CRITICAL LIEB–THIRRING BOUNDS FOR ONE-DIMENSIONAL SCHRÖDINGER OPERATORS AND JACOBI MATRICES WITH REGULAR GROUND STATES

BARRY SIMON*

ABSTRACT. Let V_0 be a potential so that $H_0 = -\frac{d^2}{dx^2} + V_0$ has $\inf \sigma(H_0) = E_0$. Suppose there is a function u so that $H_0 u = E_0 u$ and $0 < c_1 \leq u(x) \leq c_2$ for constants c_1, c_2. Then we prove there is a C so that

$$\sum_{\substack{E<E_0 \\ E\in\sigma(H)}} (E_0 - E)^{1/2} \leq C \int |V(x)|\, dx$$

for $H = H_0 + V$. We prove a similar result for Jacobi matrices above or below their spectrum.

1. Introduction

While Lieb–Thirring [14] developed their bounds for their proof of stability of matter, they realized that power law bounds on eigenvalues were valid in any dimension over a natural range of powers. Their method only worked for powers above the critical lower bound on possible powers. In dimension $\nu \geq 3$, the critical power is 0 and the resulting inequality is the celebrated CLR bound [3, 13, 16]. Only recently has the critical bound been found for $\nu = 2$ [12]. Here we want to focus on the critical bound in one dimension, not only for its own sake but because of its relevance in connection with variants of Szegő's theorem [15, 11, 4, 2].

The one-dimensional result takes the form

$$\sum_{E\notin\sigma(H_0)} \operatorname{dist}(E, \sigma(H_0))^{1/2} \leq C \int_{-\infty}^{\infty} |V(x)|\, dx \tag{1.1}$$

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* Mathematics 253-37, California Institute of Technology, Pasadena, CA 91125. E-mail: bsimon@caltech.edu. Supported in part by NSF grant DMS-0140592 and U.S.–Israel Binational Science Foundation (BSF) Grant No. 2002068.

where $H_0 = -\frac{d^2}{dx^2}$ and the sum is over eigenvalues of $H = H_0 + V$. It was first proven by Weidl [21] with $C \sim 1.005$. Hundertmark, Lieb, and Thomas [6] then provided a proof with the optimal constant $C = 1$.

We are interested in cases where

$$H_0 = -\frac{d^2}{dx^2} + V_0(x) \tag{1.2}$$

and a Jacobi analog, especially where V_0 is periodic or finite gap almost periodic (so-called algebraic-geometric potential [5]). We have proven an analog of (1.1), alas not for all eigenvalues but for eigenvalues outside the gaps of $\sigma(H_0)$. One reason for this paper is to encourage work on the gaps for suitable V_0's such as the finite gap case. One reason that I conjecture (1.1) also holds for internal edges (i.e., for eigenvalues in gaps) is that, for periodic Jacobi matrices, it has been proven by Damanik–Killip–Simon [4] by a mapping to block Jacobi matrices.

For technical simplicity, we will suppose V_0 is bounded, although it is clear one can handle uniformly L^1_{loc} V_0's and probably as well any locally L^1 limit point case where H_0 is bounded below.

Definition. We say H_0 has a *regular ground state* if

$$E_0 = \inf \sigma(H_0) \tag{1.3}$$

and there is a function u_0 obeying

$$-u_0'' + V_0 u_0 = E_0 u_0 \tag{1.4}$$

$$0 < c_1 \leq u_0(x) \leq c_2 \tag{1.5}$$

for finite positive c_1, c_2.

Our main result is the following:

Theorem 1.1. *Let H_0 have a regular ground state and let E_0 be given by* (1.3). *Then for a suitable constant C,*

$$\sum_{\substack{E \in \sigma(H_0+V_0) \\ E<E_0}} (E_0 - E)^{1/2} \leq C \int_{-\infty}^{\infty} |V(x)|\, dx \tag{1.6}$$

Remarks. 1. In the usual way [1], one can go from (1.6) to bounds on the sum of $(E_0 - E)^p$ by $C \int_{-\infty}^{\infty} |V(x)|^{p+1/2}\, dx$.

2. We have not tried to optimize C, but by following the proof, one gets a bound $C = 2c_2^2/\sqrt{3}\, c_1^2$, which is not much worse than optimal if $c_1 = c_2$.

The proof of [6] is elegant and powerful but rigid in that it requires a strong monotonicity of the Green's function as energy varies. We can prove monotonicity on the rate of decay in finite gap almost periodic cases but not on the edge terms, which are 1 in the free case.

Thus, we will follow the proof of Weidl [21]. Indeed, since we are not seeking optimal constants, we will only need half his proof since the second half of his proof can replace the first half with nonoptimal constants. Indeed, this led to a surprise: When I began, I assumed I would need some kind of strong assumption about the resolvent of $(H_0 - E + \varepsilon)^{-1}$ as $\varepsilon \downarrow 0$ to apply a Birman–Schwinger-type estimate. Precisely because I didn't need the first half of Weidl's proof, I didn't need such a bound. If Weidl had followed this strategy, his constant would have been $2/\sqrt{3} \approx 1.155$.

The key to our proof is what to take for Neumann decoupling. This is discussed in Section 2. In Section 3, we make explicit a bound in Weidl that he only has if $\int_0^\ell f(x)\,dx = 0$. In Section 4, we put these together with Weidl's tactics to prove Theorem 1.1. Sections 5–7 repeat this pattern for Jacobi matrices where we find, in particular, a Dirichlet form that may be useful in other contexts.

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2. Schrödinger Operators: Dirichlet Forms and Neumann B.C.

We begin by recalling the Dirichlet form way of writing Schrödinger operators, a notion going back to Jacobi [9].

Theorem 2.1. *Let H_0 be* (1.2) *with V_0 bounded. Suppose that* (1.3), (1.4)*, and* (1.5) *hold. Then*

(i)
$$Q(H_0) = \{gu_0 \mid g \in L^2(\mathbb{R});\ \nabla g \in L^2(\mathbb{R})\} \tag{2.1}$$

(ii) *For $g \in Q(H_0)$,*
$$\langle gu_0, (H_0 - E_0)gu_0\rangle = \int (\nabla g)^2 u_0^2\,dx \tag{2.2}$$

Proof. By a formal calculation,
$$[g,[g,H_0]] = -2(\nabla g)^2 \tag{2.3}$$
Replace H_0 by $(H_0 - E)$ and take "expectation values" in u_0 and get (2.2).

For $g \in C_0^\infty$, (2.3) applied to u_0 is an integration by parts, proving (2.2) in this case. The general result follows by taking limits and using the easy fact that $\{gu_0 \mid g \in C_0^\infty\}$ is a form core for H_0; see, for example, Simon [19]. $\square$

Our goal is to pick Neumann boundary conditions so u_0 remains in $D(H_0^N)$ and so that $H_0^N \leq H_0$. That will ensure that $H_0^N \geq E_0$ but Neumann decoupling provides lower bounds on the spectrum of H_0+V. We will define it in terms of the quadratic form (2.2).

Definition. Let $a,b \in \mathbb{R}$ with $a < b$. We define $H_{0;(a,b)}^N$ to be the operator with quadratic form

$$Q(H_{0;(a,b)}^N) = \{gu_0 \mid g \in L^2(a,b),\, \nabla g \in L^2(a,b)\} \tag{2.4}$$

with quadratic form given by (2.2).

Remark. Here and in (2.1), by $g \in L^2$, $\nabla g \in L^2$, we mean $g \in L^2$ and its distributional derivative lies in L^2. This is equivalent to g being absolutely continuous with derivative in L^2, or equivalently, to g continuous and $g(x) - g(a) = \int_a^x h(y)\,dy$ for some $h \in L^2$.

Theorem 2.2. *Let $x_{n-1} < x_n < x_{n+1}$ $(-\infty < n < \infty)$ be a two-sided sequence in $\mathbb{R}$ with $x_n \to \pm\infty$ as $n \to \pm\infty$. Associate $L^2(\mathbb{R})$ with $\oplus_n L^2((x_n, x_{n+1}))$ and let H_0^N be the direct sum $\oplus H_{0;(x_n,x_{n+1})}^N$. Then*

(i)
$$H_0^N \leq H_0 \tag{2.5}$$

(ii) *$f = gu_0 \in D(H_{0;(a,b)}^N)$ if and only if g and g' are absolutely continuous and obey the boundary conditions $g'(a) = g'(b) = 0$; equivalently, if and only if f obeys the boundary conditions*

$$f'(a)u_0(a) - f(a)u_0'(a) = 0 \tag{2.6}$$

$$f'(b)u_0(b) - f(b)u_0'(b) = 0 \tag{2.7}$$

(iii) *$u_0 \restriction (a,b) \in D(H_{0;(a,b)}^N)$ and*

$$H_{0;(a,b)}^N u_0 = E_0 u_0 \tag{2.8}$$

(iv)
$$H_{0;(a,b)}^N \geq E_0 \tag{2.9}$$

Remark. (2.5) is intended as shorthand for $(H_0^N + c)^{-1} \geq (H_0 + c)^{-1}$ for c large. It is known [10, 17, 18] to be equivalent to

$$Q(H_0) \subset Q(H_0^N) \quad \text{and} \quad f \in Q(H_0) \Rightarrow (f, H_0 f) \leq (f, H_0^N f) \tag{2.10}$$

Proof. (i) By construction, $Q(H_0) \subset Q(H_0^N)$. They differ in that $f \in Q(H_0)$ are continuous with $f, f' \in L^2$ while $f \in Q(H_0^N)$ is continuous on each $[x_n, x_{n+1}]$ but can be discontinuous at each x_n. Thus, by (2.10), we have (2.5).

(ii) For g which has both g, g' absolutely continuous,

$$(H_0 - E)gu_0 = -2g'u_0' - g''u_0$$

so

$$\int [(g')^2 u_0^2 - [(gu_0)((H_0 - E)gu_0)]]\,dx = \int_a^b (gg'u_0^2)'\,dx$$
$$= g(b)g'(b)u_0^2(b) - g(a)g'(a)u_0^2(a)$$

By (2.2), the left side is zero. Given that Q has vectors which are nonvanishing at a and/or b, we see the boundary conditions are $g'(a) = g'(b) = 0$, which is equivalent to (2.6) and (2.7) since $(fu_0^{-1})' = u_0^{-2}(f'u_0 - u_0'f)$.

(iii) $u \restriction (a,b)$ obeys the boundary conditions (2.6) and (2.7), and (2.8) clearly holds by taking inner products with arbitrary $f \in C_0^\infty(a,b)$.

(iv) is immediate from (2.2). □

As a final remark, we want to note that these Dirichlet form formulae are powerful enough to prove the lowest eigenvalue gap for $H^N_{0;(a,b)}$ is $O(\ell^{-2})$:

Proposition 2.3. *Let $E_1^{(\ell)}$ be the second lowest eigenvalue for $H^N_{0;(0,\ell)}$. Then*

$$\left(\frac{c_1}{c_2}\right)^2 \frac{1}{\ell^2} \leq (E_1^{(\ell)} - E_0) \leq \left(\frac{c_2}{c_1}\right)^2 \frac{\pi^2}{\ell^2} \tag{2.11}$$

Proof. Let

$$g(x) = \cos\left(\frac{\pi x}{\ell}\right) - c \tag{2.12}$$

where

$$c = \frac{\int_0^\ell (\cos \pi x) u_0^2\,dx}{\int_0^\ell u_0^2\,dx}$$

Since gu is orthogonal to u, we have

$$E_1^{(\ell)} - E_0 \leq \frac{\int_0^\ell (g')u_0^2\,dx}{\int_0^\ell g^2 u_0^2\,dx} \tag{2.13}$$
$$\leq \frac{c_2^2 \int_0^\ell (g')^2\,dx}{c_1^2 \int_0^\ell g^2\,dx}$$

But $\int_0^\ell g^2\,dx = \frac{1}{2} + c^2 \geq \frac{1}{2}$, so the right inequality in (2.11) results.

On the other hand, let u_1 be the normalized eigenvector associated to E_1 and let $g = u_1/u_0$. First

$$1 = \int_0^\ell g^2 u_0^2 \leq c_2^2 (\max|g|)^2 \ell \tag{2.14}$$

Since $\int_0^\ell g u_0^2 = 0$, g must vanish somewhere. Suppose c, d are picked so $\max|g(x)| = |g(c)|$ and $g(d) = 0$. For notational simplicity, suppose $c < d$. Then

$$\begin{aligned} \max(|g|)^2 &= \left| \int_c^d g'(x) \right|^2 \leq (d-c) \int_c^d (g')^2 \, dx \\ &\leq \ell \left(\int_0^\ell (g')^2 u_0^2 \, dx \right) c_1^{-2} \\ &= \ell \, c_1^{-2} (E_1 - E_0) \end{aligned} \tag{2.15}$$

(2.14) and (2.15) imply the other half of (2.11). □

3. Schrödinger Operators: Conditional Sobolev Estimates

We need the following estimate which is essentially in Weidl [21] (he states it only if $\int_0^\ell f(x) \, dx = 0$):

Proposition 3.1. *For any C^1 function, f, on $[0, \ell]$ and any $x \in [0, \ell]$,*

$$|f(x)| \leq \left| \frac{1}{\ell} \int_0^\ell f(y) \, dy \right| + \sqrt{\frac{\ell}{3}} \left(\int_0^\ell |f'(y)|^2 \, dy \right)^{1/2} \tag{3.1}$$

Proof. By an integration by parts,

$$x_0 f(x_0) = \int_0^{x_0} y f'(y) \, dy + \int_0^{x_0} f(y) \, dy \tag{3.2}$$

and

$$(\ell - x_0) f(x_0) = \int_{x_0}^\ell (y - \ell) f'(y) + \int_{x_0}^\ell f(y) \, dy \tag{3.3}$$

So, adding

$$|f(x_0)| \leq \left| \frac{1}{\ell} \int_0^\ell f(y) \, dy \right| + \left| \frac{1}{\ell} \int_0^{x_0} [y f'(y)] + \frac{1}{\ell} \int_{x_0}^\ell (y - \ell) f'(y) \right| \tag{3.4}$$

By the Schwarz inequality,

$$|f(x_0)| \leq \left| \frac{1}{\ell} \int_0^\ell f(y) \, dy \right| + C(x_0, \ell) \left(\int |f'(y)|^2 \, dy \right)^{1/2} \tag{3.5}$$

where

$$C(x_0, \ell)^2 = \frac{1}{\ell^2} \left[\int_0^{x_0} y^2 \, dy + \int_{x_0}^\ell (\ell - y)^2 \, dy \right]$$

Clearly,

$$\sup_{x_0} C(x_0, \ell)^2 = \frac{1}{\ell^2} \int_0^\ell y^2 \, dy = \frac{\ell}{3}$$

which implies (3.1). □

4. Schrödinger Operators: Proof of the Main Theorem

Our goal here is to prove Theorem 1.1. Here is the key:

Theorem 4.1. *Let (a,b) be an interval of length ℓ. Let $V \geq 0$ (and not a.e. 0). Then, if*

$$\frac{1}{\ell}\int_a^b V(x)\,dx \leq \frac{3c_1^2}{\ell^2 c_2^2} \tag{4.1}$$

then $H_{0;(a,b)}^N - V$ has exactly one eigenvalue, E, below E_0, and if

$$\alpha \equiv \frac{\ell c_2^2}{3c_1^2}\int_a^b V(x)\,dx < 1 \tag{4.2}$$

then

$$E_0 - E \leq \frac{1}{1-\alpha}\,\frac{c_2^2}{c_1^2}\,\frac{1}{\ell}\int_a^b V(x)\,dx \tag{4.3}$$

Remark. The first-order perturbation theory term for $E_0 - E$ is $\int_a^b u^2(x)V(x)\,dx / \int_a^b u^2(x)\,dx = \delta_1 E$ which obeys

$$\frac{c_1^2}{c_2^2}\,\frac{1}{\ell}\int_a^b V(x)\,dx \leq \delta_1 E \leq \frac{c_2^2}{c_1^2}\,\frac{1}{\ell}\int_a^b V(x)\,dx$$

We know that the first excited state for $H_{0;(a,b)}^N$ has energy $E_0 + O(\frac{1}{\ell^2})$. (4.1) is a condition that the first-order energy shift is also $O(\frac{1}{\ell^2})$ and so is a natural condition for only one state below E_0.

Because E is concave in coupling constant with derivative given by first-order perturbation theory, the first-order term alone cannot give a lower bound on E, but we learn that if we scale by $(1-\alpha)^{-1}$, it does.

Proof. By (3.1), we have that

$$\langle u_0 g, V u_0 g\rangle \leq c_2^2\biggl(\int_a^b V(x)\,dx\biggr)[A+B]^2 \tag{4.4}$$

where

$$A = \frac{1}{\ell}\,\biggl|\int_0^\ell g(x)\,dx\biggr| \tag{4.5}$$

and

$$\begin{aligned} B &= \sqrt{\frac{\ell}{3}}\biggl(\int_a^b (g'(x))^2\,dx\biggr)^{1/2} \\ &\leq \sqrt{\frac{\ell}{3}}\biggl(c_1^{-2}\int_a^b u_0^2 (g'(x))^2\,dx\biggr)^{1/2} \end{aligned}$$

$$= \sqrt{\frac{\ell}{3}}\, c_1^{-1} \langle u_0 g, (H^N_{0;(a,b)} - E_0) u_0 g\rangle^{1/2} \equiv C \tag{4.6}$$

For later purposes, we note that by the Schwarz inequality,

$$\begin{aligned} A &\le \left(\frac{1}{\ell} \int_a^b g(x)^2\, dx\right)^{1/2} \\ &\le c_1^{-1} \left(\frac{1}{\ell} \int_a^b (u_0 g)^2(x)\, dx\right)^{1/2} \equiv D \end{aligned} \tag{4.7}$$

If $A = 0$,

$$\begin{aligned} \langle u_0 g, V u_0 g\rangle &\le c_2^2 \left(\int_a^b V(x)\, dx\right) \frac{\ell}{3c_1^2} \langle u_0 g, (H^N_{0;(a,b)} - E_0) u_0 g\rangle \\ &\le \langle u_0 g, (H^N_{0;(a,b)} - E_0) u_0 g\rangle \end{aligned} \tag{4.8}$$

if (4.1) holds.

Thus $(H_0 - V - E_0) \ge 0$ on a space of codimension one, so there is at most one eigenvalue below E_0 if (4.1) holds.

For any β,

$$\begin{aligned} (A+B)^2 &\le (D+C)^2 \\ &\le (1+\beta^{-1}) D^2 + (1+\beta) C^2 \end{aligned}$$

so if

$$Q = \left(\frac{c_2^2}{c_1^2}\, \frac{1}{\ell} \int_a^b V(x)\, dx\right) \tag{4.9}$$

then

$$\begin{aligned} \text{RHS of (4.4)} \le Q\bigg[&(1+\beta^{-1}) \int_a^b (u_0 g)^2(x)\, dx \\ &+ (1+\beta)\, \frac{\ell^2}{3} \langle u_0 g, (H^N_{0;(a,b)} - E_0) u_0 g\rangle\bigg] \\ = (1+\beta)&\alpha \langle u_0 g, (H^N_{0;(a,b)} - E_0) u_0 g\rangle \\ &+ Q(1+\beta^{-1}) \int_a^b (u_0 g)^2(x)\, dx \end{aligned} \tag{4.10}$$

Pick β so $(1+\beta)\alpha = 1$, that is, $\beta = (1-\alpha)/\alpha$, so

$$1 + \beta^{-1} = \frac{1}{1-\alpha} \tag{4.11}$$

and get

$$\langle u_0 g, (H^N_{0;(a,b)} - V - E_0) u_0 g\rangle \ge -\frac{Q}{1-\alpha} \langle u_0 g, u_0 g\rangle \tag{4.12}$$

which implies (4.3). $\square$

Proof of Theorem 1.1. For simplicity of notation, we suppose $V \in L^1$ but is not supported on any half-line. Without loss, we can take V negative and then look instead at $-V$ with $V \geq 0$. Fix $\alpha \in (0,1)$ to be picked later. Let $x_0 = 0$ and define $x_{\pm n}$ inductively with $\ell_n = x_{n+1} - x_n$ by requiring

$$\ell_n \int_{x_n}^{x_{n+1}} V(x)\, dx = \frac{3c_1^2 \alpha}{c_2^2} \tag{4.13}$$

Since the left side is monotone in ℓ_n (setting $x_{n+1} = x_n + \ell_n$ if $n \geq 0$ and $x_n = x_{n+1} - \ell_n$ if $n \leq -1$) and goes from 0 to infinity, (4.3) has a unique solution. $V \in L^2$ implies initially that ℓ_n is uniformly bounded below and then that $\ell_n \to \infty$. In particular, $x_{\pm n} \to \pm\infty$ as $n \to +\infty$.

Let H_0^N be the direct sum of $H_{0;(x_n + x_{n+1})}$ and $H^N = H_0^N - V$. By (2.5), it suffices to prove

$$\sum_{j, E_j < E_0} |E_0 - E_j^N|^{1/2} \leq C \int_{-\infty}^{\infty} V(x) \tag{4.14}$$

since $E_j^N \leq E_j$. By $\alpha < 1$, (4.1) holds on each interval, so there is one eigenvalue below E_0 on each interval, so we label the E_j^N by $j \in \mathbb{Z}$.

Since (4.3) says

$$\ell_n^{-1} = \frac{c_2^2}{3c_1^2 \alpha} \int_{x_n}^{x_{n+1}} V(x)\, dx \tag{4.15}$$

(4.3) implies

$$E_0 - E_j^N \leq \frac{c_2^4}{3c_1^4 \alpha (1-\alpha)} \left(\int_{x_j}^{x_{j+1}} V(x)\, dx \right)^2 \tag{4.16}$$

This is optimized by $\alpha = \frac{1}{2}$ and leads to

$$\sum_j (E_0 - E_j^N)^{1/2} \leq \frac{2c_2^2}{\sqrt{3}\, c_1^2} \int_{-\infty}^{\infty} V(x)\, dx \qquad \square$$

As an application, we note that if V is a finite gap almost periodic potential (as discussed, e.g., in Gesztesy–Holden [5]), then there is an almost periodic ground state given in terms of those functions which obey (1.5).

Of course, by Dirichlet decoupling, if we have a bound for whole-line V_0, we also have a bound for the Dirichlet restriction to $(0, \infty)$.

5. Jacobi Matrices: Dirichlet Forms and Neumann B.C.

Here we want to consider two-sided Jacobi matrices on $\ell^2(\mathbb{Z})$ given by

$$J_{k\ell} = \begin{cases} b_k & \text{if } k = \ell \\ a_k & \text{if } \ell = k+1 \\ a_{k-1} & \text{if } \ell = k-1 \\ 0 & \text{if } |k-\ell| \geq 2 \end{cases} \tag{5.1}$$

where $a_k > 0$, $b_k \in \mathbb{R}$, and $\sup(|a_k| + |b_k|) < \infty$. We denote this by $J(\{a_k\}_{k=-\infty}^{\infty}, \{b_k\}_{k=-\infty}^{\infty})$. One is also interested in semi-infinite matrices obtained by restricting this to $\ell^2(\{1, 2, \dots\})$. We will focus at what happens above the top of the spectrum, but as we will in explain in Section 7, one can easily also control the perturbed eigenvalues below the bottom of the spectrum.

We are interested in $J_0 = J(\{a_k^{(0)}\}, \{b_k^{(0)}\})$ for which if $E_0 = \sup \sigma(J_0)$, there is a solution $u_n^{(0)}$ of

$$a_k^{(0)} x_{k+1} + b_k^{(0)} x_k + a_{k-1}^{(0)} x_{k-1} = E_0 x_k \tag{5.2}$$

obeying

$$0 < c_1 \leq u_n^{(0)} \leq c_2 \tag{5.3}$$

We will also need

$$\inf_j a_j^{(0)} > 0 \tag{5.4}$$

In Section 7, we will prove:

Theorem 5.1. *Let J_0 be such that* (5.4) *holds and there is a solution $u^{(0)}$ of* (5.2) *obeying* (5.3). *Let J have Jacobi parameters $\{a_k^{(0)} + \delta a_k, b_k^{(0)} + \delta b_k\}_{k=-\infty}^{\infty}$. Let $\{E_j\}$ label the eigenvalues of J above E_0. Then, for a constant C, we have*

$$\sum_j (E_j - E_0)^{1/2} \leq C\biggl(\sum_\ell (|\delta b_\ell| + 2|\delta a_\ell|)\biggr) \tag{5.5}$$

Remark. (5.5) is intended in the sense that if the right side is finite, then $\sigma(J)$ is discrete above E (obvious by Weyl's theorem) and the inequality holds.

In this section, we will first reduce to the case $\delta a_k = 0$, $\delta b_k \geq 0$, then find a Dirichlet form formula for Jacobi matrices (something new here and potentially useful in other contexts) and define Neumann boundary conditions.

Proposition 5.2. *It suffices to prove* (5.5) *when $\delta a_\ell = 0$ and $\delta b_\ell \geq 0$.*

Proof. We follow Hundertmark–Simon [7] here. Since

$$\begin{pmatrix} 0 & \delta a_j \\ \delta a_j & 0 \end{pmatrix} \leq \begin{pmatrix} \delta a_j & 0 \\ 0 & \delta a_j \end{pmatrix} \tag{5.6}$$

(the difference is rank one and positive), we have

$$J(\{a_j^{(0)} + \delta a_j\}, \{b_j^{(0)} + \delta b_j\}) \leq J(\{a_j^{(0)}\}, \{b_j^{(0)} + c_j\}) \tag{5.7}$$

where

$$c_j = |\delta b_j| + |\delta a_j| + |\delta a_{j-1}|$$

Thus, the bound for the J on the right side of (5.7) implies it for the J on the left side. □

Lemma 5.3. *Let f be a bounded two-sided sequence and let M_f be the diagonal matrix with elements f_k. Then*

$$[M_f, J(\{a_j\}, \{b_j\})] = J(\{a_j(f_j - f_{j+1})\}, \{b_j \equiv 0\}) \tag{5.8}$$

$$[M_f, [M_f, J(\{a_j\}, \{b_j\})]] = J(\{a_k(f_j - f_{j+1})^2\}, \{b_j \equiv 0\}) \tag{5.9}$$

Proof. (5.8) is an elementary calculation, and (5.8) implies (5.9). □

Theorem 5.4 (Dirichlet Form for Jacobi Matrices)**.** *If J has a solution $u^{(0)}$ of* (5.2) *obeying* (5.3)*, then for any $f \in \ell^2(\mathbb{Z})$,*

$$\langle fu^{(0)}, (E - J_0) fu^{(0)} \rangle = \sum_{j=-\infty}^{\infty} a_j^{(0)} u_j^{(0)} u_{j+1}^{(0)} (f_j - f_{j+1})^2 \tag{5.10}$$

Proof. It suffices to prove it in case f has compact support, in which case every term in $[M_f, M_f, [J_0 - E]]$ is finite rank and we can take "expectations" in u. Since $(J_0 - E)u^{(0)} = 0$, we obtain (5.10) from (5.9). □

Finally, we turn to Neumann boundary conditions.

Definition. Let $n \leq m$. Let $\mathcal{H}_{[n,m]}$ be the $m-n+1$-dimensional space $\mathbb{C}^{m-n+1}$ with vectors labelled by $j \in \{n, n+1, \dots, m\}$. Define the symmetric matrix $J_{0;[m,n]}^N$ by

$$\langle fu^{(0)}, (E - J_{0;[m,n]}^N) fu^{(0)} \rangle = \sum_{j=n}^{m-1} a_j^{(0)} u_j^{(0)} u_{j+1}^{(0)} (f_j - f_{j+1})^2 \tag{5.11}$$

Theorem 5.5. (a) $J^N_{0;[n,m]}$ *has the following matrix elements*

$$(J^N_{0;[n,m]})_{k\ell} = \begin{cases} a_k^{(0)} & \ell = k+1 \\ a_{k-1}^{(0)} & \ell = k-1 \\ b_k^{(0)} & k=\ell \in \{n+1,\dots,m-1\} \\ b_n^{(0)} + a_{n-1}^{(0)} \big(\frac{u_{n-1}^{(0)}}{u_n^{(0)}}\big) & k=\ell=n \\ b_m^{(0)} + a_m^{(0)} \big(\frac{u_{m+1}^{(0)}}{u_m^{(0)}}\big) & k=\ell=m \\ 0 & |k-\ell| \geq 2 \end{cases} \tag{5.12}$$

(b)

$$(J^N_{0;[n,m]} - E_0)[u^{(0)} \restriction [n,m]] = 0 \tag{5.13}$$

(c)

$$E_0 = \sup \sigma(J^N_{0;[n,m]}) \tag{5.14}$$

(d) *If* $\{n_j\}$ *is a sequence in* $\mathbb{Z}$ *with* n_j, n_{j+1} *and* $J_0^N = \oplus J^N_{0,[n_j,n_{j+1}-1]}$, *then*

$$J_0 \leq J_0^N \tag{5.15}$$

Remark. Because we have defined $a_j > 0$ and look above the spectrum, directions are reversed relative to the differential operators.

Proof. (a) For notational simplicity, set $Q = J^N_{0;[n,m]}$. By (5.11), $Q_{k\ell} = 0$ if $|k-\ell| \geq 2$, and using symmetries of Q,

$$2Q_{k\,k+1} = 2Q_{k+1\,k} = 2a_k^{(0)}$$

yielding (5.12) for $|k-\ell| = 1$. For the diagonal terms, take $f = \delta_k$ and get

$$Q_{k\ell}(u_k^{(0)})^2 = E(u_k^{(0)})^2 - \alpha_k[a_k^{(0)} u_k^{(0)} u_{k+1}^{(0)}] - \alpha_{k-1}[a_{k-1}^{(0)} u_k^{(0)} u_{k-1}^{(0)}] \tag{5.16}$$

where

$$\alpha_k = \begin{cases} 1 & k = n+1,\dots,m-1 \\ 0 & k = n,m \end{cases}$$

Since

$$Eu_k^{(0)} = bu_k^{(0)} + a_k^{(0)} u_{k+1}^{(0)} + a_{k-1} u_{k-1}^{(0)} \tag{5.17}$$

(5.12) for $k = \ell$ follows.

(b) Immediate from (5.17) and (5.12).

(c) This is true for any matrix which is positive off-diagonal and has a positive eigenfunction.

(d) By (5.10) and (5.11),

$$\langle fu^{(0)}, (J_0^N - J_0)fu^{(0)}\rangle = \sum_{\ell=-\infty}^{\infty} a_{n_\ell-1}^{(0)} u_{n_\ell-1}^{(0)} u_{n_\ell}^{(0)} (f_{n_\ell-1} - f_{n_\ell})^2$$

n is positive. □

Remark. As in the continuum case, one sees $O(\ell^{-2})$ upper and lower bounds on the top gap in $H^N_{0;[n,m]}$ if $|n-m| = \ell$.

6. Jacobi Matrices: Conditional Sobolev Estimates

We need a discrete analog of Proposition 3.1:

Proposition 6.1. *For any ℓ and any finite sequence $\{f_j\}_{j=1}^{\ell}$, we have*

$$|f_j| \le \left|\frac{1}{\ell}\sum_{k=1}^{\ell} f_k\right| + \sqrt{\frac{\ell}{3}}\left(\sum_{k=1}^{\ell-1} |f_{k+1} - f_k|^2\right)^{1/2} \tag{6.1}$$

Proof. By cancelling terms, one sees that

$$jf_j = \sum_{k=1}^{j-1} k(f_{k+1} - f_k) + \sum_{k=1}^{j} f_k$$

$$(\ell - j)f_j = \sum_{k=j}^{\ell-1} (\ell - k)(f_k - f_{k+1}) + \sum_{k=j+1}^{\ell} f_k$$

So, by the Schwarz inequality,

$$\left|\ell f_j - \sum_{k=1}^{\ell} f_k\right| \le \left[\sum_{k=1}^{j-1} k^2 + \sum_{k=j}^{\ell-1} (\ell-k)^2\right]^{1/2} \left(\sum_{k=1}^{\ell-1} |f_{k+1} - f_k|^2\right)^{1/2} \tag{6.2}$$

The extreme case of the first sum of the right occurs when $j = 1$ or ℓ and is

$$\sum_{j=1}^{\ell-1} j^2 = \frac{(\ell-1)\ell(2\ell-1)}{6} < \frac{\ell^2}{3}$$

Thus (6.2) implies (6.1). □

7. Jacobi Matrices: The Main Theorem

Here is the analog of Theorem 4.1:

Theorem 7.1. *Let $[n, m]$ be an interval of length ℓ (i.e., $\ell = m - n + 1$). If $\delta b \ge 0$ and*

$$\frac{1}{\ell}\sum_{j=n}^{m} \delta b_j \le \frac{3\min(a_j^{(0)})c_1^2}{\ell^2 c_2^2} \tag{7.1}$$

then $J^N_{0;[n,m]} + \delta b$ *has exactly one eigenvalue in* (E_0, ∞) *and if*

$$\alpha \equiv \frac{\ell c_2^2}{3c_2^2 \min(a_j^{(0)})} \left(\sum_{j=1}^{n} \delta b_j \right) < 1 \tag{7.2}$$

then

$$E - E_0 \leq \frac{1}{1-\alpha} \, \frac{c_2^2}{c_1^2} \left(\frac{1}{\ell} \sum_{j=n}^{m} \delta b_j \right) \tag{7.3}$$

Proof. Let

$$A = \sum_{j=m}^{n} \delta b_j \tag{7.4}$$

and suppose $\sum_{j=n}^{m} g_j = 0$, then by (6.1),

$$\begin{aligned}
\langle u^0 g, (\delta b) u^0 g \rangle &\leq A c_2^2 \sup_j |g_j|^2 \\
&\leq A c_2^2 \, \frac{\ell}{3} \sum_{j=n}^{m-1} |g_{j+1} - g_j|^2 \\
&\leq \frac{A c_2^2}{\min a_j^{(0)} c_1^2} \, \frac{\ell}{3} \sum_{j=n}^{m-1} a_j^{(0)} u_j^{(0)} u_{j+1}^{(0)} |g_{j+1} - g_j|^2
\end{aligned}$$

As in the Schrödinger case, this implies that when (7.1) holds, $J + \delta b - E_0 \leq 0$ off a one-dimensional space and then implies (7.3) as in that case. $\square$

The discreteness of Jacobi matrices produces two potential problems in extending Theorem 1.1 to Theorem 5.1:

(i) Individual δb's may be so large that (7.1) fails even for $\ell = 1$.

(ii) We cannot arrange to pick ℓ so that equality holds in (7.2) for a fixed α.

As we will see, neither difficulty is hard to overcome but each involves increases in constants. It will be useful to define

$$D = \tfrac{1}{2} \left(\frac{3c_1^2}{c_2^2} \, \min(a_j^{(0)}) \right) \tag{7.5}$$

Proof of Theorem 5.1. We suppose first that for all j,

$$0 \leq \delta b_j < D \tag{7.6}$$

and that δb is not supported on a half-line. We define $n_0 = 0$ and $\{n_j\}_{j=-\infty}^{\infty}$ inductively with $\ell_j = n_j - n_{j-1}$ by requiring for $j \geq 1$ that

$$\ell_j \sum_{k=n_{j-1}}^{n_j - 1} \delta b_k \leq D \tag{7.7}$$

and

$$(\ell_j + 1) \sum_{k=n_{j-1}}^{n_j} \delta b_k > D \tag{7.8}$$

For $j \leq 0$, we require (7.7) and

$$(\ell_j + 1) \sum_{k=n_{j-1}}^{n_j} \delta b_j > D \tag{7.9}$$

By (7.6), we have (7.7) for $\ell_j = 1$, and for $j \geq 1$,

$$\ell_j \sum_{k=n_{j-1}}^{n_{j-1}+\ell_j-1} \delta b_k$$

is monotone in ℓ_j going to infinity. So we can find ℓ_j inductively for $j \geq 1$, so (7.7) and (7.8). Similarly, we can find ℓ_j for $j \leq 0$, so (7.7), (7.9) hold.

(7.7) implies that (7.1) holds. Indeed, (7.2) holds with $\alpha < \frac{1}{2}$. Thus, if we use n_j for Neumann boundary conditions, each $J_{0;[n_{j-1},n_{j-1}]} + \delta b$ has exactly one eigenvalue in (E_0, ∞) and it obeys (7.3) with $\alpha = \frac{1}{2}$. Since the eigenvalues E_j for $J_{0;[n_{j-1},n_{j-1}]} + \delta b$ obeys

$$(E_j - E_0) = \frac{2c_2^2}{c_1^2} \frac{1}{\ell_j} \sum_{k=n_{j-1}}^{n_j - 1} \delta b_k$$

For $j \leq 1$, by (7.8),

$$\frac{1}{\ell_j} \leq \frac{2}{\ell_j + 1} \leq 2D^{-1} \sum_{k=n_{j-1}}^{n_j} \delta b_k$$

Thus

$$\begin{aligned} \sum_{j \geq 1} (E_j - E_0)^{1/2} &\leq \frac{2c_2}{c_1 D^{1/2}} \biggl(\sum_{j \geq 1} \biggl(\sum_{k=n_{j-1}}^{n_j} \delta b_k \biggr) \biggr) \\ &\leq \frac{4c_2}{c_1 D^{1/2}} \biggl[\sum_{k=0}^{\infty} \delta b_k \biggr] \end{aligned}$$

where we need to take $4 = 2 \cdot 2$ because some δb_k occur twice.

A similar argument works for $j \leq 0$, and we find that if (7.6) holds, then

$$\sum_j (E_j - E_0)^{1/2} \leq \frac{4c_2}{c_1 D^{1/2}} \sum_{k=0}^{\infty} (\delta b_j) \tag{7.10}$$

where now E_j are the eigenvalues for $J_0 + \delta b$ without the Neumann conditions.

For general $\delta b > 0$ with $\sum_k \delta b_k < \infty$, we single out the necessarily finite number $\{\delta b_{k_n}\}_{n=1}^N$ of δb's with $\delta b_k \geq D$ ordered so that

$$\delta b_{k_1} \leq \delta b_{k_2} \leq \cdots \leq \delta b_{k_N} \tag{7.11}$$

We consider sequences $\delta^0 b, \delta^1 b, \dots, \delta b^N$ so that $\delta^0 b$ has none of the b_{k_n} turned on and $\delta^n b$ has m turned on, that is,

$$(\delta^m b)_k = \begin{cases} \delta b_k & k \notin \{k_n\}_{n=1}^N \\ \delta b_k & k \in \{k_n\}_{n=1}^m \\ 0 & k \in \{k_n\}_{n=m+1}^N \end{cases} \tag{7.12}$$

By the first part of the proof, (7.10) holds for $\delta^0 b$. $\delta^1 b - \delta^0 b$ is rank one, so all the eigenvalues of $J_0 + \delta^1 b$, excluding the top 1, are bounded above by eigenvalues of $J_0 + \delta^0 b$ and that other eigenvalue is bounded by $E_0 + \delta b_{k_1}$ since $\|\delta^1 b\| = \delta b_{k_1}$. Thus

$$\sum (E(\delta^1 b) - E_0)^{1/2} \leq \sqrt{\delta b_{k_1}} + \sum (E(\delta^0 b) - E_0)^{1/2}$$

Proceeding inductively, using (7.11) to see $\|\delta^m b\| = \delta b_{k_m}$ and using $\delta b_{k_j} \geq D$ and

$$\sqrt{\delta b_{k_j}} \leq D^{-1/2} \delta b_{k_j} \leq \frac{4c_2}{c_1 D^{1/2}}\, \delta b_{k_j} \tag{7.13}$$

we see that (7.10) holds for any δb with $\sum \delta b < \infty$. $\square$

While we have focused on eigenvalues below the spectrum of J_0, since

$$UJ(\{a_n\}, \{b_n\})U^{-1} = -J(\{a_n\}, \{-b_n\})$$

with $(U\eta)_n = (-1)^n \eta_n$, we can obtain theorems below the spectrum of J_0 if $E_1 = \inf \sigma(J_0)$, and there is a solution of $(J_0 - E_1)u^{(1)} = 0$ where $0 < c_1 \leq (-1)^n u^{(1)} < c_2$.

Using results of Sodin–Yuditskii [20], one can prove that the hypotheses of Theorem 5.1 apply to finite gap almost periodic Jacobi matrices. We are especially interested in extending $\frac{1}{2}$ power bounds to the gap in this case because of potential applications [2]. For slightly weaker $\frac{1}{2}$ power bounds in the gaps for this case, see [8].

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