SUM RULES FOR JACOBI MATRICES AND DIVERGENT LIEB-THIRRING SUMS

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Abstract. Let E_j be the eigenvalues outside $[-2,2]$ of a Jacobi matrix with $a_n - 1 \in \ell^2$ and $b_n \to 0$, and μ' the density of the a.c. part of the spectral measure for the vector δ_1. We show that if $b_n \notin \ell^4$, $b_{n+1} - b_n \in \ell^2$, then

$$\sum_j (|E_j| - 2)^{5/2} = \infty,$$

and if $b_n \in \ell^4$, $b_{n+1} - b_n \notin \ell^2$, then

$$\int_{-2}^{2} \ln(\mu'(x))(4-x^2)^{3/2}\, dx = -\infty.$$

We also show that if $a_n - 1, b_n \in \ell^3$, then the above integral is finite if and only if $a_{n+1} - a_n, b_{n+1} - b_n \in \ell^2$. We prove these and other results by deriving sum rules in which the a.c. part of the spectral measure and the eigenvalues appear on opposite sides of the equation.

1. Introduction

In the present paper we consider Jacobi matrices

$$J \equiv \begin{pmatrix} b_1 & a_1 & 0 & \dots \\ a_1 & b_2 & a_2 & \dots \\ 0 & a_2 & b_3 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}$$

with $a_n > 0$, $b_n \in \mathbb{R}$, and $a_n \to 1$, $b_n \to 0$. These are compact perturbations of the *free matrix* J_0 with $a_n \equiv 1$ and $b_n \equiv 0$. If only $a_n \equiv 1$, then J is the discrete half-line Schrödinger operator with the decaying potential b_n.

J is a self-adjoint operator acting on $\ell^2(\{1,2,\dots\})$. We denote by μ the spectral measure of the (cyclic for J) vector δ_1 and by μ' the density of its a.c. part. For J_0, the measure μ_0 is absolutely continuous with $\mu_0'(x) = (2\pi)^{-1}\sqrt{4-x^2}\chi_{[-2,2]}(x)$, and so by Weyl's theorem, $\sigma_{\text{ess}}(J) = \sigma_{\text{ess}}(J_0) = [-2,2]$. Hence, outside $[-2,2]$ spectrum of J consists only of

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eigenvalues (of multiplicity 1), with ± 2 the only possible accumulation points. We will denote the negative ones $E_1, E_3, \dots$ and the positive ones $E_2, E_4, \dots$, with the convention that $E_{2j-1} \equiv -2$ ($E_{2j} \equiv 2$) if J has fewer than j eigenvalues below -2 (above 2).

We let $\partial a_n \equiv a_{n+1} - a_n$, $\partial b_n \equiv b_{n+1} - b_n$, and define

$$r_n \equiv b_n^4 - 2(\partial b_n)^2 - 8(\partial a_n)^2 + 4(a_n^2 - 1)(b_n^2 + b_n b_{n+1} + b_{n+1}^2).$$

The following are our main results.

Theorem 1. *Assume $a_n - 1 \in \ell^3$ and $b_n \to 0$.*

(i) *If $\sum_{n=1}^\infty r_n = \infty$ or does not exist, then $\sum_{j=1}^\infty (|E_j| - 2)^{5/2} = \infty$.*

(ii) *If $\sum_{n=1}^\infty r_n = -\infty$ or does not exist, then $\int_{-2}^2 \ln(\mu'(x))(4-x^2)^{3/2}\, dx = -\infty$.*

Remark. One can actually dispense with the assumption $a_n - 1 \in \ell^3$, but the corresponding r_n is less transparent (it is the diagonal element of the matrix $P_w(J)$ from the proof of Theorem 1).

Corollary 2. *Assume $a_n - 1 \in \ell^2$ and $b_n \to 0$.*

(i) *If $b_n \notin \ell^4$ and $\partial b_n \in \ell^2$, then $\sum_{j=1}^\infty (|E_j| - 2)^{5/2} = \infty$.*

(ii) *If $b_n \in \ell^4$ and $\partial b_n \notin \ell^2$, then $\int_{-2}^2 \ln(\mu'(x))(4 - x^2)^{3/2}\, dx = -\infty$.*

Proof. Since $a_n - 1 \in \ell^2$, we have $\partial a_n \in \ell^2$. Also,

$$|4(a_n^2 - 1)(b_n^2 + b_n b_{n+1} + b_{n+1}^2)| \le 72(a_n^2 - 1)^2 + \tfrac{1}{4}(b_n^4 + b_{n+1}^4)$$

and $a_n^2 - 1 \in \ell^2$, so the result follows from Theorem 1. $\square$

The sum in (i) is a Lieb-Thirring sum and most results go in the direction opposite to (i), bounding sums of eigenvalue moments from above in terms of the matrix elements. See [5], where it is proved that

$$\sum_j (|E_j| - 2)^p \le c_p \Big(\sum_n |a_n - 1|^{p+1/2} + \sum_n |b_n|^{p+1/2} \Big) \tag{1}$$

for any $p \ge \frac{1}{2}$ and some $c_p > 0$, and references therein.

The integral in (ii) is one from a family of Szegő-type integrals recently studied, among others, in [3, 6, 7, 8, 9, 10, 11, 12]. The actual Szegő integral has the weight $(4 - x^2)^{-1/2}$ instead of $(4 - x^2)^{3/2}$ and is an important object in the theory of orthogonal polynomials.

We also single out the following of our results (cf. Corollary 9).

Theorem 3. *Assume $a_n - 1, b_n \in \ell^3$. Then $\partial a_n, \partial b_n \in \ell^2$ if and only if $\int_{-2}^2 \ln(\mu'(x))(4 - x^2)^{3/2}\, dx > -\infty$.*

Remarks. 1. The "only if" part was proved in [7].

2. Note that $a_n - 1, b_n \in \ell^3$ and (1) imply $\sum_{j=1}^\infty (|E_j| - 2)^{5/2} < \infty$.

We briefly review here related results. In [6], which started recent development in the area of sum rules, it is proved that $a_n - 1, b_n \in \ell^2$ if and only if $\sum_j (|E_j| - 2)^{3/2} < \infty$ and $\int_{-2}^{2} \ln(\mu'(x))(4 - x^2)^{1/2}\, dx > -\infty$. Using a higher sum rule [8] shows that $a_n - 1, b_n \in \ell^4$ and $\partial^2 a_n, \partial^2 b_n \in \ell^2$ if and only if $\sum_j (|E_j| - 2)^{7/2} < \infty$ and $\int_{-2}^{2} \ln(\mu'(x))(4 - x^2)^{5/2}\, dx > -\infty$. Finally, [9] shows that $a_n - 1, b_n \in \ell^4$ and $a_{n+1} + a_n, b_{n+1} + b_n \in \ell^2$ if and only if $\sum_j (|E_j| - 2)^{3/2} < \infty$ and $\int_{-2}^{2} \ln(\mu'(x)) x^2 (4 - x^2)^{1/2}\, dx > -\infty$. Closely related to our work is also a general "existence" result in [10].

From most such results one can conclude that a Lieb-Thirring sum or a Szegő-type integral is infinite for certain a_n, b_n, but is not able to say which one of these happens. We achieve this by obtaining sum rules in which these two quantities appear on opposite sides of the equation (Theorem 7(i)). This is in the spirit of Theorem 4.1 in [11], which shows that $\limsup_n \sum_{j=1}^{n} \ln(a_n) = \infty$ implies $\sum_j (|E_j| - 2)^{1/2} = \infty$ and $\liminf_n \sum_{j=1}^{n} \ln(a_n) = -\infty$ implies $\int_{-2}^{2} \ln(\mu'(x))(4 - x^2)^{-1/2}\, dx = -\infty$ (see also Theorem 10 below).

The paper is organized as follows. In Section 2 we introduce the necessary tools, *Case sum rules for Jacobi matrices* (see [1, 6, 11, 12]), and then extend these to a form we will need here (Theorem 7). In Section 3 we use them to prove Theorems 1 and 3 and related results.

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2. Sum Rules for Jacobi Matrices

In this section we use the notation of and extend results from [11]. If for some $\{c_\ell\}_{\ell=0}^{k}$ we have $w(\theta) \equiv \sum_{\ell=0}^{k} c_\ell \cos(\ell\theta) \geq 0$, we define

$$
\begin{aligned}
Z_w(J) &\equiv -\frac{1}{2\pi} \int_0^{\pi} \ln\left(\frac{\pi\mu'(2\cos\theta)}{\sin\theta}\right) w(\theta)\, d\theta \\
&= -\frac{1}{2\pi} \int_{-2}^{2} \ln\left(\frac{\mu'(x)}{\mu_0'(x)}\right) \sum_{\ell=0}^{k} c_\ell T_\ell\left(\frac{x}{2}\right) \frac{dx}{\sqrt{4 - x^2}}, \qquad (2)
\end{aligned}
$$

where $T_\ell(\cos\theta) \equiv \cos \ell\theta$ is the ℓ^{th} Chebyshev polynomial (of degree ℓ), and the second equality follows from the substitution $x = 2\cos\theta$. Since $\ln(\mu'(x)) \leq \mu'(x)\sqrt{4 - x^2} - \ln(\sqrt{4 - x^2})$, $\mu(\mathbb{R}) = 1$, and $w(\theta) \geq 0$, the positive part of the integral is bounded, that is,

$$
Z_w(J) \geq C_w \qquad (3)
$$

with $C_w > -\infty$ (but $Z_w(J) = \infty$ is possible). Note that $Z_w(J_0) = 0$.

We also let $|\beta_j| \geq 1$ be such that $E_j = \beta_j + \beta_j^{-1}$. Hence

$$
|\beta_j| - 1 = (|E_j| - 2)^{1/2} + O(|E_j| - 2).
$$

We define

$$J^{(n)} = \begin{pmatrix} b_{n+1} & a_{n+1} & 0 & \dots \\ a_{n+1} & b_{n+2} & a_{n+2} & \dots \\ 0 & a_{n+2} & b_{n+3} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}$$

that is, $J^{(n)}$ is the matrix we obtain from J by removing the first n rows and columns. We let $E_j^{(n)} \equiv E_j(J^{(n)})$ and $\beta_j^{(n)} \equiv \beta_j(J^{(n)})$. We also let J_n be the matrix one obtains from J by replacing a_j by 1 and b_{j+1} by 0 for $j \geq n$. Notice that $(J_n)^{(n)} = J_0$.

We denote (with $\ell \geq 1$)

$$X_0^{(n)}(J) \equiv \sum_{j=1}^{\infty} \Big[\ln(|\beta_j|) - \ln(|\beta_j^{(n)}|) \Big],$$

$$X_\ell^{(n)}(J) \equiv \frac{1}{2\ell} \sum_{j=1}^{\infty} \Big[\big(\beta_j^\ell - \beta_j^{-\ell}\big) - \big((\beta_j^{(n)})^\ell - (\beta_j^{(n)})^{-\ell}\big) \Big].$$

These sums are always convergent because $X_\ell^{(n)}(J) = \sum_{j=0}^{n-1} X_\ell^{(1)}(J^{(j)})$ (where $J^{(0)} \equiv J$), and the finiteness of $X_\ell^{(1)}(J)$ follows from the fact that positive (resp. negative) eigenvalues of J and $J^{(1)}$ interlace [11].

Finally, if B is a semi-infinite matrix, we let $B(n)$ be the matrix we obtain from B by adding to it, from the top and left, n rows and columns containing only zeros. For instance, $J^{(n)}(n)$ is the matrix one obtains from J by replacing a_j, b_j for $j \leq n$ by zeros. We then define

$$\xi_0^{(n)}(J) \equiv - \sum_{j=1}^{n} \ln(a_j)$$

$$\xi_\ell^{(n)}(J) \equiv -\frac{1}{\ell} \operatorname{Tr} \Big(T_\ell\big(\tfrac{1}{2}J\big) - T_\ell\big(\tfrac{1}{2}J^{(n)}\big)(n) \Big)$$

for $\ell \geq 1$. These are well defined because the diagonal of the matrix $T_\ell(\frac{1}{2}J) - T_\ell(\frac{1}{2}J^{(n)})(n)$ eventually vanishes (starting from $(n+\ell)^{\text{th}}$ diagonal element), although the matrix need not be trace class.

With this notation one has the following *step-by-step sum rule*:

Lemma 4. *If* $w(\theta) = \sum_{\ell=0}^{k} c_\ell \cos(\ell\theta) \geq 0$, *then*

$$Z_w(J) = \sum_{\ell=0}^{k} c_\ell \xi_\ell^{(n)}(J) + \sum_{\ell=0}^{k} c_\ell X_\ell^{(n)}(J) + Z_w(J^{(n)}). \tag{4}$$

Remark. Here both sides can be $+\infty$. In particular, $Z_w(J) = \infty$ if and only if $Z_w(J^{(n)}) = \infty$.

Proof. One proves the statement for $n = 1$ and then iterates the obtained formula n times. The proof is identical to that of Theorems 3.1–3.3 in [11] (using their Remark 1 before Theorem 2.1), where $w(\theta) \equiv 1$, $w(\theta) \equiv 1 \pm \cos\theta$, and $w(\theta) \equiv 1 - \cos 2\theta$ (the proofs, with more detail, also appear in [12]). □

A natural question here is what happens when we take $n \to \infty$. To do this we need to determine the convergence of the terms on the right hand side of (4). Following [11], one can use two approximations — J by J_n, and J_0 by $J^{(n)}$ — to treat the second and third term. We define

$$f_w(\beta) \equiv c_0 \ln(|\beta|) + \sum_{\ell=1}^{k} \frac{c_\ell}{2\ell}\big(\beta^\ell - \beta^{-\ell}\big) \tag{5}$$

so that

$$\sum_{\ell=0}^{k} c_\ell X_\ell^{(n)}(J) = \sum_{j=1}^{\infty} \Big[f_w(\beta_j) - f_w(\beta_j^{(n)})\Big].$$

We also let $X_{\ell,+}^{(n)}(J)$ be defined as $X_\ell^{(n)}(J)$ but with the sum taken only over positive eigenvalues. Similarly we define $X_{\ell,-}^{(n)}(J)$, with only negative eigenvalues. We then have $X_\ell^{(n)}(J) = X_{\ell,+}^{(n)}(J) + X_{\ell,-}^{(n)}(J)$ and

$$\sum_{\ell=0}^{k} c_\ell X_{\ell,+}^{(n)}(J) = \sum_{E_j \geq 2} \Big[f_w(\beta_j) - f_w(\beta_j^{(n)})\Big],$$

$$\sum_{\ell=0}^{k} c_\ell X_{\ell,-}^{(n)}(J) = \sum_{E_j \leq -2} \Big[f_w(\beta_j) - f_w(\beta_j^{(n)})\Big].$$

Lemma 5. *If $a_n \to 1$, $b_n \to 0$, and $w(\theta) = \sum_{\ell=0}^{k} c_\ell \cos(\ell\theta) \geq 0$, then*

$$\liminf_{n\to\infty} Z_w(J^{(n)}) \geq Z_w(J_0) = 0, \tag{6}$$

$$\liminf_{n\to\infty} Z_w(J_n) \geq Z_w(J). \tag{7}$$

Also,

$$\lim_{n\to\infty} \sum_{\ell=0}^{k} c_\ell X_{\ell,\pm}^{(n)}(J) = \sum_{\pm E_j \geq 2} f_w(\beta_j), \tag{8}$$

$$\lim_{n\to\infty} \sum_{\ell=0}^{k} c_\ell X_{\ell,\pm}^{(n)}(J_n) = \sum_{\pm E_j \geq 2} f_w(\beta_j). \tag{9}$$

Remarks. 1. Eqs. (8), (9) are intended as two statements each — one with the plus signs and one with the minus signs. This will be the case in Theorems 7(ii) and 10 as well.

2. The sums on the left hand sides of (8), (9) both exist but could be $\pm\infty$. We separate the sums over positive and negative eigenvalues from each other because one could be ∞ and the other $-\infty$.

Proof. Eqs. (5), (6) follow directly from Corollary 5.3 in [6].

Let us prove (8), (9) with the plus signs (the second case is identical). Notice that f_w is continuous on $[1,\infty)$ with $f_w(1) = 0$. Since also $f_w \in C^\infty$ and not all its derivatives at 1 vanish (unless $f_w \equiv 0$), it is monotone on some interval $[1, 1+\varepsilon]$, $\varepsilon > 0$ (and so the sums in (8), (9) exist). For such functions (8) holds by Lemma 4.6 in [11]. Similarly, (9) holds by Theorem 6.2 in [6], using that $(J_n)^{(n)} = J_0$ has no eigenvalues (and so the left hand side is just $\lim_{n\to\infty} \sum_{E_j \ge 2} f_w(\beta_j(J_n))$). □

To treat the first sum in (4) we define

$$P_w(J) \equiv S - c_0 A - \sum_{\ell=1}^{k} \frac{c_\ell}{\ell} T_\ell(\tfrac{1}{2}J) \tag{10}$$

where A is the matrix with $\ln(a_j)$ on the diagonal, and S is the matrix with $S_{1,1} = -\sum_{\ell=1}^{k} \frac{1}{4\ell}(1+(-1)^\ell)c_\ell$ and all other elements zero.

Lemma 6. *If $n > k$, then with $o(1) = o(n^0)$,*

$$\sum_{\ell=0}^{k} c_\ell \xi_\ell^{(n)}(J) = \sum_{j=1}^{n} \big(P_w(J)\big)_{j,j} + o(1). \tag{11}$$

Proof. As already mentioned, diagonal elements of $T_\ell(\frac{1}{2}J) - T_\ell(\frac{1}{2}J^{(n)})(n)$ vanish starting from $(n+k)^{\text{th}}$. The first n of them are equal to those of $T_\ell(\frac{1}{2}J)$, so we are left with proving that the sum of the remaining $k-1$ is $\frac{1}{4}(1+(-1)^\ell) + o(1)$.

The $(n+1)^{\text{st}}$ through $(n+k-1)^{\text{st}}$ diagonal elements of $T_\ell(\frac{1}{2}J)$ differ by $o(1)$ from those of $T_\ell(\frac{1}{2}J_0)$ (since $a_n \to 1$, $b_n \to 0$), and these are 0 when $n > k$ [12, Lemma 3.29]. The $(n+1)^{\text{st}}$ through $(n+k-1)^{\text{st}}$ diagonal elements of $T_\ell(\frac{1}{2}J^{(n)})(n)$ differ by $o(1)$ from the 1^{st} through $(k-1)^{\text{st}}$ of $T_\ell(\frac{1}{2}J_0)$, which sum up to $-\frac{1}{4}(1+(-1)^\ell)$ [12, Lemma 3.29]. The proof is finished. □

With this preparation we can obtain the final form of the sum rules.

Theorem 7. *Let $a_n \to 1$, $b_n \to 0$, and $w(\theta) = \sum_{\ell=0}^{k} c_\ell \cos(\ell\theta) \ge 0$.*

(i) *If $f_w \geq 0$ on $[1, 1+\varepsilon] \cup [-1-\varepsilon, -1]$ for some $\varepsilon > 0$, and either $Z_w(J) < \infty$ or $\sum_{j=1}^\infty f_w(\beta_j) < \infty$, then* $\mathrm{Tr}(P_w(J))$ *exists and*

$$Z_w(J) = \mathrm{Tr}(P_w(J)) + \sum_{j=1}^\infty f_w(\beta_j).$$

(ii) *If $\pm f_w \geq 0$ on $[1, 1+\varepsilon]$ and $\pm f_w \leq 0$ on $[-1-\varepsilon, -1]$ for some $\varepsilon > 0$, and either $Z_w(J) < \infty$ and $\sum_{\pm E_j \leq -2} f_w(\beta_j) > -\infty$ or $\sum_{\pm E_j \geq 2} f_w(\beta_j) < \infty$, then* $\mathrm{Tr}(P_w(J))$ *exists and*

$$Z_w(J) - \sum_{\pm E_j \leq -2} f_w(\beta_j) = \mathrm{Tr}(P_w(J)) + \sum_{\pm E_j \geq 2} f_w(\beta_j).$$

(iii) *If $f_w \leq 0$ on $[1, 1+\varepsilon] \cup [-1-\varepsilon, -1]$ for some $\varepsilon > 0$, then* $\mathrm{Tr}(P_w(J))$ *exists and*

$$Z_w(J) - \sum_{j=1}^\infty f_w(\beta_j) = \mathrm{Tr}(P_w(J)).$$

Remarks. 1. The matrix $P_w(J)$ need not be trace-class, but its trace, given by the sum of its diagonal elements, exists in (i)–(iii).

2. We use here the convention that $\pm\infty + a = \pm\infty$ for $a \in \mathbb{R}$ and $\infty - \infty$ can be anything. For example, if in (i) $Z_w(J) < \infty$ and $\sum_j f_w(\beta_j) = \infty$, then $\mathrm{Tr}(P_w(J))$ must be $-\infty$. Notice that in the above sum rules, $\mathrm{Tr}(P_w(J))$ is the only term that can be $-\infty$.

3. Theorem 7(iii) is just the main result of [10] in a different guise. It provides a characterization of the a_n's and b_n's which correspond to matrices with spectral measures for which a certain Szegő-type integral involving μ' and a certain Lieb-Thirring sum are both finite.

4. In the proofs of Theorems 1 and 3 we will use Theorem 7(i) with

$$w(\theta) \equiv 3 - 4\cos 2\theta + \cos 4\theta = 2(1 - \cos 2\theta)^2. \tag{12}$$

The previously mentioned results from [6, 8] can be obtained from Theorem 7(iii) by taking $w(\theta) \equiv (1 - \cos 2\theta)^k$ for $k = 1, 3$, respectively.

Proof. (i) We take $n \to \infty$ in (4). Using (6), (8), and (11) we obtain

$$Z_w(J) \geq \limsup_{n\to\infty} \sum_{j=1}^n (P_w(J))_{j,j} + \sum_{j=1}^\infty f_w(\beta_j).$$

Similarly, writing (4) for J_n in place of J (with $(J_n)^{(n)} = J_0$) and taking $n \to \infty$, from (6), (9), and (11) we obtain

$$Z_w(J) \leq \liminf_{n\to\infty} \sum_{j=1}^n (P_w(J))_{j,j} + \sum_{j=1}^\infty f_w(\beta_j).$$

Here we used the fact that the first $n-k$ diagonal elements of $P_w(J)$ and $P_w(J_n)$ are the same, whereas the next k differ by $o(1)$. Unless both $Z_w(J)=\infty$ and $\sum_j f_w(\beta_j)=\infty$, these inequalities can both be satisfied only if the $\limsup = \liminf$.

The proofs of (ii) and (iii) are analogous. $\square$

3. Spectral Consequences

Proof of Theorem 1. First we note that

$$T_0(x)=1, \quad T_2(x)=2x^2-1, \quad T_4(x)=8x^4-8x^2+1,$$

and so with w as in (12) we have $\sum_{\ell=0}^k c_\ell T_\ell(\frac{x}{2}) = \frac12(4-x^2)^2$. Hence by (2), $\int_{-2}^2 \ln(\mu'(x))(4-x^2)^{3/2}\,dx=-\infty$ if and only if $Z_w(J)=\infty$.

Next, we have

$$f_w(\beta)\equiv 3\ln(|\beta|)-(\beta^2-\beta^{-2})+\tfrac18(\beta^4-\beta^{-4}) = \tfrac85(|\beta|-1)^5+O((|\beta|-1)^6).$$

In particular, $\sum_j(|E_j|-2)^{5/2}=\infty$ if and only if $\sum_j f_w(\beta_j)=\infty$.

Finally, with $S_{i,j}=\frac78\delta_{1,i}\delta_{1,j}$, we have

$$P_w(J)=S-3A+2T_2(\tfrac12 J)-\tfrac14 T_4(\tfrac12 J) = S-3A-\tfrac18(J^4-12J^2+18).$$

If all $a_j=1$, then for $j\ge 4$ the j^{th} diagonal element of $P_w(J)$ is

$$-\tfrac18\big[(b_j^4+6b_j^2+b_{j-1}^2+b_{j+1}^2+2b_j(b_{j+1}+b_{j-1})+6)-12(b_j^2+2)+18\big].$$

Since $b_j\to 0$, we get that the limit $\mathrm{Tr}(P_w(J))$ exists if and only if $\sum_{j=1}^\infty[b_j^4-2(\partial b_j)^2]$ exists, and

$$\mathrm{Tr}(P_w(J)) = -\frac18\sum_{j=1}^\infty\big[b_j^4-2(\partial b_j)^2\big]+O\big(1+\|b_j\|_\infty\big).$$

For general $d_j\equiv a_j-1$ we get with $O(\|J\|_\infty)=O(\|a_j\|_\infty+\|b_j\||_\infty)$,

$$\begin{aligned}-8\,\mathrm{Tr}(P_w(J)) = \sum_{j=1}^\infty\big[&b_j^4-2(\partial b_j)^2-8(\partial d_j)^2\\ &+8d_j(2d_j^2+d_jd_{j+1}+d_{j+1}^2+b_j^2+b_jb_{j+1}+b_{j+1}^2)\\ &+4d_j^2(-d_j^2+d_{j+1}^2+b_j^2+b_jb_{j+1}+b_{j+1}^2)+O(d_j^5)\big]\\ &+O\big(\|J\|_\infty\big). \end{aligned} \tag{13}$$

If $a_j-1\in\ell^3$, then this is $\sum_j r_j+O(\|d_j\|_3^3+\|J\|_\infty)$.

(i) From the hypothesis and (13), we have $\mathrm{Tr}(P_w(J))=-\infty$ or does not exist. Thus $\sum_j f_w(\beta_j)=\infty$ by Theorem 7(i) and (3).

(ii) Now $\mathrm{Tr}(P_w(J))=\infty$ or does not exist, and we use Theorem 7(i) and $\sum_j f_w(\beta_j)>-\infty$ to get $Z_w(J)=\infty$. $\square$

By a careful examination of (13), one can prove the following variation on Theorem 1, allowing $a_n - 1 \notin \ell^3$. We let $a_\pm \equiv \max\{\pm a, 0\}$.

Corollary 8. (i) *If $(a_n-1)_- \in \ell^2$, $\partial a_n, \partial b_n \in \ell^2$, and either $a_n - 1 \notin \ell^3$ or $b_n \notin \ell^4$, then $\sum_j (|E_j|-2)^{5/2} = \infty$.*
(ii) *If $(a_n-1)_+ \in \ell^2$, $b_n \in \ell^4$ and either $a_n - 1 \notin \ell^3$ or $\partial a_n \notin \ell^2$ or $\partial b_n \notin \ell^2$, then $\int_{-2}^2 \ln(\mu'(x))(4-x^2)^{3/2}\, dx = -\infty$.*

Proof. (i) Note that once d_j is small enough, then for $d_j \le 0$ the sum of the second and third lines in (13) is bounded below by $-Cd_j^2 - \varepsilon(|d_{j+1}|^3 + b_j^4 + b_{j+1}^4)$ (for any $\varepsilon > 0$ and $C = C(\varepsilon) < \infty$), and for $d_j \ge 0$ it is bounded below by $8d_j^3$. So the whole sum is bounded below by $\sum_j [(1-2\varepsilon)b_j^4 + (8-\varepsilon)d_j^3 - q_j]$ for some summable q_j, proving $\mathrm{Tr}(P_w(J)) = -\infty$. The result follows as in the proof of Theorem 1(i).

(ii) One shows that $\mathrm{Tr}(P_w(J)) = \infty$ in a similar way as in (i), this time bounding the sum of the second and third lines of (13) above by $Cd_j^2 + \varepsilon(|d_{j+1}|^3 + b_j^4 + b_{j+1}^4)$ for $d_j \ge 0$ and by $8d_j^3$ for $d_j \le 0$. ☐

Proof of Theorem 3. The hypothesis and (1) give $\sum_j (|E_j|-2)^{5/2} < \infty$. Hence, by Theorem 7(i) with w given by (12), $\mathrm{Tr}(P_w(J))$ exists. And it is finite if and only if $Z_w(J) < \infty$. But by the assumptions and (13), the former happens precisely when $\partial a_n, \partial b_n \in \ell^2$. As in Theorem 1, the latter happens if and only if $\int_{-2}^2 \ln(\mu'(x))(4-x^2)^{3/2}\, dx > -\infty$. ☐

Here is an application of Theorem 7(i) to *oscillatory* Jacobi matrices:

Corollary 9. *If $\limsup_n \sum_{j=1}^n (|\partial a_j|^2 + |\partial b_j|^2) / \sum_{j=1}^n (|a_j - 1|^3 + |b_j|^3) = \infty$, then $\int_{-2}^2 \ln(\mu'(x))(4-x^2)^{3/2}\, dx = -\infty$.*

Remark. This applies, for example, in the case $a_n = 1 + \alpha_1 \cos(\mu n)/n^{\gamma_1}$ and $b_n = \alpha_2 \cos(\mu n)/n^{\gamma_2}$ when $\mu \notin 2\pi\mathbb{Z}$ and $\alpha_j \neq 0$, $\gamma_j \le \frac{1}{2}$ for either $j = 1$ or $j = 2$. In [3] it was proved that in this case, with $\alpha_1 = 0$, $\int_{-2}^2 \ln(\mu'(x))(4-x^2)^{-1/2}\, dx = -\infty$.

Proof. For w as in the proof of Theorem 1 we get $\mathrm{Tr}(P_w(J)) = \infty$ (from (13)). Then we continue as in (ii) of that proof. ☐

Finally, here are two results illustrating the use of Theorem 7(ii). The first has been proved in [11] for the case $a_n - 1, b_n \in \ell^2$. The second is related to results in [2, 4].

Theorem 10. *If $a_n \to 1$, $b_n \to 0$, and $\limsup_n \sum_{j=1}^n [\ln(a_j) \pm \frac{1}{2} b_j] = \infty$, then*

$$\sum_{\pm E_j \ge 2} (|E_j| - 2)^{1/2} = \infty.$$

Proof. Let $w(\theta) \equiv 1 \pm \cos\theta$ so that $f_w(\beta) = 2(|\beta| - 1) + O((|\beta| - 1)^2)$ for $\pm\beta \downarrow 1$ and $f_w(\beta) = -\frac{1}{6}(|\beta|-1)^3 + O((|\beta|-1)^4)$ for $\pm\beta \uparrow -1$. Then $P_w(J) = -A \mp \frac{1}{2}J$, and so its j^{th} diagonal element is $-[\ln(a_j) \pm \frac{1}{2}b_j]$. Theorem 7(ii) finishes the proof. $\square$

Theorem 11. *If $a_n \to 1$, $b_n \to 0$, and one of $\sum_{n=1}^{\infty}[\ln(a_n) \pm \frac{1}{2}b_n]$ is larger than $\frac{1}{2}$ or does not exist, then J has at least one eigenvalue outside* $[-2, 2]$.

Remark. The bound $\frac{1}{2}$ is optimal as can be seen by taking $a_n \equiv 1$ and $|b_n| \le \delta_{1,n}$. The corresponding Jacobi matrix has no eigenvalues.

Proof. Take again $w(\theta) \equiv 1 \pm \cos\theta$ in Theorem 7(ii). By (2.45) in [12],

$$\begin{aligned} Z_w(J) &\ge \int_0^{\pi} (1 - \cos\theta) \ln(2 + 2\cos\theta) \frac{d\theta}{2\pi} \\ &= \frac{1}{2} \int_0^{2\pi} (1 - \cos\theta) \ln\left|1 + 2e^{i\theta} + e^{2i\theta}\right| \frac{d\theta}{2\pi}. \end{aligned}$$

Jensen's formulae for the function $\ln|1+2z+z^2| = \Re(2z+O(z^2))$ show that the last integral equals -1. If J had no eigenvalues, we would have $-\frac{1}{2} \le Z_w(J) = \mathrm{Tr}(P_w(J)) = -\sum_{n=1}^{\infty}[\ln(a_n) \pm \frac{1}{2}b_n]$, a contradiction. $\square$

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