+|E_n|)}\right]^{-1}e^{-\lambda(b-a)}.$$

Theorem 2. *Let V be continuous on R (but perhaps not bounded above), and suppose that for $\alpha>0$, $V(x)\geqq E_n+\alpha^2$ on $R\setminus[a,b]$, where $E_n>E_{n-1}$ are eigenvalues of $-d^2/dx^2+V(x)$. Then*

$$E_n-E_{n-1}\geqq\pi\lambda^2\alpha(\lambda+\alpha)^{-1}e^{-\lambda(b-a)}.$$

As a "warm-up," we will prove Theorem 1 under the extra assumption that $V(x)$ is even (and $a=-b$) in Sect. 2 and the general results in Sect. 3. In Sect. 4, we give bounds on widths of bands in one dimensional solids. Our proofs in Sect. 2, 3 use the Prüfer variable $\operatorname{Arctan}(u'/-\lambda u)$.

In order to understand the above bounds, we point out several facts:

(a) The proof only uses λ as a bound, so λ may be replaced by any larger constant even if that increases the right side of the bounds, i.e. $\pi\lambda^2\alpha(\lambda+\alpha)^{-1}e^{-\lambda(b-a)}$ can be replaced by $\max_{\mu\geqq\lambda}\pi\mu^2\alpha(\mu+\alpha)^{-1}e^{-\mu(b-a)}$.

(b) There is a scaling covariance here: Making the unitary transformation that takes $x\to\mu x$, and multiplying H by μ^2 takes us to $-d^2/dx^2+\mu^2V(\mu x)$. This change multiplies λ^2 and E_n, E_{n-1} by μ^2 and b, a by μ^{-1}. One can check that both sides of the various bounds only get multiplied by the same factor of μ^2.

(c) Let χ_c be the characteristic function of $(-c,c)$ and let $V_{c,\ell}(x)=-(\chi_c(x)+\chi_c(x-\ell))$. Then, so long as c is chosen so large that E_0 for ℓ large is smaller than $-\frac{1}{2}$ (this is certainly true since $\lim_{c\to\infty}\lim_{\ell\to\infty}E_0=-1$), $\Delta E\sim e^{-\lambda\ell}$ for ℓ large (see [5]), so that the factor $e^{-\lambda(b-a)}$ cannot be replaced by $e^{-\lambda(1+\varepsilon)(b-a)}$ for any $\varepsilon>0$. In this sense, these are precisely tunneling type lower bounds. In fact, the proofs show that, in a sense we will make precise, the results must be fairly close to tunneling examples to saturate the exponential factors in the bounds when $(b-a)\lambda$ is large.

(d) From the point of view of tunneling, $(b-a)\lambda$ should be replaced by $\int_a^b\sqrt{(V(x)-E)_+}\,dx=t$ (where $y_+=\max(y,0)$). With our methods, one can probably replace λ by $[(b-a)^{-1}\int_a^b(V(x)-E)dx]^{1/2}$, which is better than $\max|V(x)-E|^{1/2}$ but not as good as $(b-a)^{-1}t$. By making assumptions on derivatives of V one might be able to get t out by using an x-dependent scaling factor where we use the constant scale factor λ in defining Prüfer variables. Of course, most detailed tunneling analyses require some control on derivatives.

(e) Our results are a kind of analog of those of Harrell [6] for resonances. Davies [1, 2] has emphasized the need for bounds valid in more than an asymptotic regime.

(f) While we stated the results for $(-\infty, \infty)$, there are results for finite volume with various boundary conditions. See, for example, the end of Sect. 2.

2. Even V of Compact Support: A Warm-Up

Our goal here is to prove Theorem 1 under the additional assumption that V is even in x (so $a=-b$). We use Prüfer variables defined with an extra factor (following [3]):

$$u(x)=r(x)\cos(\theta(x)), \tag{2.1a}$$

$$u'(x)=-\lambda r(x)\sin(\theta(x)), \tag{2.1b}$$

where λ is given by (1.1) and u solves

$$-u''+Vu=Eu. \tag{2.2}$$

θ is only determined $\bmod 2\pi$; we will determine it completely by appropriate boundary conditions. From the Ricatti equation: $(u'/u)'=(V-E)-(u'/u)^2$, one immediately obtains

$$\theta'(x)=\lambda^{-1}(E-V(x))\cos^2\theta(x)+\lambda\sin^2\theta(x). \tag{2.3}$$

For each $E<0$, let u solve (2.2) with the boundary condition $u(x)=\exp(\sqrt{-E}x)$ for $x\in(-\infty,a)$. Then $\tan\theta(x,E)=-\lambda^{-1}\sqrt{-E}$ on $(-\infty,a)$ and θ is normalized by

$$\theta(x,E)=-\operatorname{Arctan}[\sqrt{-E}/\lambda]; \quad -\infty\subset x<a, \tag{2.4}$$

i.e. by requiring $\theta(-\infty,E)\in(-\pi/2,0)$. We will see in the next section (as is well-known) that for x fixed, $\theta(x,E)$ is increasing in E. From (2.3), we see that if $\theta=\pm\pi/2,\ 3\pi/2,\ldots$, then $\theta'>0$ so that one can count up zeros of u by looking at $\arg\theta$. In particular, on account of the symmetry

$$\theta(0,E_n)=n\pi/2, \tag{2.5}$$

where E_n is the $(n+1)^{\text{st}}$ eigenvalue.

Define $\varphi(x,E)=\partial\theta/\partial E(x,E)$, so by (2.4):

$$\varphi(a,E)=\lambda(2\sqrt{-E})^{-1}(\lambda^2-E)^{-1}. \tag{2.6}$$

Taking a derivative in (2.3)

$$\varphi'=\{\lambda-\lambda^{-1}[E-V(x)]\}[\sin 2\theta]\varphi+\lambda^{-1}\cos^2\theta \tag{2.7}$$

which, by (1.1), has the form when $E\in[E_{n-1},E_n]$,

$$\varphi'(x)=f(x)\varphi(x)+g(x);\ |f(x)|\leqq 2\lambda;\ |g(x)|\leqq\lambda^{-1}. \tag{2.8}$$

From (2.7)

$$(e^{-2\lambda(x-a)}\varphi)'=e^{-2\lambda(x-a)}(\varphi'-2\lambda\varphi)\leqq g(x)e^{-2\lambda(x-a)}\leqq\lambda^{-1}e^{-2\lambda(x-a)}.$$

Integrating (recall $a<0$)

$$\varphi(0)e^{2\lambda a} \leqq \varphi(a) + \tfrac{1}{2}\lambda^{-2}[1-e^{2\lambda a}] \leqq \varphi(a) + \tfrac{1}{2}\lambda^{-2} \tag{2.9}$$

(in most cases of interest $|\lambda a| \gg 1$, so we drop the $e^{-2|\lambda a|}$ term but it could be retained). Using (2.6) and the monotonicity of $\sqrt{|E|}(\lambda^2+|E|)$ in $|E|$, we see that

$$\varphi(0) \leqq e^{2|\lambda a|}[(2\lambda^2)^{-1} + \tfrac{1}{2}\lambda\{\sqrt{|E_n|}(\lambda^2+|E_n|\}^{-1}].$$

If we note that $2|a| = b-a$, the bound in Theorem 1 results if we note that

$$\frac{\pi}{2} = \theta(0,E_n) - \theta(0,E_{n-1}) \leqq [\max_{E\in[E_{n-1},E_n]} \varphi(0,E)](E_n - E_{n-1}).$$

This completes the proof of Theorem 1 in the symmetric case. Note that in going from (2.8) to (2.9), we could have used Gronwall's inequality, replacing $2\lambda(x-a)$ by $\int_0^x f(y)\,dy$ and have improved our result (but make it appear more complicated; we would adjust λ differently). We could also deal with Dirichlet or Neumann boundary conditions on an interval. We state the results in general, although the above proof only works if V is even (the ideas in the next section handle the general case). Note that with these fixed boundary conditions, $\varphi(a)=0$, so the bound is simpler to state:

Theorem 2.1. *Let E_{n-1}, E_n be two successive eigenvalues of $-d^2/dx^2 + V(x)$ on $[a,b]$ with either Dirichlet or Newman boundary conditions at both a and b. Let λ be given by (1.1). Then*

$$E_n - E_{n-1} \geqq \pi\lambda^2 \exp(-\lambda(b-a)).$$

3. The General Case

In handling the general case (V may be not of compact support and not necessarily even) there are two issues which must be addressed in using the idea of the last section:

(i) Because V is not even, we cannot be sure that at $(a+b/2)$ $\theta(x,E_n) - \theta(x,E_{n-1})$ isn't very small.

(ii) We cannot compute $\theta(a,E)$ and $\phi(a,E) = \partial\theta/\partial E(a,E)$ exactly and so we need a separate argument to see that $\phi(a,E)$ isn't too large.

Let us solve (i) first; by doing that, we will have explained how to prove Theorem 1 and Theorem 2.1 in the non-even case. For this step it is useful to consider $\tilde{V}(x) = V(a+b-x)$. Since $H = -d^2/dx^2 + V$ and $-d^2/dx^2 + \tilde{V}$ are unitarily equivalent, they have the same eigenvalues. For $E < \inf\sigma_{\mathrm{ess}}(H)$, let $\theta(x,E)$, $\tilde{\theta}(x,E)$ denote the Prüfer angle associated to the solution which is L^2 at $-\infty$ via the transformation (2.1). Because E_n and E_{n-1} are eigenvalues, we have

$$\tilde{\theta}(x,E_{n-1}) = (n-1)\pi - \theta(a+b-x,E_{n-1}), \tag{3.1a}$$

$$\tilde{\theta}(x,E_n) = n\pi - \theta(a+b-x,E_n), \tag{3.1b}$$

where this relation only holds for eigenvalues E. The minus sign comes from the flip of sign in u', and we obtain the factors of π by noting that as $x \to -\infty$, $\theta(x, E_{n-1})$, $\tilde{\theta}(x, E_{n-1}) \in (-\pi/2, 0)$ and as $x \to \infty$, θ must pass through the values $\pi/2$, $3\pi/2, \ldots$ exactly n times, each once. From (3.1), we immediately obtain

Lemma 3.1. *One of* $\tilde{\theta}((a+b)/2, E_n) - \tilde{\theta}((a+b)/2, E_{n-1})$ *or* $\theta((a+b)/2, E^n) - \theta((a-b)/2, E_{n-1})$ *is at least* $\pi/2$.

Proof. By (3.1), the two numbers sum up to π. ■

Thus we can make the analysis on either V or $\tilde{V}$, and so, without loss, we can suppose that

$$\theta\left(\frac{a+b}{2}, E_n\right) - \theta\left(\frac{a+b}{2}, E_{n-1}\right) \geqq \pi/2. \tag{3.2}$$

As for problem (ii), we will use an explicit formula for $\varphi = \partial\theta/\partial E$:

Theorem 3.2. *Let* $E < \inf \text{ess spec}(-d^2/dx^2 + V)$,

$$\varphi(x, E) = \lambda \int_{-\infty}^{x} u(y)^2 \, dy / [\lambda^2 u(x)^2 + u'(x)^2] \tag{3.3}$$

where u *is the solution of* (2.2) *which is* ℓ^2 *at* $-\infty$.

Proof. In order to check that u can be chosen to be smooth in E near some E_0 (so that θ is C^1), we pick $W = V$ near $\pm\infty$ so $\inf \text{spec}(W) > E_0$ and W is bounded below. Let $f \in C_0^\infty$ have support in $(-1, 1)$. Then, on $(-\infty, -1)$, we can pick

$$u(x) = \left[\left(-\frac{d^2}{dx^2} + W - E\right)^{-1} f\right](x) \tag{3.4}$$

(u is non-zero since $(-d^2/dx^2 + W - E)^{-1}$ has a strictly positive integral kernel). From (3.4) and the fact that $D(d/dx) \subset Q(-d^2/dx^2 + W)$, we see that u, u' are in L^2 at $-\infty$. Similarly

$$\dot{u}(x) \equiv \frac{\partial u}{\partial E} = \left[\left(-\frac{d^2}{dx^2} + W - E\right)^{-2} f\right](x) \tag{3.5}$$

obeys $\dot{u}$, $\dot{u}' \in L^2$ at $-\infty$. We note that u is C^1 in E (in L^2_{loc} in x-sense) because of the smooth dependence of $u(x)$ on $u(\frac{1}{2})$, $u'(-\frac{1}{2})$. From $\theta = \text{Arctan}(-u'/\lambda u)$ we see that

$$\varphi \equiv \dot{\theta} = \lambda(\dot{u}u' - u\dot{u}')/[\lambda^2 u^2 + (u')^2]. \tag{3.6}$$

Let

$$\eta(x) = \dot{u}(x)u'(x) - u(x)\dot{u}'(x).$$

Then, by (2.2) and $-\dot{u}'' + V\dot{u} = E\dot{u} + u$, we see that $d\eta/dx = u^2$. Since η is L^1 at $-\infty$, we see that

$$\eta(x) = \int_{-\infty}^{x} u^2(y) \, dy$$

which, given (3.6), proves (3.3). ■

Before turning to the proof of Theorem 2, we make two remarks about (3.3). First of all, it provides the promised proof that $\varphi > 0$. Secondly, the only way that $\varphi((a+b)/2, E)$ can be exponentially large for $E \in [E_{n-1}, E_n]$, which is required for our bounds in Theorems 1, 2 to be saturated is if $\lambda^2 u(x)^2 + u'(x)^2$ is exponentially small. This is precisely typical of tunneling situations, that these u's which are small at $-\infty$ are also small in the center of the region (a,b) of importance.

We can now solve problem (ii) by using:

Lemma 3.3. *Let*

$$V(x) \geqq E + \alpha^2 \tag{3.7}$$

on $(-\infty, a]$, *and let* u *solve* (2.2) *and be* L^2 *and positive at* $-\infty$. *Then for* $x \in (-\infty, a]$:

$$u(x) \leqq e^{\alpha(x-a)} u(a). \tag{3.8}$$

Proof. We will show that $e^{-\alpha x} u(x)$ is monotone increasing on $(-\infty, a]$. Since

$$(e^{-\alpha x} u(x))' = e^{-\alpha x}(u' - \alpha u) = \lambda e^{-\alpha x} r(x)(-\sin\theta(x) - \sqrt{\varepsilon}\cos\theta(x))$$

(where $\varepsilon = \alpha^2/\lambda^2$) and $\theta(x) \in (-\pi, 0)$ on $(-\infty, a)$, it suffices that

$$\sin^2\theta(x) \geqq \varepsilon \cos^2\theta(x) \tag{3.9}$$

on $(-\infty, a)$.

Note first that since $V - E > 0$ on $(-\infty, a)$, u and u' are both positive there by a standard ODE argument. Thus, on $(-\infty, a)$, $\theta(x) < 0$.

By (2.3) and (3.7)

$$\theta'(x) < \lambda(\sin^2\theta - \varepsilon\cos^2\theta). \tag{3.10}$$

Pick $\varepsilon' < \varepsilon$. We will show that (3.9) holds with ε replaced by ε' and then make a limiting argument. Let $\theta_0 = -\operatorname{Arctan}\sqrt{\varepsilon'}$. By (3.10), $\theta'(x) \leqq c < 0$ if $\theta(x) \in (\theta_0, 0)$. But, if $\theta(x) > \theta_0$ for some $x \in (-\infty, a)$, this inequality implies that $\theta(y) = 0$ for some $y \in (x - \theta_0/2, x)$ which is impossible by the above remarks. Thus, (3.9) holds. ■

Proof of Theorem 2. By (3.3) and (3.8)

$$\varphi(a) \leqq \lambda \int_{-\infty}^{a} e^{2\lambda\bar{\varepsilon}(x-a)} u(a)^2\, dx / \lambda^2 u(a)^2 = 1/2\lambda^2\sqrt{\varepsilon}.$$

By (2.7) and the argument following it

$$\varphi\left(\frac{a+b}{2}\right) \leqq e^{\lambda(b-a)}[\varphi(a) + \tfrac{1}{2}\lambda^{-2}].$$

But, by (3.2),

$$\frac{\pi}{2} \leqq (E_n - E_{n-1}) \sup_{E \in [E_{n-1}, E_n]} \varphi\left(\frac{a+b}{2}\right) \leqq (E_n - E_{n-1}) e^{\lambda(b-a)}[(2\lambda^2\sqrt{\varepsilon})^{-1} + (2\lambda^2)^{-1}]$$

which yields the bound of Thm. 2. ■

4. Widths of Bands in One-Dimensional Solids

Another situation where non-zero objects can be exponentially small due to tunneling is the case of band widths in one dimensional periodic potentials [4, 11]. Here, we want to note an elementary lower bound on such widths. It is related to what has gone earlier in two interlocking ways: (i) One could think of the argument in Sect. 2 as comparing operators on $(-\infty, 0]$ with Dirichlet and Newmann boundary conditions; band widths compare a periodic and antiperiodic eigenvalue. (ii) We will use the discriminant which is intimately related to θ.

Theorem 4.1. *Let* $[E_b, E_t]$ *be a band of the spectrum of* $-d^2/dx^2 + V(x)$, *where* $V(x+L) = V(x)$. *Let* $E_m = \max(|E_b|, |E_t|)$. *Then*

$$E_t - E_b \geqq 2\exp[-(\sqrt{\|V\|_\infty} + \sqrt{|E_m|} + 1)L]. \tag{4.1}$$

Remark. The tunneling results of [4, 11] show this is optimal in the sense that L cannot be replaced by $(1+\varepsilon)L$.

Proof. Let $\Delta(E)$ be the discriminant. Then [10]

$$|\Delta(E)| \leqq 2\exp(L\sqrt{|E|})\cosh(L\sqrt{\|V\|_\infty}). \tag{4.2}$$

([10] proves this for $L = \pi$; the general case follows by scaling.) Since $\Delta(E)$ is analytic and (4.2) holds for all *complex* E, a Cauchy estimate using the circle $|E' - E| = 1$ shows that

$$|\Delta'(E)| \leqq 2\exp[(\sqrt{\|V\|_\infty} + \sqrt{|E|} + 1)]. \tag{4.3}$$

Since, by the theory of the discriminant [10]: $|\Delta(E_t) - \Delta(E_b)| = 4$, and (4.3) implies (4.1). ■

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