Sum Rules and the Szegő Condition for Jacobi Matrices

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Abstract

We consider Jacobi matrices J with $b_n \in \mathbb{R}$ on the diagonal, $a_n > 0$ on the next two diagonals, and with spectral measure $d\nu(x) = \nu'(x)dx + d\nu_{\text{sing}}(x)$. In particular, we are interested in compact perturbations of the free matrix J_0, that is, such that $a_n \to 1$ and $b_n \to 0$. We study the Case sum rules for such matrices. These are trace formulae relating sums involving the a_n's and b_n's on one side and certain quantities in terms of ν on the other. We establish situations where the sum rules are valid, extending results of Case and Killip-Simon.

The matrix J is said to satisfy the Szegő condition whenever the integral

$$\int_0^\pi \ln\bigl[\nu'(2\cos\theta)\bigr]\,d\theta,$$

which appears in the sum rules, is finite. Applications of our results include an extension of Shohat's classification of certain Jacobi matrices satisfying the Szegő condition to cases with infinite point spectrum, and a proof that if $n(a_n - 1) \to \alpha$, $nb_n \to \beta$, and $2\alpha < |\beta|$, then the Szegő condition fails. Related to this, we resolve a conjecture by Askey on the Szegő condition for Jacobi matrices which are Coulomb perturbations of J_0. More generally, we prove that if

$$a_n \equiv 1 + \frac{\alpha}{n^\gamma} + O(n^{-1-\varepsilon}), \qquad b_n \equiv \frac{\beta}{n^\gamma} + O(n^{-1-\varepsilon})$$

with $0 < \gamma \le 1$ and $\varepsilon > 0$, then the Szegő condition is satisfied if and only if $2\alpha \ge |\beta|$.

Contents

Chapter 1

Introduction

This thesis discusses the spectral theory of Jacobi matrices. A *Jacobi matrix* is the tri-diagonal semi-infinite self-adjoint matrix

$$J = \begin{pmatrix} b_1 & a_1 & 0 & \dots \\ a_1 & b_2 & a_2 & \dots \\ 0 & a_2 & b_3 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \tag{1.1}$$

with $a_n > 0$ and $b_n \in \mathbb{R}$. We will mainly be interested in matrices which are compact perturbations of the *free matrix* J_0 (with $a_n \equiv 1$ and $b_n \equiv 0$). For such J we have $a_n \to 1$, $b_n \to 0$, and $\sigma_{\text{ess}}(J) = [-2, 2]$. Outside this interval J can have only simple isolated eigenvalues, with ± 2 the only possible accumulation points. We denote them $E_1^+ > E_2^+ > \cdots > 2$ and $E_1^- < E_2^- < \cdots < -2$.

There is an intimate connection between Jacobi matrices and *orthogonal polynomials* on the real line, that is, polynomials orthonormal with respect to a (positive) measure on $\mathbb{R}$. Actually, when we restrict ourselves to bounded Jacobi matrices on one side, and to probability measures with bounded infinite supports on the other, then these two objects are one. Indeed, there is a special spectral measure ν for J as an operator on $\ell^2(\{0, 1, \dots\})$, namely, the spectral measure with respect to the vector δ_0. It turns out that the orthogonal polynomials $P_n(x)$ for this measure are at the same time *Dirichlet eigenfunctions* for J, when energy x is fixed and n is varied.

In particular, they obey the *three-term recurrence relation*

$$xP_n(x) = a_{n+1}P_{n+1}(x) + b_{n+1}P_n(x) + a_nP_{n-1}(x) \tag{1.2}$$

with $P_{-1} \equiv 0$ and $P_0 \equiv 1$. So given a measure ν, one can construct the corresponding J by means of P_n and (1.2). This gives a one-to-one correspondence of matrices and measures.

Although Jacobi matrices and orthogonal polynomials have a lot in common, it seems that there has not been much interaction between these two areas. In the present work we would like to join efforts in this direction by applying methods from one area to answer questions in the other. This aim is reflected in the fact that our work has two main parts. In the first part, Chapter 3, we develop the *sum rules* for Jacobi matrices, tools which we then apply in the second part, Chapter 4, to solve an open problem and some related questions in the theory of orthogonal polynomials.

The sum rules are trace formulae which relate spectral information of J and sums involving the a_n's and b_n's. They were first written down by Case [2] (motivated by Flaschka's work on the Toda lattice [10]), who proved them for J's with $J - J_0$ finite rank, and his methods probably also work in the case $\sum n(|a_n - 1| + |b_n|) < \infty$. An important contribution in this respect was recently obtained by Killip-Simon [13], who extended the sum rules to $J - J_0$ trace class. The sum rule part of the present thesis is motivated by their work. In this introduction we will only state the first of the sum rules, leaving the rest for later. But before we can do this, we need to define its constituents.

An object of particular interest, both for us and in the theory of orthogonal polynomials, is the *Szegő integral*

$$Z(J) \equiv \frac{1}{2\pi} \int_{-2}^{2} \ln\left(\frac{\sqrt{4-x^2}}{2\pi\nu'(x)}\right) \frac{dx}{\sqrt{4-x^2}} \tag{1.3}$$

with $\nu'(x) \equiv d\nu_{\rm ac}(x)/dx$. It is often taken in the literature as

$$\frac{1}{2\pi}\int_0^\pi \ln\bigl[\nu'(2\cos\theta)\bigr]\,d\theta,$$

which differs from $Z(J)$ by a constant and a minus sign. This is a natural analogue of the Szegő integral for measures supported on the unit circle, which is one of the central objects in the theory of orthogonal polynomials on the unit circle.

We say that J satisfies the *Szegő condition* (or J is *Szegő*) if $Z(J)$ is finite. The negative part of the integrand in (1.3) is always integrable, and $Z(J) \geq -\frac{1}{2}\ln(2)$. Hence, we are left with the question whether $Z(J) < \infty$. There is extensive literature on when this is the case. See, for example, [1, 2, 8, 11, 17, 18, 20, 21, 22, 28, 33, 34].

We are interested in this question for two reasons. One is that $Z(J)$ and similar integrals appear in the sum rules which we study here. The other is that the open problem we want to solve is exactly this question for certain special J's, as we shall see later.

Next, we introduce the eigenvalue sum

$$\mathcal{E}_0(J) \equiv \sum_{\pm}\sum_j \ln\biggl[\tfrac{1}{2}\Bigl(|E_j^\pm| + \sqrt{(E_j^\pm)^2 - 4}\Bigr)\biggr]. \tag{1.4}$$

It is not hard to see that $\mathcal{E}_0(J) < \infty$ if and only if

$$\sum_{\pm}\sum_j \sqrt{|E_j^\pm| - 2} < \infty. \tag{1.5}$$

The last quantity we need is

$$A_0(J) \equiv \lim_{N\to\infty}\biggl(-\sum_{n=1}^N \ln(a_n)\biggr), \tag{1.6}$$

which we define if the limit exists, even if it is $+\infty$ or $-\infty$.

Now we are ready to formulate the Z sum rule, called C_0 in [13]:

$$Z(J) = A_0(J) + \mathcal{E}_0(J). \tag{1.7}$$

In this equality two terms come from the spectral measure ν, whereas the third comes from the matrix J. In this light, the form $Z(J) - \mathcal{E}_0(J) = A_0(J)$ might seem more appropriate, but we will see that the form (1.7) enters naturally.

As noted above, Killip-Simon proved (1.7) for $J - J_0$ trace class, in which case $A_0(J)$ is well defined and all three terms can be shown to be finite. It is not a priori clear what happens if we abandon this assumption. The interest in this question is justified, besides the quest for broadening of mathematical knowledge, by the main result of Killip-Simon. They were able to prove one of the sum rules (P_2, called Z_2^- here) for *all* Jacobi matrices, and using it they obtained a characterization of all Hilbert-Schmidt perturbations of J_0. This result (motivated in turn by previous work on Schrödinger operators by Deift-Killip [5] and Denisov [6]) shows how to exploit the sum rules as a spectral tool. In particular, Killip-Simon emphasized the importance of proving the sum rules for as large a class of J's as possible.

In Chapter 3 of our thesis we will address this question and extend all the sum rules to full generality. One of our main results in that chapter is the following:

Theorem 1.1. *Suppose the limit* (1.6) *exists. If any two of the three quantities* $Z(J)$, $A_0(J)$, *and* $\mathcal{E}_0(J)$ *are finite, then all three are, and* (1.7) *holds.*

Remarks. 1. The full theorem (Theorem 3.14) does not require the limit (1.6) to exist, but is more complicated to state in that case.

2. If the three quantities are finite, many additional sum rules hold.

3. Peherstorfer-Yuditskii [22] (see their remark after Lemma 2.1) prove that if $Z(J) < \infty$, $\mathcal{E}_0(J) = \infty$, then the limit in (1.6) is also infinite.

Theorem 1.1 is a real line analogue of a seventy-year-old theorem for orthogonal polynomials on the unit circle:

$$\frac{1}{2\pi}\int_0^{2\pi} \ln\bigl[\nu'(e^{i\theta})\bigr]\, d\theta = \sum_{n=0}^{\infty} \ln(1 - |\alpha_j|^2), \tag{1.8}$$

where $\{\alpha_j\}_{j=1}^{\infty}$ are the Verblunsky coefficients (also called reflection, Geronimus, Schur, or Szegő coefficients) of ν. This result was first proven by Verblunsky [39] in 1935, although it is closely related to Szegő's 1920 paper [34].

One application we will make of Theorem 1.1 and related ideas is to prove the following ($\equiv$ Theorem 3.20):

Theorem 1.2. *Suppose* $\sigma_{\text{ess}}(J) \subseteq [-2,2]$ *and* (1.5) *holds. Then* J *is Szegő if and only if*

$$\liminf_{N\to\infty}\left(-\sum_{n=1}^{N}\ln(a_n)\right) < \infty. \tag{1.9}$$

Moreover, if these conditions hold, then

(i) *the limit* (1.6) *exists and is finite,*

(ii) $\lim_{N\to\infty}\sum_{n=1}^{N} b_n$ *exists and is finite,*

(iii)

$$\sum_{n=1}^{\infty}\left[(a_n-1)^2+b_n^2\right] < \infty. \tag{1.10}$$

Results of this genre when it is assumed that $\sigma(J) = [-2,2]$ go back to Shohat [28], with important contributions by Nevai [18]. The precise form is from Killip-Simon [13]. Nikishin [21] showed how to extend this to Jacobi matrices with finitely many eigenvalues. Peherstorfer-Yuditskii [22] proved $Z(J) < \infty$ implies (i) under the condition $\mathcal{E}_0(J) < \infty$, allowing an infinity of eigenvalues for the first time. Our result cannot extend to situations with $\mathcal{E}_0(J) = \infty$ since Theorem 1.1 says that if (i) holds and $Z(J) < \infty$, then $\mathcal{E}_0(J) < \infty$.

We will highlight one other result from Chapter 3 (see Theorem 3.24):

Theorem 1.3. *Suppose* (1.10) *holds and either* $\limsup[-\sum_{n=1}^{N}(a_n - 1 + \frac{1}{2}b_n)] = \infty$ *or* $\limsup[-\sum_{n=1}^{N}(a_n - 1 - \frac{1}{2}b_n)] = \infty$. *Then* $Z(J) = \infty$.

One of the main results of [13] is the proof of a conjecture of Nevai [20]. It states that if the perturbation $J - J_0$ is trace class, then $Z(J) < \infty$. Killip-Simon were able to prove this by extending the sum rule (1.7) to $J - J_0$ trace class, and by using a result of Hundertmark-Simon [12] that $\mathcal{E}_0(J) < \infty$ in that case. In Chapter 4 we will address a related question involving non-trace-class $J - J_0$. This is yet another reason for us to extend the sum rules to full generality. The question is the following conjecture of Askey about Coulomb-decay Jacobi matrices, reported by Nevai in [17]:

Askey's Conjecture. If

$$a_n \equiv 1 + \frac{\alpha}{n} + O\left(\frac{1}{n^2}\right), \qquad\qquad b_n \equiv \frac{\beta}{n} + O\left(\frac{1}{n^2}\right),$$

and $\alpha^2 + \beta^2 > 0$, then J is not Szegő.

These a_n, b_n are natural because they are just at the borderline beyond $J - J_0$ trace class. It has been known for some time that in the case of $\alpha = \beta = 0$, one has $Z(J) < \infty$. These results predate Killip-Simon by more than twenty years, for example, Nevai's result in [17] that if $\sum \ln(n)|a_n - 1| < \infty$ and $\sum \ln(n)|b_n| < \infty$, then $Z(J) < \infty$.

The other cases have remained open and will be treated in this work. Actually, we will consider more general errors here, namely, $O(n^{-1-\varepsilon})$ for $\varepsilon > 0$. Before stating our main result in this respect, let us first discuss the history of these kinds of problems.

In the late 1940's Pollaczek [23, 24, 25] found an explicit class of examples in the region (in our language) $|\beta| < -2\alpha$, one example for each such (α, β), with further study by Szegő [34, 36]. They found that in these cases the Szegő condition fails.

In 1979 Nevai [17] reported the above conjecture of Askey. However, in 1984 Askey-Ismail [1, p.102] gave some explicit examples with $b_n \equiv 0$ and $\alpha > 0$, and noted that the Szegő condition holds (!), so they concluded the conjecture needed to be modified.

In 1986 Dombrowski-Nevai [8] proved a general result that Szegő condition holds when $b_n \equiv 0$ and $\alpha > 0$ with $o(n^{-2})$ errors. And finally, in 1987 Charris-Ismail [3] computed the weights for Pollaczek-type examples in the entire (α, β) plane. Although they did not note it, their examples are Szegő if and only if $2\alpha \geq |\beta|$. We will see that this is the general picture for this problem, and the "right" form of the conjecture.

Here is our result for this class:

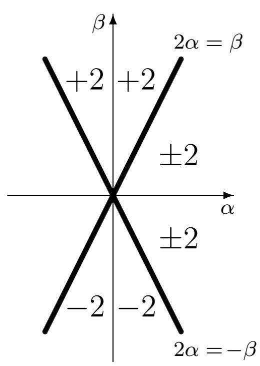
Theorem 1.4. *Let*

$$a_n \equiv 1 + \frac{\alpha}{n^\gamma} + O(n^{-1-\varepsilon}), \qquad\qquad b_n \equiv \frac{\beta}{n^\gamma} + O(n^{-1-\varepsilon})$$

with $0 < \gamma \le 1$ *and* $\varepsilon > 0$. *Then* J *is Szegő if and only if* $2\alpha \ge |\beta|$.

Remark. This is a corollary of more general results, in particular, of Theorem 4.16.

We will prove even more for $\frac{1}{2} < \gamma \le 1$. In Section 4.4 we discuss some situations when the Szegő integral is allowed to diverge at one end of $[-2, 2]$ and study its convergence at the other end (*one-sided Szegő conditions*). This is of particular interest when the perturbation $J - J_0$ is Hilbert-Schmidt (which is the origin of the requirement $\gamma > \frac{1}{2}$). In that case the abovementioned P_2 sum rule of Killip-Simon shows that the Szegő integral (1.3) can only diverge at ± 2. We establish here the following picture for these γ:



Legend:
± 2 – Szegő condition holds
$+2$ – Szegő condition at 2 holds
-2 – Szegő condition at -2 holds

The (α, β) plane is divided into four regions by the lines $2\alpha = \pm\beta$. Inside the right-hand region $Z(J)$ converges at both ends, inside the top and bottom regions $Z(J)$ converges only at, respectively, 2 and -2, and inside the left-hand region $Z(J)$ diverges at both ends. As for the borderlines $2\alpha = \pm\beta$, if $\alpha \ge 0$, then $Z(J)$ converges at both ends, and if $\alpha < 0$, then $Z(J)$ diverges at ± 2 (convergence at ∓ 2 is left open). The divergence results follow from the material in Chapter 3, whereas the convergence results are proved in Chapter 4. We note that the divergence results hold for more general errors, trace class in particular.

The thesis is organized as follows. In Chapter 2 we collect most of the background material we need. With a couple of exceptions, proofs are provided for the reader's convenience. Some more specialized results are left for the appendices to Chapters 3 and 4.

In Chapter 3 we extend the sum rules to general Jacobi matrices, non-trace-class in particular, and prove Theorem 1.1. We then give various applications, including Theorems 1.2 and 1.3, the second of which can be viewed as a general *necessary* condition for $Z(J) < \infty$.

In Chapter 4 we apply the sum rules to derive *sufficient* conditions for $Z(J) < \infty$. These are stated in the form of a relation between the sizes of the on-diagonal and off-diagonal pieces of the perturbation $J - J_0$, and are in line with the (α, β) picture above. In particular, we obtain Theorem 1.4.

Chapter 2

Background

In this chapter we collect most of the background material used in this work. The majority of the results are common knowledge about Jacobi matrices and orthogonal polynomials. In Section 2.1 we develop the basic relationships between these objects. In Section 2.2 we state results concerning bound states: Sturm oscillation theory and Lieb-Thirring inequalities. Section 2.3 deals with the behavior of spectral measures and eigenvalues for converging sequences of matrices. Section 2.4 introduces the Szegő integral and derives some of its important properties. Finally, Section 2.5 contains some basic facts about the m-function, the Borel transform of the spectral measure.

2.1 Jacobi Matrices, Spectral Measures, and Orthogonal Polynomials

The main object of our investigation is the *Jacobi matrix*

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

with $a_n > 0$ and $b_n \in \mathbb{R}$. In this work we will only consider cases where $\{a_n\}$ and $\{b_n\}$ are bounded. Hence J is a bounded self-adjoint operator on the Hilbert space

$\ell^2(\mathbb{Z}^+) = \ell^2(\{0, 1, \dots\})$. Usually, J is extended to map the set of complex sequences $\{u_n\}_{n=-1}^{\infty}$ to the set of complex sequences $\{v_n\}_{n=0}^{\infty}$ by taking $a_0 \equiv 1$ and defining

$$(Ju)_n \equiv a_{n+1}u_{n+1} + b_{n+1}u_n + a_n u_{n-1}$$

for $n \geq 0$. If such a sequence satisfies the eigenfunction equation

$$(Ju)_n = \zeta u_n \tag{2.1}$$

for some $\zeta \in \mathbb{C}$ and all $n \geq 0$, then u is called a *generalized eigenfunction* (or simply *eigenfunction*) of J for *energy* ζ. It is clear from (2.1) that any eigenfunction u for energy ζ is uniquely determined by u_n and u_{n-1} (for arbitrary n). Consequently, eigenfunctions for a given energy form a two-dimensional vector space. Notice that if $u_n = u_{n-1} = 0$, then the eigenfunction u is identically zero.

For any energy there are two special eigenfunctions. If $u_{-1} = 0$ and $u_0 = 1$, then the eigenfunction u is the *Dirichlet eigenfunction*, and if $u_{-1} = 1$ and $u_0 = 0$, then it is the *Neumann eigenfunction*. Obviously, ζ is an eigenvalue of J if and only if the Dirichlet eigenfunction for ζ is in $\ell^2(\mathbb{Z}^+)$. By self-adjointness of J, this can only happen for $\zeta \in \mathbb{R}$. If $\zeta \in \mathbb{C}\backslash\mathbb{R}$, then there is always an eigenfunction $u \in \ell^2(\mathbb{Z}^+)$ for ζ, but it has $u_{-1} \neq 0$. Indeed, one can take

$$u_n \equiv -\big((J - \zeta)^{-1}\delta_0\big)_n \tag{2.2}$$

for $n \geq 0$, and $u_{-1} = 1$. This is well defined because $(J - \zeta)^{-1} : \ell^2(\mathbb{Z}^+) \to \ell^2(\mathbb{Z}^+)$ is a bounded operator. Obviously $(J - \zeta)u = -\delta_0 + a_0 u_{-1}\delta_0 = 0$.

We define the *Wronskian* of two sequences $\{u_n\}_{n=-1}^{\infty}$ and $\{v_n\}_{n=-1}^{\infty}$ to be

$$W_n(u, v) \equiv a_n(u_n v_{n-1} - u_{n-1}v_n) \tag{2.3}$$

for $n \geq 0$. Clearly $W_n(u, u) \equiv 0$. The most useful property of this object is that if u, v are two eigenfunctions of J for energy ζ, then $W(u, v) \equiv W_n(u, v)$ is independent of n. This is well known and can be checked easily using (2.1). Notice that then $W(u,v) = 0$ if and only if u and v are linearly dependent. This shows that for any energy there can be only one ℓ^2-eigenfunction (up to a multiplicative constant).

The vector $\delta_0 = (1,0,0,\dots)$ is a cyclic vector for J. Indeed, if Q_n is a real polynomial of degree n with leading coefficient $q \neq 0$, then it is clear that

$$Q_n(J)\delta_0 = q\Big(\prod_{j=1}^{n} a_j\Big)\delta_n + \sum_{j=0}^{n-1} r_j\delta_j$$

for some $r_j \in \mathbb{R}$. This of course means that there is a unique real polynomial P_n of degree n such that $P_n(J)\delta_0 = \delta_n$ (and since $a_n > 0$, the leading coefficient of P_n must be positive). Hence δ_0 must be cyclic. It follows that the spectrum of J is simple and the spectral measure for δ_0 (which we will call ν) is a spectral measure for J, in the sense that J is isomorphic to the operator of multiplication by x on $L^2(\mathbb{R}, d\nu)$.

By the spectral theorem,

$$\langle \delta_0, (J-\zeta)^{-1}\delta_0\rangle = \int \frac{d\nu(x)}{x-\zeta}$$

for $\zeta \in \mathbb{C}\backslash\mathbb{R}$ (all integrals in this chapter are taken from $-\infty$ to ∞ unless indicated otherwise). More generally, we have

$$\langle \delta_0, f(J)\delta_0\rangle = \int f(x)\, d\nu(x) \tag{2.4}$$

for any $f \in L^1(\mathbb{R}, d\nu)$. Notice also that $\nu(\mathbb{R}) = \|\delta_0\|_2 = 1$, that is, ν is a probability measure, and the support of ν is bounded. Also, it is an infinite set, because by the spectral theorem $L^2(\mathbb{R}, d\nu) \cong \ell^2(\mathbb{Z}^+)$ is infinite-dimensional.

Next we turn to the polynomials P_n. By (2.4) and $P_n(x) \in \mathbb{R}$ we have

$$\int P_n(x)P_m(x)\, d\nu(x) = \langle P_m(J)\delta_0, P_n(J)\delta_0\rangle = \delta_{m,n}.$$

Hence the polynomials $P_0 \equiv 1, P_1, P_2, \dots$ are an orthonormal set in $L^2(\mathbb{R}, d\nu)$. Since the degree of P_n is n and P_n is real with positive leading coefficient, these must be the *orthogonal polynomials* for ν, which one obtains by applying the Gram-Schmidt procedure to the set $\{1, x, x^2, \dots\} \subset L^2(\mathbb{R}, d\nu)$. This latter set is a basis and thus so must $\{P_0, P_1, \dots\}$ be. Moreover, we have

$$\int xP_n(x)P_m(x)\,d\nu(x) = \langle P_m(J)\delta_0, JP_n(J)\delta_0\rangle = a_{n+1}\delta_{m,n+1} + b_{n+1}\delta_{m,n} + a_n\delta_{m,n-1}$$

and it follows that with $P_{-1} \equiv 0$,

$$xP_n(x) = a_{n+1}P_{n+1}(x) + b_{n+1}P_n(x) + a_nP_{n-1}(x) \tag{2.5}$$

for $n \geq 0$. This is the so-called *three-term recurrence relation*. It shows that $\{P_n(x)\}_{n=0}^{\infty}$ is the Dirichlet eigenfunction for J and energy x. It also shows that multiplication by x on $L^2(\mathbb{R}, d\nu)$ is unitarily equivalent to J acting on $\ell^2(\mathbb{Z}^+)$ (the corresponding bases being $\{P_0, P_1, \dots\}$ and $\{\delta_0, \delta_1, \dots\}$). This follows from the spectral theorem as well.

In the above, we have constructed a measure ν (and its orthogonal polynomials) associated to a given bounded Jacobi matrix. One can also go in the opposite direction. Given a probability measure ν with bounded infinite support, one first constructs its orthogonal polynomials P_n using the Gram-Schmidt procedure in the Hilbert space $L^2(\mathbb{R}, d\nu)$ with inner product $\langle f, g\rangle_\nu \equiv \int \bar{f} g\, d\nu$. Again, P_n are all real and have positive leading coefficients. Since $xP_n(x)$ is a polynomial of degree $n+1$, it is orthogonal to $P_m(x)$ for $m \geq n+2$. It is also orthogonal to $P_m(x)$ for $m \leq n-2$ because $\langle xP_n(x), P_m(x)\rangle_\nu = \langle P_n(x), xP_m(x)\rangle_\nu$ and $xP_m(x)$ is of degree at most $n-1$. If we denote the leading coefficient of P_n by γ_n, then

$$a_n \equiv \langle xP_n(x), P_{n-1}(x)\rangle_\nu = \langle P_n(x), xP_{n-1}(x)\rangle_\nu = \langle P_n(x), \frac{\gamma_{n-1}}{\gamma_n}P_n(x)\rangle_\nu = \frac{\gamma_{n-1}}{\gamma_n} > 0$$

because P_n is orthogonal to polynomials of degree less than n. Hence with

$$b_n \equiv \langle xP_{n-1}(x), P_{n-1}(x)\rangle_\nu \tag{2.6}$$

we have (2.5). This gives rise to a Jacobi matrix J. By (2.5), the spectral measure for δ_0 and J coincides with the one for $P_0(x) \equiv 1$ and the operator of multiplication by x on $L^2(\mathbb{R}, d\nu)$. This latter measure is clearly ν.

We have just seen that there is a bijection between matrices and measures, so that bounded Jacobi matrices and probability measures with bounded infinite support are essentially two guises of the same object.

For future reference we note that by (2.5), the leading coefficient of the polynomial P_n is $\gamma_n = (a_1 \dots a_n)^{-1}$, and thus by Gram-Schmidt

$$P_n(x) = \frac{1}{a_1 \dots a_n}\Big[x^n - \sum_{j=0}^{n-1} \langle x^n, P_j(x)\rangle_\nu P_j(x)\Big]. \tag{2.7}$$

Then from orthonormality of the P_j's we obtain

$$1 = \langle P_n(x), P_n(x)\rangle_\nu = \Big(\frac{1}{a_1 \dots a_n}\Big)^2 \Big[\langle x^n, x^n\rangle_\nu - \sum_{j=0}^{n-1} \langle x^n, P_j(x)\rangle_\nu^2\Big]$$

and therefore

$$a_n = \frac{1}{a_1 \dots a_{n-1}} \sqrt{\langle x^n, x^n\rangle_\nu - \sum_{j=0}^{n-1} \langle x^n, P_j(x)\rangle_\nu^2}\,. \tag{2.8}$$

Let us now consider the "basic" matrix

$$J_0 \equiv \begin{pmatrix} 0 & 1 & 0 & \dots \\ 1 & 0 & 1 & \dots \\ 0 & 1 & 0 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}.$$

This is the free half-line discrete Schrödinger operator, and therefore will be called the *free matrix*. It is a direct computation that for $\theta \in (0, \pi)$,

$$2\cos\theta\cos n\theta = \cos(n+1)\theta + \cos(n-1)\theta \tag{2.9}$$

$$2\cos\theta\sin n\theta = \sin(n+1)\theta + \sin(n-1)\theta$$

and so $\{\cos n\theta\}_n$ and $\{\sin n\theta\}_n$ are eigenfunctions of J_0 for energy $2\cos\theta$. Using (2.9) and induction, one can show that $\cos n\theta$ and $\sin(n+1)\theta/\sin\theta$ are polynomials of degree n in $\cos\theta$. We call

$$T_n(\cos\theta) \equiv \cos n\theta \tag{2.10}$$

the *Chebyshev polynomials of the first kind* and

$$U_n(\cos\theta) \equiv \frac{\sin(n+1)\theta}{\sin\theta} \tag{2.11}$$

the *Chebyshev polynomials of the second kind* (when extended to all of $\mathbb{R}$). By (2.9), $\{U_n(\frac{x}{2})\}_n$ is the Dirichlet eigenfunction for J_0 and energy x, so $U_n(\frac{x}{2})$ is the n^{th} orthogonal polynomial for ν_0, the spectral measure of J_0. For later reference we note that

$$T_0(x) = 1, \qquad T_1(x) = x, \qquad T_2(x) = 2x^2 - 1. \tag{2.12}$$

The above, of course, shows that the free eigenfunctions for energy $2\cos\theta \in (-2,2)$ are of the form $c_1 e^{in\theta} + c_2 e^{-in\theta}$. For the sake of completeness, we note that one can easily see that the free eigenfunctions for any energy $x \in \mathbb{R}$ are

$$u_n = \begin{cases} c_1 e^{in\theta} + c_2 e^{-in\theta} & x = 2\cos\theta \in (-2,2), \\ c_1 n + c_2 & x = 2, \\ (-1)^n (c_1 n + c_2) & x = -2, \\ c_1 e^{n\theta} + c_2 e^{-n\theta} & x = 2\cosh\theta > 2, \\ (-1)^n (c_1 e^{n\theta} + c_2 e^{-n\theta}) & x = -2\cosh\theta < -2. \end{cases} \tag{2.13}$$

In general, if $\zeta \in \mathbb{C}$ is different from ± 2 and $z + z^{-1} = \zeta$, then the eigenfunctions for energy ζ are $u_n = c_1 z^n + c_2 z^{-n}$.

Finally, the spectral measure for J_0 is

$$d\nu_0(x) = \chi_{[-2,2]}(x) \frac{\sqrt{4-x^2}}{2\pi} dx, \tag{2.14}$$

as can be seen from

$$\int_{-2}^{2} U_n(\tfrac{x}{2})U_m(\tfrac{x}{2})\sqrt{4-x^2}\,dx = \int_0^\pi 4\sin(n+1)\theta\,\sin(m+1)\theta\,d\theta = 2\pi\delta_{m,n}$$

by using the change of variables $x = 2\cos\theta$.

We close this section with an estimate of the norm of the difference $J - J_0$ in the Schatten classes $\mathfrak{I}_p$ [29]. This appears in [13] and will be useful in our considerations of compact perturbations of J_0.

Lemma 2.1. *If* $c_n \equiv \max\{|a_n - 1|, |b_n|, |a_{n-1} - 1|\}$, *then for any* $p \in [1, \infty)$,

$$\tfrac{1}{3}\Big(\sum_{n=1}^{\infty} c_n^p\Big)^{1/p} \le \|J - J_0\|_p \le 3\Big(\sum_{n=1}^{\infty} c_n^p\Big)^{1/p}.$$

Proof. Let C be the diagonal matrix with c_n's on the diagonal. Then the tri-diagonal matrix S given by $C^{1/2}SC^{1/2} = J - J_0$ has all elements bounded by 1, so that the operator norm $\|S\| \le 3$. By Hölder's inequality for $\mathfrak{I}_p$ [29] we have

$$\|J - J_0\|_p \le \|C^{1/2}\|_{2p}\,\|S\|\,\|C^{1/2}\|_{2p} \le 3\Big(\sum_{n=1}^{\infty} c_n^p\Big)^{1/p}.$$

On the other hand,

$$\Big(\sum_{n=1}^{\infty} c_n^p\Big)^{1/p} \le \Big(\sum_{n=1}^{\infty} |b_n|^p\Big)^{1/p} + 2\Big(\sum_{n=1}^{\infty} |a_n - 1|^p\Big)^{1/p} \le 3\|J - J_0\|_p,$$

using

$$\|A\|_p^p = \sup\Big\{\sum_n |\langle\varphi_n, A\psi_n\rangle|^p \Big| \{\varphi_n\}, \{\psi_n\} \text{ orthonormal sets}\Big\}$$

from [29]. □

In this context, we also mention the obvious fact that

$$\sup_n\{c_n\} \le \|J - J_0\| \le 3\sup_n\{c_n\} \tag{2.15}$$

which was used to obtain $\|S\| \le 3$.

2.2 Bound States

In this work we will mostly consider Jacobi matrices whose essential spectrum is $[-2, 2]$. We will call such matrices *BW matrices* (for Blumenthal-Weyl). Note that this class includes compact perturbations of J_0, that is, such that $a_n \to 1$ and $b_n \to 0$. Hence from now on, unless stated otherwise, all matrices will be assumed to be BW matrices.

The condition $\sigma_{\text{ess}}(J) = [-2, 2]$ and boundedness of J imply that outside of $[-2, 2]$ there can be only simple isolated eigenvalues, with ± 2 the only possible accumulation points. We denote these $E_1^+ > E_2^+ > \cdots > 2$ and $E_1^- < E_2^- < \cdots < -2$, and call them *bound states*. To avoid possible notational problems, we define $E_j^\pm \equiv \pm 2$ whenever J has less than j positive/negative bound states.

In many of our considerations we will deal with positive bound states only. The reason is the following. If we define $\tilde{J}$ to have $\tilde{a}_n \equiv a_n$ and $\tilde{b}_n \equiv -b_n$, then $\tilde{J} = U(-J)U$ where $U = U^*$ is the unitary transformation taking a vector $\{u_n\} \in \ell^2$ to $\{(-1)^n u_n\}$. Due to this symmetry, negative bound states of J are negatives of positive bound states of $\tilde{J}$ and any results for the latter translate to the former. Note that $J_0 = \tilde{J}_0$, which is reflected in the fact that the free eigenfunctions (2.13) for energies x and $-x$ differ by $(-1)^n$.

We quote here without proof two important results involving eigenvalues. The first is from Sturm oscillation theory (see, e.g., [37]), which relates behavior of eigenfunctions for some energy $x \geq 2$ ($x \leq -2$) and the number of eigenvalues above (below) this energy. We say that a real sequence $\{u_n\}_{n=-1}^\infty$ *crosses zero* at $n \geq 0$ if $u_m u_{n-1} < 0$, with $m \geq n$ smallest such that $u_m \neq 0$. For non-zero eigenfunctions, this is the same as saying that u crosses zero at n if $u_n u_{n-1} < 0$ or $u_n = 0$, because in the latter case $u_n = 0$ implies $u_{n+1} u_{n-1} < 0$.

Theorem 2.2. *Let J be a BW matrix.*

(i) *If $x \geq 2$, then the number of eigenvalues of J strictly above x equals the number of times the Dirichlet eigenfunction for x crosses zero on the interval* $[1, \infty)$.

(ii) *If u, v are non-zero eigenfunctions for energies $x > y$, respectively, and u crosses* *zero at both* $n < m$*, then* v *crosses zero at least at one of* $n, n+1, \dots, m$*.*

(iii) *If* $x \leq -2$*, then the number of eigenvalues of* J *strictly below* x *equals the number of times the Dirichlet eigenfunction for* x *fails to cross zero on the interval* $[1, \infty)$*.*

(iv) *If* u, v *are non-zero eigenfunctions for energies* $x < y$*, respectively, and* u *fails to cross zero at both* $n < m$*, then* v *fails to cross zero at least at one of* $n, n+1, \dots, m$*.*

Remarks. 1. So, for example, (i) shows that the Dirichlet eigenfunction for $x \geq E_1^+$ stays positive.

2.(iii) and (iv) follow from (i) and (ii) by the above symmetry argument.

The second result is a Lieb-Thirring inequality for Jacobi matrices [12], bounding the distance of eigenvalues from the essential spectrum in terms of a certain $\mathfrak{I}_p$ norm of the difference $J - J_0$.

Theorem 2.3. *For any* $p \geq \frac{1}{2}$ *there exists* $c_p < \infty$ *such that for any* J

$$\sum_j \left(|E_j^+ - 2|^p + |E_j^- + 2|^p \right) \leq c_p \sum_n \left(|a_n - 1|^{p+1/2} + |b_n|^{p+1/2} \right).$$

Remarks. 1. By Lemma 2.1, the right-hand side is comparable to $\|J - J_0\|_{p+1/2}^{p+1/2}$.

2. We will mainly use this result for $p = \frac{1}{2}$ and $J - J_0 \in \mathfrak{I}_1$, that is, trace class.

2.3 Convergence of Jacobi Matrices

Most of the techniques we develop here will, in one way or another, involve successive approximation of a Jacobi matrix of interest by other Jacobi matrices. We will therefore need various results on limits of matrices. We collect these in this section.

The first is a well-known theorem relating convergence of the matrix elements and of the spectral measure.

Theorem 2.4. *Assume that* J_m*,* $m = 1, 2, \dots,$ *and* J *are uniformly bounded Jacobi matrices with spectral measures* ν_m *and* ν*, respectively, and matrix elements* $a_n^{(m)}, b_n^{(m)}$

and a_n, b_n, respectively. Then $\nu_m \rightharpoonup \nu$ (weak convergence) if and only if for all n

$$\lim_{m\to\infty} a_n^{(m)} = a_n, \qquad \lim_{m\to\infty} b_n^{(m)} = b_n. \tag{2.16}$$

Proof. Let M be the uniform bound on $\|J\|$ and $\|J_m\|$. This means that all spectral measures are supported on $[-M, M]$. Let us first assume that $\nu_m \rightharpoonup \nu$. We will show by induction that for all n

$$\lim_{m\to\infty} |a_n^{(m)} - a_n| = 0, \qquad \lim_{m\to\infty} \left(\sup_{|x|\le M} |P_n^{(m)}(x) - P_n(x)| \right) = 0. \tag{2.17}$$

Clearly $|a_0^{(m)} - a_0| = 0$ and $|P_0^{(m)}(x) - P_0(x)| = 0$. The induction step for a_n follows from (2.8), the assumption $\nu_m \rightharpoonup \nu$, $\nu_m(\mathbb{R}) = \nu(\mathbb{R}) = 1$, and from the induction hypothesis. The induction step for P_n then follows from the same facts, (2.7), and from the convergence for a_n which has just been established. This proves (2.17). Eq. (2.6) then proves the convergence for b_n.

Now we assume that (2.16) holds for all n. Notice that

$$\int x^j d\nu(x) = \langle \delta_0, J^j \delta_0 \rangle = (J^j)_{1,1}$$

and $(J_m^j)_{1,1} \to (J^j)_{1,1}$ for each j by the hypothesis. Hence, $\int Q(x) d\nu_m(x) \to \int Q(x) d\nu(x)$ for every polynomial Q. Using the uniform approximation of continuous functions by polynomials on $[-M, M]$ and an $\frac{\varepsilon}{3}$ argument, we obtain

$$\int \varphi(x) d\nu_m(x) \to \int \varphi(x) d\nu(x)$$

for any $\varphi \in C(\mathbb{R})$. Therefore $\nu_m \rightharpoonup \nu$. $\square$

From now on we shall say that J_m *converge* to J (denoted $J_m \to J$) whenever (2.16) holds, or equivalently, whenever $\nu_m \rightharpoonup \nu$.

In much of what follows, we will consider two natural approximating sequences connected to a matrix J. We let

$$J_n \equiv \begin{pmatrix} b_1 & a_1 & & & & & & \\ a_1 & b_2 & \dots & & & & & \\ & \dots & \dots & \dots & & & & \\ & & \dots & b_{n-1} & a_{n-1} & & & \\ & & & a_{n-1} & b_n & 1 & & \\ & & & & 1 & 0 & 1 & \\ & & & & & 1 & 0 & \dots \\ & & & & & & \dots & \dots \end{pmatrix} \tag{2.18}$$

be the matrix obtained from J by changing b_m to 0 and a_{m-1} to 1 for $m > n$. Clearly $J_n - J_0$ has rank at most n and so has only finitely many bound states. Notice that $J_n \to J$ in the above sense. This sequence will play an important role in proving one inequality in the sum rules in Chapter 3.

It will be useful to define $J_{n;F}$ to be the upper left-hand $n \times n$ corner of J (or J_n). For J_0 we will denote this matrix $J_{0,n;F}$. We have the following result.

Lemma 2.5.

$$\det(z - J_{n;F}) = a_1 \dots a_n P_n(z). \tag{2.19}$$

Proof. It is easy to check that (2.19) holds for $n = 0, 1$ (with the determinant of the 0×0 matrix being 1). Then by expanding in the last row, we obtain

$$\det(z - J_{n+1;F}) = (z - b_{n+1}) \det(z - J_{n;F}) - a_n^2 \det(z - J_{n-1;F})$$

which, by (2.5), also holds for $a_1 \dots a_n P_n(z)$ in place of $\det(z - J_{n;F})$. This finishes the proof. $\square$

The second sequence is formed by the matrices

$$J^{(n)} \equiv \begin{pmatrix} b_{n+1} & a_{n+1} & 0 & \dots \\ a_{n+1} & b_{n+2} & a_{n+2} & \dots \\ 0 & a_{n+2} & b_{n+3} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \tag{2.20}$$

obtained from J be deleting the first n rows and columns. Note that $J^{(n)} \to J_0$ whenever $J - J_0$ is compact. This property will prove useful for obtaining the opposite inequality in the sum rules in Chapter 3.

We have the following application of Sturm oscillation theory.

Corollary 2.6. *If $\varepsilon \geq 0$ and J has only finitely many eigenvalues above $2+\varepsilon$/below $-2-\varepsilon$, then there is n such that $J^{(n)}$ has no such eigenvalues.*

Proof. If there are only finitely many eigenvalues above $2+\varepsilon$, we only need to choose n to be larger than the last crossing of zero of some eigenfunction for energy $2+\varepsilon$. By Theorem 2.2(ii), the Dirichlet eigenfunction for $J^{(n)}$ and energy $2+\varepsilon$, which crosses zero at -1, cannot cross zero at $m \geq 0$. Theorem 2.2(i) then gives the result. The case $-2-\varepsilon$ is similar. □

Next, we prove two results on the convergence of sums of eigenvalues. These involve the matrices J_n and $J^{(n)}$ which we have just introduced. In the following we assume that f is a continuous function on $\mathbb{R}$ such that f is even, $f(x) = 0$ for $|x| \leq 2$, and f is monotone increasing on $[2, \infty)$. We have the following result from [13].

Lemma 2.7. *For any J and all n,*

(i) $|E_1^{\pm}(J_n)| \leq |E_1^{\pm}(J)| + 1$,

(ii) $|E_{j+1}^{\pm}(J_n)| \leq |E_j^{\pm}(J)|$.

In particular, for any f as above,

$$\sum_{j=1}^{\infty} f(E_j^{\pm}(J_n)) \leq f(E_1^{\pm}(J) \pm 1) + \sum_{j=1}^{\infty} f(E_j^{\pm}(J)). \tag{2.21}$$

Moreover, if $J - J_0$ is compact, then

$$\lim_{n\to\infty} \sum_{j=1}^{\infty} f(E_j^{\pm}(J_n)) = \sum_{j=1}^{\infty} f(E_j^{\pm}(J)). \tag{2.22}$$

Remarks. 1. Each of (i), (ii), (2.21), and (2.22) is intended as two statements — one with all plus signs and one with all minus signs.

2. Recall that $E_j^{\pm} \equiv \pm 2$ if there are less than j positive/negative bound states.

3. The sums for J are allowed to be infinity. Since J_n has only finitely many bound states, the corresponding sums are finite.

Proof. By the symmetry discussed in Section 2.2, we only need to consider E_j^+. We follow the proof in [13]. We start by proving (i),(ii) in 4 steps.

First, we compare J and $J_{n;F}$. Since the latter is a restriction of the former to $\ell^2(\{0, 1, \dots, n-1\})$, the min-max principle [26] shows that

$$E_j^+(J_{n;F}) \leq E_j^+(J).$$

Second, we let $J_{n;F}^+$ be the matrix obtained from $J_{n;F}$ by adding 1 to its bottom right-hand corner (changing it to $b_n + 1$). Obviously

$$E_1^+(J_{n;F}^+) \leq E_1^+(J_{n;F}) + 1 \leq E_1^+(J) + 1 \tag{2.23}$$

and since the change is a rank 1 perturbation, we also have (again by the min-max principle)

$$E_{j+1}^+(J_{n;F}^+) \leq E_j^+(J_{n;F}) \leq E_j^+(J). \tag{2.24}$$

Next, we let J_0^+ be J_0 with its upper left-hand corner changed to 1 (instead of 0).

We let $J_n^+ = J_{n;F}^+ \oplus J_0^+$, that is,

$$(J_n^+)_{k,l} = \begin{cases} (J_{n;F}^+)_{k,l} & 0 \le k,l < n, \\ (J_0^+)_{k-n,l-n} & k,l \ge n, \\ 0 & \text{otherwise.} \end{cases}$$

Here we denote by $A_{k,l}$ the (k,l) element of the matrix A, with the upper left-hand corner being $A_{0,0}$. Since J_0^+ has no eigenvalues by Theorem 2.2 (the Dirichlet eigenfunction for energy 2 is $u_n \equiv 1$), inequalities (2.23) and (2.24) hold with J_n^+ in place of $J_{n;F}^+$.

Finally, J_n is obtained from J_n^+ by adding the matrix

$$dJ^+ \equiv \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}$$

at sites $n, n+1$. Since $\langle \varphi, dJ^+ \varphi \rangle \le 0$ for any $\varphi \in \mathbb{R}^2$, this change decreases all eigenvalues. This proves (i),(ii), and (2.21) follows immediately.

To prove (2.22) we note that if $J - J_0$ is compact, then $\|J_n - J\| \to 0$. Hence also

$$\|E_j^+(J_n) - E_j^+(J)\| \to 0. \tag{2.25}$$

Thus if $\sum_{j=1}^\infty f(E_j^+(J)) < \infty$, then (ii) and the dominated convergence theorem imply (2.22). If $\sum_{j=1}^\infty f(E_j^+(J)) = \infty$, then Fatou's lemma gives

$$\liminf_{n\to\infty} \sum_{j=1}^\infty f(E_j^\pm(J_n)) \ge \sum_{j=1}^\infty f(E_j^\pm(J)) = \infty$$

and (2.22) holds again. □

We finish this section with proving a related result for $J^{(n)}$.

Lemma 2.8. *For any BW matrix J and all n we have*

$$|E^{\pm}_{j+n}(J)| \leq |E^{\pm}_j(J^{(n)})| \leq |E^{\pm}_j(J)|. \tag{2.26}$$

If f is as in Lemma 2.7, then

$$\lim_{n\to\infty} \sum_{j=1}^{\infty} \Big[f(E^{\pm}_j(J)) - f(E^{\pm}_j(J^{(n)})) \Big] = \sum_{j=1}^{\infty} f(E^{\pm}_j(J)). \tag{2.27}$$

Remarks. 1. Again, each of (2.26) and (2.27) represents two statements.

2. By (2.26), the sum on the left-hand side of (2.27) has non-negative summands and is finite for every n.

3. In (2.27) both sides can be infinity.

Proof. Again consider only E^+_j. Since $J^{(n)}$ is a restriction of J to $\ell^2(\{n, n+1, \dots\})$, (2.26) holds by the min-max principle.

Call the sum on the left of (2.27) $\delta^{\pm}_n(f, J)$. Since $E^+_j(J^{(n)}) \leq E^+_j(J)$, we have for any m,

$$\delta^+_n(f, J) \geq \sum_{j=1}^{m} \big[f(E^+_j(J)) - f(E^+_j(J^{(n)})) \big].$$

From Corollary 2.6 we know that for each j

$$\lim_{n\to\infty} E^+_j(J^{(n)}) = 2.$$

Hence we have by taking $n \to \infty$ and then $m \to \infty$,

$$\liminf_{n\to\infty} \delta^+_n(f, J) \geq \sum_{j=1}^{\infty} f(E^+_j(J)).$$

On the other hand, since $f \geq 0$,

$$\limsup_{n\to\infty} \delta^+_n(f, J) \leq \sum_{j=1}^{\infty} f(E^+_j(J))$$

is obvious. This proves (2.27). □

2.4 The Szegő Integral and Its Siblings — a Semi-Continuous Family

This section follows the exposition in [13]. One of the main objects of study in this thesis is the *Szegő integral*

$$Z(J) \equiv \frac{1}{2\pi} \int_{-2}^{2} \ln\biggl(\frac{\sqrt{4-x^2}}{2\pi\nu'(x)}\biggr) \frac{dx}{\sqrt{4-x^2}}, \tag{2.28}$$

where $\nu'(x)\,dx \equiv d\nu_{\rm ac}(x)$ is the absolutely continuous part of ν. With the change of variables $x = 2\cos\theta$, this integral can be written as

$$Z(J) = \frac{1}{2\pi} \int_{0}^{\pi} \ln\biggl(\frac{\sin\theta}{\pi\nu'(2\cos\theta)}\biggr) d\theta. \tag{2.29}$$

Before we proceed, let us introduce two classes of related integrals. For $\ell \geq 1$ we define

$$Y_\ell(J) \equiv -\frac{1}{\pi} \int_{0}^{\pi} \ln\biggl(\frac{\sin\theta}{\pi\nu'(2\cos\theta)}\biggr) \cos(\ell\theta)\,d\theta \tag{2.30}$$

$$= -\frac{1}{\pi} \int_{-2}^{2} \ln\biggl(\frac{\sqrt{4-x^2}}{2\pi\nu'(x)}\biggr) T_\ell\Bigl(\frac{x}{2}\Bigr) \frac{dx}{\sqrt{4-x^2}} \tag{2.31}$$

and

$$Z_\ell^\pm(J) \equiv \frac{1}{2\pi} \int_{0}^{\pi} \ln\biggl(\frac{\sin\theta}{\pi\nu'(2\cos\theta)}\biggr) (1 \pm \cos(\ell\theta))\,d\theta \tag{2.32}$$

$$= \frac{1}{2\pi} \int_{-2}^{2} \ln\biggl(\frac{\sqrt{4-x^2}}{2\pi\nu'(x)}\biggr) \Bigl(1 \pm T_\ell\Bigl(\frac{x}{2}\Bigr)\Bigr) \frac{dx}{\sqrt{4-x^2}} \tag{2.33}$$

with T_ℓ from (2.10). Of course,

$$Z_\ell^\pm(J) = Z(J) \mp \tfrac{1}{2} Y_\ell(J) \tag{2.34}$$

when all integrals converge.

Many authors consider the integral

$$\frac{1}{2\pi}\int_0^{\pi} \ln\bigl[\nu'(2\cos\theta)\bigr]\,d\theta \tag{2.35}$$

instead of $Z(J)$. By (2.29), this differs from $Z(J)$ by a sign and a constant. Our choice of $Z(J)$ has two reasons. The form (2.28) appears in the sum rules which play a major role in this work, and from (2.14)

$$Z(J_0) = Z_\ell^{\pm}(J_0) = Y_\ell(J_0) = 0.$$

We add that each of $Z_\ell^{\pm}$, Y_ℓ will have its own sum rule, as Z has (1.7) (see Chapter 3).

The first question to be answered at this point is the convergence of the above integrals. Let $\ln_\pm$ be defined by

$$\ln_\pm(y) = \max\{0, \pm\ln(y)\},$$

so that

$$\ln(y) = \ln_+(y) - \ln_-(y),$$
$$|\ln(y)| = \ln_+(y) + \ln_-(y).$$

Lemma 2.9. *The* $\ln_-$ *piece of* (2.28), (2.30), *and* (2.32) *always converges.*

Proof. Since $1 \pm \cos(\ell\theta) \le 2$, we only need to treat (2.28):

$$\begin{aligned}\int_{-2}^{2} \ln_-\left(\frac{\sqrt{4-x^2}}{2\pi\nu'(x)}\right)\frac{dx}{\sqrt{4-x^2}} &\le \int_{-2}^{2} \ln_-\left(\frac{1}{2\pi\nu'(x)\sqrt{4-x^2}}\right) + \ln_-\left(4-x^2\right)\frac{dx}{\sqrt{4-x^2}}\\ &\le \int_{-2}^{2} 2\pi\nu'(x)\,dx + \int_{-2}^{2} \ln_-\left(4-x^2\right)\frac{dx}{\sqrt{4-x^2}} < \infty\end{aligned}$$

using $\ln_-(xy) \le \ln_-(x) + \ln_-(y)$ and $\ln_-(x) \le x^{-1}$. □

It follows that the integrals defining $Z(J)$ and $Z_\ell^{\pm}(J)$ either converge or diverge to

$+\infty$. We therefore always define $Z(J)$ and $Z_\ell^\pm(J)$, although they may take the value $+\infty$. Since the weight in $Y_\ell(J)$ does not have a definite sign, $Y_\ell(J)$ cannot always be defined. However, $Z(J) < \infty$ clearly implies the convergence of both $Z_\ell^\pm(J)$ and $Y_\ell(J)$, so we define $Y_\ell(J)$ by (2.34) if and only if $Z(J) < \infty$.

Note that the proof of Lemma 2.9 actually gives a lower bound on $Z(J)$ and $Z_\ell^\pm(J)$, since $\int \nu'(x)dx \leq 1$. We will improve this bound for $Z(J)$ and $Z_2^-(J)$ in Lemma 2.12. These two integrals are of special interest among the Z family, as will be seen in Chapter 3. The weights in them, in terms of θ, are 1 and $2\sin^2(\theta)$ and so represent the two types of decay at ± 2 which are exhibited by the weights $1 \pm \cos(\ell\theta)$.

It is clear from their definitions that $Z(J)$ and $Z_\ell^\pm(J)$ can be $+\infty$ when $\nu'(x)$ is small on a large enough set. For example, if it decays fast enough at ± 2 (which will be the case in one part of Askey's conjecture as we shall see in Chapter 3) or if it vanishes on a set of positive Lebesgue measure. Conversely, $Z(J) < \infty$ implies that the essential support of ν_{ac} is $[-2, 2]$.

If $Z(J) < \infty$, we say that J obeys the *Szegő condition* or J is *Szegő*. This condition is a natural object in the theory of orthogonal polynomials (see, e.g., [36]). If $Z_1^\pm(J) < \infty$, we say J is *Szegő at* ± 2. This is because if $Z_1^+(J) < \infty$, then the integral in (2.28) can only diverge at $x = -2$ and if $Z_1^-(J) < \infty$, the integral can only diverge at $x = 2$, as can be seen from changing variables to θ. Note that if $Z_1^-(J) < \infty$, then $Z_2^-(J) < \infty$ because

$$1 - \cos(2\theta) = 2\sin^2(\theta) \leq 8\sin^2\left(\tfrac{\theta}{2}\right) = 4(1 - \cos\theta).$$

Similarly $Z_1^+(J) < \infty$ implies $Z_2^-(J) < \infty$. As in [13], we will call $Z_2^-(J) < \infty$ the *quasi-Szegő condition*.

In the remaining part of this section we will prove a result of Killip-Simon [13], who realized that integrals like $Z(J)$ are just negative entropies. Entropies are upper semi-continuous w.r.t. weak convergence of spectral measures, which translates, via Theorem 2.4, into lower semi-continuity of $Z(J)$ w.r.t. pointwise convergence of matrix elements. That is,

$$Z(J) \leq \liminf_{n\to\infty} Z(J(n)) \tag{2.36}$$

whenever $J(n) \to J$ (and similarly for $Z_\ell^\pm(J)$). This will be proved by obtaining variational principles for $Z(J)$ and similar integrals, as suprema of (weakly) continuous functions. Inequality (2.36) is the cornerstone of the passage from step-by-step sum rules to "full size" sum rules (see Chapter 3), and plays an important role in the proofs of the main results of Chapter 4.

Following [13], if μ, ν are two finite measures, we define the *entropy* of μ relative to ν to be

$$S(\mu|\nu) \equiv \begin{cases} -\int \ln\left(\frac{d\mu}{d\nu}\right) d\mu & \text{if } \mu \text{ is } \nu\text{-a.c.,} \\ -\infty & \text{otherwise.} \end{cases} \tag{2.37}$$

Notice that if $d\mu = f\, d\nu$, then

$$S(\mu|\nu) = -\int \ln(f(x)) f(x)\, d\nu(x), \tag{2.38}$$

the usual definition of entropy. In that case

$$\int \ln_-\left(\frac{d\mu}{d\nu}\right) d\mu \leq \int f^{-1}(x)\, d\mu(x) = \nu(\{x|f(x) \neq 0\}) \leq \nu(\mathbb{R}) < \infty, \tag{2.39}$$

so that the integral in (2.37) can only diverge to $-\infty$.

Lemma 2.10.

$$S(\mu|\nu) \leq \mu(\mathbb{R}) \ln\left(\frac{\nu(\mathbb{R})}{\mu(\mathbb{R})}\right) \tag{2.40}$$

with equality if and only if μ is a multiple of ν.

Proof. If μ is not ν-a.c., then there is nothing to prove, so assume $d\mu = f\, d\nu$. Then by the concavity of ln and Jensen's inequality for the probability measure $d\mu/\mu(\mathbb{R})$,

$$\begin{aligned} S(\mu|\nu) &= \mu(\mathbb{R}) \int \ln\left(f^{-1}(x)\right) \frac{d\mu(x)}{\mu(\mathbb{R})} \\ &\leq \mu(\mathbb{R}) \ln\left(\int f^{-1}(x) \frac{d\mu(x)}{\mu(\mathbb{R})}\right) \end{aligned}$$

$$= \mu(\mathbb{R}) \ln \left(\frac{\nu(\{x | f(x) \neq 0\})}{\mu(\mathbb{R})} \right)$$
$$\leq \mu(\mathbb{R}) \ln \left(\frac{\nu(\mathbb{R})}{\mu(\mathbb{R})} \right).$$

Since ln is strictly convex, equality in the first inequality holds only if $f^{-1}(x)$ is a constant where $f(x) \neq 0$, and in the second inequality only if $f(x) \neq 0$ everywhere on the essential support of ν. This proves the claim. □

Theorem 2.11.

$$S(\mu|\nu) = \inf_F \left[\int F(x)\, d\nu(x) - \int \big(1 + \ln F(x)\big)\, d\mu(x) \right] \tag{2.41}$$

where the infimum is taken over all real-valued bounded continuous functions F with $\inf_{x \in \mathbb{R}} F(x) > 0$. *So if $\mu_n \rightharpoonup \mu$ and $\nu_n \rightharpoonup \nu$ and the supports of μ_n, μ, ν_n, ν are uniformly bounded, then*

$$S(\mu|\nu) \geq \limsup_{n \to \infty} S(\mu_n|\nu_n).$$

Proof. Let us define

$$\mathfrak{S}(F) \equiv \mathfrak{S}(F; \mu, \nu) \equiv \int F(x)\, d\nu(x) - \int \big(1 + \ln F(x)\big)\, d\mu(x)$$

for $F > 0$ with $F \in L^1(d\nu)$ and $\ln F \in L^1(d\mu)$. For any fixed continuous F this function is weakly jointly continuous in μ and ν on the set of measures with uniformly bounded supports. Since the infimum of continuous functions is upper semicontinuous, the second claim of the theorem follows from the first. We are left with proving (2.41).

First consider μ to be ν-a.c., so assume that $d\mu = f\, d\nu$. Then

$$\ln \frac{F(x)}{f(x)} \leq \frac{F(x)}{f(x)} - 1$$

whenever $f(x) > 0$, which is equivalent to

$$-f(x) \ln f(x) \leq F(x) - f(x)(1 + \ln F(x)).$$

Integrating w.r.t. $d\nu$ gives $S(\mu|\nu) \le \mathfrak{S}(F)$, and so $S(\mu|\nu) \le \inf_F \mathfrak{S}(F)$.

To obtain equality, one could take $F \equiv f$. But f might not be continuous nor bounded away from $0, \infty$, so we will have to approximate it instead. First take

$$f_N(x) \equiv \begin{cases} N & f(x) > N, \\ f(x) & \frac{1}{N} \le f(x) \le N, \\ \frac{1}{N} & f(x) \le \frac{1}{N}, \end{cases}$$

and pick continuous $F_{N;n}$ such that $\frac{1}{N} \le F_{N;n} \le N$ and $F_{N;n} \to f_N$ in $L^1(d\mu + d\nu)$. We have

$$\begin{aligned} \Big|\mathfrak{S}(F_{N;n}) - \mathfrak{S}(f_N)\Big| &= \left| \int (F_{N;n} - f_N)\, d\nu - \int (\ln F_{N;n} - \ln f_N)\, d\mu \right| \\ &\le \int |F_{N;n} - f_N|\, d\nu + \int |F_{N;n} - f_N| N\, d\mu(x) \end{aligned}$$

and so $\lim_{n\to\infty} \mathfrak{S}(F_{N;n}) = \mathfrak{S}(f_N)$. Moreover,

$$\mathfrak{S}(f_N) = \int (f_N - f)\, d\nu - \int \ln_+ f_N\, d\mu + \int \ln_- f_N\, d\mu.$$

Clearly $f_N \to f$ in $L^1(d\nu)$, so the first integral converges to 0 as $n \to \infty$. By monotone convergence theorem (and using (2.37) and (2.39)), the rest converges to

$$-\int \ln_+ f\, d\mu + \int \ln_- f\, d\mu = S(\mu|\nu).$$

Hence $\inf_F \mathfrak{S}(F) \le \inf_{N,n} \mathfrak{S}(F_{N;n}) = S(\mu|\nu)$, as was to prove.

Now assume μ is not ν-a.c. Then there is a set $A \subset \mathbb{R}$ such that $\mu(A) > 0$ and $\nu(A) = 0$. Let $f_N(x) \equiv 1 + N\chi_A(x)$, and let $F_{N;n}$ be continuous and such that $1 \le F_{N;n} \le N+1$ and $F_{N;n} \to f_N$ in $L^1(d\mu + d\nu)$. Then as above, $\lim_{n\to\infty} \mathfrak{S}(F_{N;n}) = \mathfrak{S}(f_N)$. But

$$\mathfrak{S}(f_N) = \nu(\mathbb{R}) - \mu(\mathbb{R}) - \mu(A)\ln(N+1),$$

that is, $\mathfrak{S}(f_N) \to -\infty$. Hence $\inf_{N,n} \mathfrak{S}(F_{N;n}) = -\infty = S(\mu|\nu)$. $\square$

This result can now be applied to Szegő-type integrals via the following lemma.

Lemma 2.12. *Let ν be the spectral measure of J and let*

$$d\mu_0(x) \equiv \frac{dx}{\pi\sqrt{4-x^2}}, \tag{2.42}$$

$$d\mu_\ell^\pm(x) \equiv \frac{1 \pm T_\ell\big(\frac{x}{2}\big)}{\pi\sqrt{4-x^2}}\, dx \tag{2.43}$$

for $\ell \geq 1$. Then there are $\kappa_0, \kappa_\ell^\pm \in \mathbb{R}$ such that

$$Z(J) = \kappa_0 - \tfrac{1}{2}S(\mu_0|\nu), \tag{2.44}$$

$$Z_\ell^\pm(J) = \kappa_\ell^\pm - \tfrac{1}{2}S(\mu_\ell^\pm|\nu). \tag{2.45}$$

Moreover, $\kappa_0 = -\frac{1}{2}\ln(2)$ and $\kappa_2^- = 0$.

Remark. Here μ_0 and $\mu_\ell^\pm$ are probability measures, as can be seen using the change of variables $x = 2\cos\theta$. Hence $Z(J) \geq \kappa_0$ and $Z_\ell^\pm(J) \geq \kappa_\ell^\pm$ by Lemma 2.10.

Proof. Notice that since μ_0, $\mu_\ell^\pm$ are absolutely continuous, $S(\mu_0|\nu) = S(\mu_0|\nu_{\rm ac})$ and $S(\mu_\ell^\pm|\nu) = S(\mu_\ell^\pm|\nu_{\rm ac})$. If μ_0, $\mu_\ell^\pm$ are not ν-a.c., that is, $\nu'(x) = 0$ on a subset of $[-2,2]$ of positive measure, then all the $-S$'s and Z's are $+\infty$. So assume the μ's are ν-a.c. Then (2.44)/(2.45) follow directly from (2.28)/(2.33) and from (2.37), if we take

$$\kappa_0 \equiv \frac{1}{2\pi}\int_{-2}^{2} \ln\left(\frac{4-x^2}{2}\right)\frac{dx}{\sqrt{4-x^2}},$$

$$\kappa_\ell^\pm \equiv \frac{1}{2\pi}\int_{-2}^{2} \ln\left(\frac{4-x^2}{2\big(1 \pm T_\ell\big(\frac{x}{2}\big)\big)}\right)\frac{1 \pm T_\ell\big(\frac{x}{2}\big)}{\sqrt{4-x^2}}\, dx.$$

Since $T_2(y) = 2y^2 - 1$, we have $\kappa_2^- = 0$. To compute κ_0 we apply once again the change of variables $x = 2\cos\theta$:

$$\begin{aligned}\kappa_0 &= \frac{1}{2\pi}\int_0^\pi \ln(2\sin^2\theta)\, d\theta \\ &= \frac{1}{2}\ln(2) + \frac{1}{2\pi}\int_0^{2\pi} \ln|\sin\theta|\, d\theta\end{aligned}$$

$$= \frac{1}{2}\ln(2) + \frac{1}{2\pi}\int_0^{2\pi} \ln\left|\frac{1-e^{2i\theta}}{2}\right| d\theta$$
$$= \frac{1}{2}\ln(2) + \ln\left(\frac{1}{2}\right) = -\frac{1}{2}\ln(2),$$

where we used Jensen's formula for $f(z) = \frac{1}{2}(1-z^2)$ to evaluate the integral. □

Hence Z and $Z_\ell^\pm$ are lower semi-continuous in J. We gather the results obtained in this section in

Theorem 2.13. *The negative parts of the integrals defining $Z(J)$ and $Z_\ell^\pm(J)$ are bounded by*

$$\kappa \equiv 2 + \frac{1}{\pi}\int_{-2}^{2} \ln_-\left(4-x^2\right)\frac{dx}{\sqrt{4-x^2}}.$$

Moreover,

$$Z(J) \geq -\tfrac{1}{2}\ln(2) \tag{2.46}$$

and

$$Z_2^-(J) \geq 0. \tag{2.47}$$

If $J(n) \to J$ (in terms of pointwise convergence of matrix elements), then

$$Z(J) \leq \liminf_{n\to\infty} Z(J(n)) \tag{2.48}$$

and

$$Z_\ell^\pm(J) \leq \liminf_{n\to\infty} Z_\ell^\pm(J(n)). \tag{2.49}$$

We note that the bounds (2.46) and (2.47) are sharp, as can be seen from Lemma 2.10 by taking $\nu = \mu_0$ and $\nu = \mu_2^- = \frac{1}{2\pi}\sqrt{4-x^2}\,dx$, respectively.

2.5 m and M

One of the central objects of spectral theory of Jacobi matrices is the m*-function.* This is the *Borel transform* of the spectral measure ν of J, defined by

$$m(\zeta) \equiv \int \frac{d\nu(x)}{x-\zeta} = \langle \delta_0, (J-\zeta)^{-1}\delta_0 \rangle \tag{2.50}$$

for $\zeta \in \mathbb{C}\backslash\mathbb{R}$. We write $m(\zeta; J)$ when we want to make the J-dependence explicit. In the case under consideration, that is, when ν is supported on $[-2, 2]$ plus the set of points $\{E_j^\pm\}$, we can write

$$m(\zeta) = \sum_{\pm}\sum_{j} \frac{\nu(\{E_j^\pm\})}{E_j^\pm - \zeta} + \int_{-2}^{2} \frac{d\nu(x)}{x-\zeta}. \tag{2.51}$$

Clearly, m is meromorphic in $\mathbb{C}\backslash[-2, 2]$ and analytic off the support of ν.

One usually looks at $m(\zeta)$ for $\zeta \in \mathbb{C}^+$, the (open) upper half-plane, since $m(\bar{\zeta}) = \overline{m(\zeta)}$. Clearly $\operatorname{Im} m(\zeta) > 0$ in $\mathbb{C}^+$. More precisely, for $E \in \mathbb{R}$ and $\varepsilon > 0$,

$$\operatorname{Im} m(E + i\varepsilon) = \int \frac{\varepsilon}{(x-E)^2 + \varepsilon^2}\, d\nu(x). \tag{2.52}$$

Using this and

$$\int \frac{\varepsilon}{(x-E)^2 + \varepsilon^2}\, dx = \pi,$$

one can show that $\operatorname{Im} m(E + i\varepsilon)\, dE$ recovers $d\nu(E)$ as $\varepsilon \downarrow 0$, as can be seen in the following standard result (see, e.g., [30]).

Theorem 2.14. *Let m be the Borel transform of the measure ν. Then*

$$\lim_{\varepsilon\downarrow 0} \operatorname{Im} m(E + i\varepsilon)\, dE = \pi d\nu(E) \tag{2.53}$$

in the sense of weak convergence of measures. Pointwise,

$$\lim_{\varepsilon\downarrow 0} \operatorname{Im} m(E + i\varepsilon) = \pi\nu'(E) \tag{2.54}$$

for almost all E (w.r.t. the Lebesgue measure), and the singular part of ν is supported on the set of those E for which

$$\lim_{\varepsilon\downarrow 0} \operatorname{Im} m(E+i\varepsilon) = \infty. \tag{2.55}$$

Remark. Actually, (2.54) and (2.55) hold with non-tangential limits from $\mathbb{C}^+$.

In light of Theorem 2.14, the following lemma relates the spectral measure and the behavior of ℓ^2-eigenfunctions at the origin (cf. Theorem 4.25).

Lemma 2.15. *If $u(\zeta)$ is an eigenfunction for J and energy $\zeta \in \mathbb{C}\backslash\mathbb{R}$ such that $u(\zeta) \in \ell^2(\mathbb{Z}^+)$, then*

$$m(\zeta) = -\frac{u_0(\zeta)}{u_{-1}(\zeta)}. \tag{2.56}$$

Proof. From (2.2) and the argument after it, we know that u must be a multiple of $\delta_{-1} - (J-\zeta)^{-1}\delta_0$. Then

$$-\frac{u_0(\zeta)}{u_{-1}(\zeta)} = \langle \delta_0, (J-\zeta)^{-1}\delta_0 \rangle,$$

which is $m(\zeta)$ by (2.50). □

This equality can be used to derive an important relation between the m-functions of J and $J^{(1)}$, which will play a crucial role in the proof of the step-by-step sum rules in Chapter 3:

Lemma 2.16.

$$m(\zeta; J)^{-1} = -\zeta + b_1 - a_1^2 m(\zeta; J^{(1)}). \tag{2.57}$$

Remark. One can iterate this to obtain a continued fraction expansion of m around ∞ (since $m(\infty) = 0$).

Proof. Let

$$u_n(\zeta) \equiv \big(\delta_{-1} - (J-\zeta)^{-1}\delta_0\big)_n$$

for $n \geq -1$ be the ℓ^2-eigenfunction for J and energy ζ. Then

$$v_n(\zeta) \equiv \begin{cases} u_{n+1}(\zeta) & n \geq 0, \\ a_1 u_0(\zeta) & n = -1 \end{cases}$$

is the ℓ^2-eigenfunction for $J^{(1)}$, as can be easily verified (notice that $a_n(J^{(1)}) = a_{n+1}(J)$ but $a_0(J^{(1)}) = 1$). Therefore

$$m(\zeta; J^{(1)}) = -\frac{u_1(\zeta)}{a_1 u_0(\zeta)} = -\frac{(\zeta - b_1)u_0(\zeta) - u_{-1}(\zeta)}{a_1^2 u_0(\zeta)} = \frac{-\zeta + b_1 - m(\zeta; J)^{-1}}{a_1^2}$$

by using (2.1) and (2.56). Eq. (2.57) is immediate. □

It will be useful to transfer everything into the unit disk $\mathbb{D} = \{z \mid |z| < 1\}$, using the fact that $z \mapsto \zeta = z + z^{-1}$ maps $\mathbb{D}$ bijectively onto the Riemann sphere cut along $[-2, 2]$. Under this mapping, the upper half-disk is mapped onto the lower half-plane and the lower half-disk onto the upper half-plane. Thus we define for $|z| < 1$

$$M(z) = -m(z + z^{-1}). \tag{2.58}$$

The minus sign is picked so that $\operatorname{Im} M(z) > 0$ if $\operatorname{Im} z > 0$. Hence M is meromorphic in $\mathbb{D}$ with poles at $(\beta_j^{\pm})^{-1}$ such that

$$E_j^{\pm} = \beta_j^{\pm} + (\beta_j^{\pm})^{-1} \tag{2.59}$$

and $|\beta_j^{\pm}| > 1$. Hence $\beta_j^{\pm} = \beta(E_j^{\pm})$ with

$$\beta(E) \equiv \frac{E + \operatorname{sgn}(E)\sqrt{E^2 - 4}}{2}$$

for $|E| \geq 2$. It is clear that the function $\beta(E)$ is well defined and increasing on $(-\infty, -2] \cup [2, \infty)$ with $\beta(\pm 2) = \pm 1$. One can easily see that $|\beta| - 1 \asymp \sqrt{|E| - 2}$ for $|E| \to 2$.

We would now like to write (2.51) (or rather its imaginary part) in terms of M.

By separating the pole terms (including those at ± 2, if they are present), we get

$$\operatorname{Im} M(z) = \operatorname{Im} \sum_{\pm} \frac{\alpha(\pm 1)}{z + z^{-1} - 2} + \operatorname{Im} \sum_{j,\pm} \frac{\alpha(\beta_j^\pm)}{z + z^{-1} - [\beta_j^\pm + (\beta_j^\pm)^{-1}]} + K(z), \tag{2.60}$$

where

$$K(z) \equiv \operatorname{Im} \int_{-2}^{2} \chi_{(-2,2)}(x) \frac{d\nu(x)}{z + z^{-1} - x}$$

and we use $\alpha(\beta_j^\pm)$ for the weights $\nu(\{E_j^\pm\})$ (and $\alpha(\pm 1)$ for $\nu(\{\pm 2\})$). Also, $\chi_{(-2,2)}$ ensures that possible mass points at ± 2 do not enter twice. We note that since $\alpha(\beta_j^\pm)$ are point masses of a probability measure, we have

$$\sum_{j,\pm} \alpha(\beta_j^\pm) \leq 1 \tag{2.61}$$

with the $\alpha(\pm 1)$ terms included in the sum as $\beta_\infty^\pm \equiv \pm 1$.

Note that $K(z)$ is a harmonic function in $\mathbb{D}$, so one should be able to rewrite it in terms of its boundary values using the *Poisson kernel*

$$P_r(\theta, \varphi) \equiv \frac{1 - r^2}{1 + r^2 - 2r\cos(\theta - \varphi)} \tag{2.62}$$

with $r < 1$ and $\theta, \varphi \in [0, 2\pi]$. Since the imaginary parts of the pole terms in (2.60) go pointwise to 0 as $r \uparrow 1$,

$$\lim_{r \uparrow 1} \left[K(re^{i\theta}) - \operatorname{Im} M(re^{i\theta}) \right] = 0$$

for any $\theta \in [0, 2\pi]$. Hence the boundary values of $K(z)$ coincide with those of $\operatorname{Im} M(z)$.

By the definition of M and by (2.54) for non-tangential limits, we have

$$\operatorname{Im} M(e^{i\theta}) = -\operatorname{Im} M(e^{-i\theta}) = \pi \nu'(2\cos\theta) \tag{2.63}$$

for a.e. $\theta \in [0, \pi]$, where

$$\operatorname{Im} M(e^{i\theta}) \equiv \lim_{r \uparrow 1} \operatorname{Im} M(re^{i\theta}) \tag{2.64}$$

exists almost everywhere. Note that by using this, one can substitute $\operatorname{Im} M(e^{i\theta})$ for $\pi\nu'(2\cos\theta)$ in (2.29), (2.30), and (2.32). In Chapter 3, the sum rules will be stated in these terms and proved using the properties of the limit in (2.64).

If $\tilde{\mu}$ is a finite measure on $[0, 2\pi]$ such that $\tilde{\mu}(\{0\}) = \tilde{\mu}(\{\pi\}) = \tilde{\mu}(\{2\pi\}) = 0$ and

$$\tilde{\mu}(I) = \pi\nu(2\cos I) \tag{2.65}$$

for any interval $I \subset (0, \pi) \cup (\pi, 2\pi)$, and we let

$$d\mu^{\#}(\theta) \equiv (2\sin\theta)^{-1}\, d\tilde{\mu}(\theta), \tag{2.66}$$

then by (2.63) and (2.65),

$$K(e^{i\theta}) = \operatorname{Im} M(e^{i\theta}) = (\mu^{\#})'(\theta) \tag{2.67}$$

for a.e. $\theta \in [0, 2\pi]$. Hence one should expect the Poisson integral formula

$$K(re^{i\theta}) = \int_0^{2\pi} P_r(\theta, \varphi)\, \frac{d\mu^{\#}(\varphi)}{2\pi} \tag{2.68}$$

to hold in some sense (see, e.g., [27]).

The problem with this identity is that the measure $\mu^{\#}$ inside the integral is signed and may be infinite, as can be seen from (2.66). One can remove the signature problem by using the symmetry of $\mu^{\#}$. If we let

$$D_r(\theta, \varphi) = P_r(\theta, \varphi) - P_r(\theta, -\varphi) \tag{2.69}$$

and define a (positive but possibly infinite) measure μ on $[0, \pi]$ by

$$d\mu(\theta) \equiv d\mu^{\#}(\theta) \restriction [0, \pi] = (2\sin\theta)^{-1}\, d\tilde{\mu}(\theta) \restriction [0, \pi], \tag{2.70}$$

then the integral in (2.68) becomes

$$\int_0^{2\pi} D_r(\theta,\varphi)\,\frac{d\mu(\varphi)}{2\pi}.$$

This is because by (2.66), $d\mu^{\#}(\theta) \restriction [\pi, 2\pi] = -d\mu(2\pi - \theta)$. Since $\varphi \in [0,\pi]$ implies $D_r(\theta,\varphi) \geq 0$ for $\theta \in [0,\pi]$ and $D_r(\theta,\varphi) \leq 0$ for $\theta \in [\pi, 2\pi]$, the integral is well defined (although, a priori, it may be infinite). It turns out that, as one expects from the above heuristic, this integral is finite and

$$\operatorname{Im} M(re^{i\theta}) = \operatorname{Im} \sum_{j,\pm} \frac{\alpha(\beta_j^{\pm})}{re^{i\theta} + r^{-1}e^{-i\theta} - [\beta_j^{\pm} + (\beta_j^{\pm})^{-1}]} + \int_0^{\pi} D_r(\theta,\varphi)\,\frac{d\mu(\varphi)}{2\pi} \tag{2.71}$$

for $r < 1$. By $M(\bar z) = \overline{M(z)}$ and $D_r(-\theta,\varphi) = -D_r(\theta,\varphi)$, we only need to consider $\theta \in [0,\pi]$:

Lemma 2.17. *If M and μ are defined by* (2.58) *and* (2.70)*, $r < 1$, and $\theta, \varphi \in [0,\pi]$, then $D_r(\theta,\varphi) \geq 0$, it is bounded and continuous in φ, and* (2.71) *holds.*

Proof. If $\theta, \varphi \in [0,\pi]$, then $D_r(\theta,\varphi) \geq 0$ and it is bounded in φ by (2.62). We use (2.62) and (2.69) to show

$$\begin{aligned} D_r(\theta,\varphi) &= \frac{(1-r^2)2r[\cos(\theta-\varphi) - \cos(\theta+\varphi)]}{[1+r^2-2r\cos(\theta-\varphi)]\,[1+r^2-2r\cos(\theta+\varphi)]} \\ &= P_r(\theta,\varphi)\frac{4r\sin\theta\sin\varphi}{1+r^2-2r\cos(\theta+\varphi)}. \end{aligned}$$

Notice that if $\theta, \varphi \in [0,\pi]$, then $2r\cos(\theta+\varphi) \leq 2r|\cos\theta|$. Since $r < 1$, we have

$$\sin^2(\theta) + 2|\cos\theta| = 1 - \cos^2(\theta) + 2|\cos\theta| \leq 2 \leq \frac{1+r^2}{r},$$

which implies

$$\frac{r\sin^2(\theta)}{1+r^2-2r|\cos\theta|} \leq 1.$$

Hence

$$0 \leq \frac{D_r(\theta,\varphi)}{\sin\varphi} \leq \frac{4P_r(\theta,\varphi)}{\sin\theta} \tag{2.72}$$

for $\theta, \varphi \in (0, \pi)$.

Since $\tilde{\mu}([0,\pi]) \leq \pi$ by (2.65), the integral in (2.71) can be estimated as

$$0 \leq \int_0^\pi \frac{D_r(\theta,\varphi)}{\sin\varphi} \frac{d\tilde{\mu}(\varphi)}{4\pi} \leq \frac{\|P_r\|_\infty}{\sin\theta}$$

and so it is finite (notice that if $\theta = 0, \pi$, then $D_r(\theta,\varphi) \equiv 0$).

To show (2.71), one can check directly that

$$D_r(\theta,\varphi) = \operatorname{Im} \frac{4\sin\varphi}{re^{i\theta} + r^{-1}e^{-i\theta} - 2\cos\varphi}.$$

Then by (2.65),

$$\begin{aligned} K(re^{i\theta}) &= \int_0^\pi \operatorname{Im} \frac{1}{re^{i\theta} + r^{-1}e^{-i\theta} - 2\cos\varphi} \frac{d\tilde{\mu}(\varphi)}{\pi} \\ &= \int_0^\pi D_r(\theta,\varphi) \frac{d\tilde{\mu}(\varphi)}{4\pi\sin\varphi} \\ &= \int_0^\pi D_r(\theta,\varphi) \frac{d\mu(\varphi)}{2\pi}, \end{aligned}$$

and so (2.71) is just (2.60). □

For later reference, notice that (2.67) shows

$$\operatorname{Im} M(e^{i\theta}) = \mu'(\theta) \tag{2.73}$$

for a.e. $\theta \in [0,\pi]$.

Finally, we note that (2.57) reads

$$-M(z;J)^{-1} = -(z+z^{-1}) + b_1 + a_1^2 M(z;J^{(1)}). \tag{2.74}$$

We have that $M(0;J) = m(\infty;J) = 0$ and similarly $M(0;J^{(1)}) = 0$. Hence if we let

$$f(z) \equiv \frac{M(z)}{z}, \tag{2.75}$$

then by (2.74), $f(0) = 1$. This will be used to prove the sum rule for Z. To prove sum rules for $Z_\ell^\pm$, we will need to compute the Taylor coefficients of $\ln f$. We will do this, using the method of [13], in the appendix to Chapter 3.

Chapter 3

Sum Rules for Jacobi Matrices

Most of the material contained in this chapter is a joint work with Barry Simon [33]. In Section 3.1 we prove a technical result on continuity of boundary values of the M-function introduced in Chapter 2. This is then applied in Section 3.2 to derive the step-by-step sum rules. Section 3.3 iterates these to obtain the "full size" sum rules, and proves Theorem 1.1 and related results. In Section 3.4 we prove Theorem 1.2 and in Section 3.5 Theorem 1.3, along with other results.

3.1 Continuity of Integrals of $\ln(\operatorname{Im} M)$

In this section, we will prove a general continuity result about boundary values for M-functions satisfying (2.71). We will consider suitable weight functions, $w(\varphi)$, on $[0, \pi]$, of which the examples of most interest are $w(\varphi) = \sin^k(\varphi)$, $k = 0$ or 2. Our goal is to prove that

$$\lim_{r \uparrow 1} \int \ln[\operatorname{Im} M(re^{i\varphi})]\, w(\varphi)\, d\varphi = \int \ln[\operatorname{Im} M(e^{i\varphi})]\, w(\varphi)\, d\varphi \tag{3.1}$$

and that the convergence is in L^1 if the integral on the right is finite. All integrals in this section are from 0 to π if not indicated otherwise. We define

$$d(\varphi) \equiv \min(\varphi, \pi - \varphi) \tag{3.2}$$

and we suppose that

$$0 \le w(\varphi) \le C_1\, d(\varphi)^{-1+\alpha} \tag{3.3}$$

for some $C_1, \alpha > 0$ and that w is C^1 with

$$|w'(\varphi)w(\varphi)^{-1}| \le C_2\, d(\varphi)^{-\beta} \tag{3.4}$$

for $C_2, \beta > 0$. For weights of interest, one can take $\alpha = \beta = 1$.

Remarks. 1. For the applications in mind, we are only interested in allowing "singularities" (i.e., w vanishing or going to infinity) at 0 or π, but all results hold with unchanged proofs if $d(\varphi) \equiv \min_j\{|\varphi - \varphi_j|\}$ for any finite set $\{\varphi_j\}$. For example, $w(\varphi) = \sin^2(m\varphi)$, as in [14], is fine.

2. By (3.3), $\int_0^\pi w(\varphi)\, d\varphi < \infty$.

3. Note that (3.1) does not contradict (2.53) because the logarithm kills the singular part of the measure under consideration, which affects $M(re^{i\varphi})$ but not $M(e^{i\varphi})$.

The main technical result we will need is

Theorem 3.1. *Let M be a function with a representation of the form* (2.71) *and let w be a weight obeying* (3.3) *and* (3.4)*. Then* (3.1) *holds. Moreover, if*

$$\int \ln[\operatorname{Im} M(e^{i\varphi})] w(\varphi)\, d\varphi > -\infty \tag{3.5}$$

(*it is never $+\infty$*)*, then*

$$\lim_{r\uparrow 1} \int \bigl|\ln[\operatorname{Im} M(re^{i\varphi})] - \ln[\operatorname{Im} M(e^{i\varphi})]\bigr|\, w(\varphi)\, d\varphi = 0. \tag{3.6}$$

We will prove Theorem 3.1 by proving

Theorem 3.2. *For any $a > 0$ and $p < \infty$, $\ln_+[\operatorname{Im} M(e^{i\varphi})/a] \in L^p\bigl((0,\pi), w(\varphi)d\varphi\bigr)$, and*

$$\lim_{r\uparrow 1} \int \left|\ln_+\left(\frac{\operatorname{Im} M(re^{i\varphi})}{a}\right) - \ln_+\left(\frac{\operatorname{Im} M(e^{i\varphi})}{a}\right)\right|^p w(\varphi)\, d\varphi = 0. \tag{3.7}$$

Theorem 3.3. *For any $a > 0$, we have*

$$\lim_{r\uparrow 1} \int \ln_-\left(\frac{\operatorname{Im} M(re^{i\varphi})}{a}\right) w(\varphi)\, d\varphi = \int \ln_-\left(\frac{\operatorname{Im} M(e^{i\varphi})}{a}\right) w(\varphi)\, d\varphi. \tag{3.8}$$

Proof of Theorem 3.1 given Theorems 3.2 and 3.3. By Fatou's lemma and the fact that for a.e. φ, $\operatorname{Im} M(re^{i\varphi}) \to \operatorname{Im} M(e^{i\varphi})$, we have

$$\liminf_{r\uparrow 1} \int \ln_-[\operatorname{Im} M(re^{i\varphi})]\, w(\varphi)\, d\varphi \geq \int \ln_-[\operatorname{Im} M(e^{i\varphi})]\, w(\varphi)\, d\varphi. \tag{3.9}$$

Since Theorem 3.2 says that $\sup_{0<r\leq 1} \int \ln_+[\operatorname{Im} M(re^{i\varphi})] w(\varphi)\, d\varphi < \infty$, it follows that if $\int \ln_-[\operatorname{Im} M(e^{i\varphi})] w(\varphi)\, d\varphi = \infty$, then (3.1) holds.

If (3.5) holds, then

$$\lim_{a\downarrow 0} \int \ln_-\left(\frac{\operatorname{Im} M(e^{i\varphi})}{a}\right) w(\varphi)\, d\varphi = 0$$

since $\ln_-(y/a)$ is monotone decreasing to 0 as a decreases. Given ε, first find a so

$$\int \ln_-\left(\frac{\operatorname{Im} M(e^{i\varphi})}{a}\right) w(\varphi)\, d\varphi < \frac{\varepsilon}{3}$$

and then, by (3.8), $r_1 < 1$ such that for $r_1 < r < 1$,

$$\int \ln_-\left(\frac{\operatorname{Im} M(re^{i\varphi})}{a}\right) w(\varphi)\, d\varphi < \frac{\varepsilon}{3}.$$

By (3.7), find $r_2 < 1$ such that for $r_2 < r < 1$,

$$\int \left| \ln_+\left(\frac{\operatorname{Im} M(re^{i\varphi})}{a}\right) - \ln_+\left(\frac{\operatorname{Im} M(e^{i\varphi})}{a}\right) \right| w(\varphi)\, d\varphi < \frac{\varepsilon}{3}.$$

Writing

$$|\ln(\alpha) - \ln(\beta)| \leq \left| \ln_+\left(\frac{\alpha}{a}\right) - \ln_+\left(\frac{\beta}{a}\right) \right| + \ln_-\left(\frac{\alpha}{a}\right) + \ln_-\left(\frac{\beta}{a}\right)$$

we see that if $\max\{r_1, r_2\} < r < 1$, then

$$\int \left|\ln[\operatorname{Im} M(re^{i\varphi})] - \ln[\operatorname{Im} M(e^{i\varphi})]\right| w(\varphi)\, d\varphi < \varepsilon,$$

so (3.6) holds. □

We will prove Theorem 3.2 by using the dominated convergence theorem and standard maximal function techniques. We let the maximal function of the measure $\tilde{\mu}$ defined in (2.65) be

$$\tilde{\mu}^*(x) = \sup_{0<a<\pi} \frac{\tilde{\mu}([x-a, x+a])}{2a}.$$

The Hardy-Littlewood maximal inequality for measures (see Rudin [27]) says that

$$|\{x \mid \tilde{\mu}^*(x) > \lambda\}| \le \frac{3\tilde{\mu}([0, 2\pi])}{\lambda} \le \frac{6\pi}{\lambda}. \tag{3.10}$$

Lemma 3.4. *Let M satisfy* (2.71). *Then for $\theta \in (0, \pi)$ and $r \in (0, 1)$,*

$$\operatorname{Im} M(re^{i\theta}) \le \frac{2\tilde{\mu}^*(\theta)}{\sin\theta} + \frac{1}{r\sin^2(\theta)}. \tag{3.11}$$

Proof. We have that P_r is a convolution operator with a positive even function of φ, decreasing on $[0, \pi]$, with $\int_0^{2\pi} P_r(\theta, \varphi)\, d\varphi/2\pi = 1$. So by standard calculations, (2.72), and (2.70),

$$\int_0^\pi D_r(\theta, \varphi)\, \frac{d\mu(\varphi)}{2\pi} \le \int_0^\pi \frac{4P_r(\theta, \varphi)}{\sin\theta}\, \frac{d\tilde{\mu}(\varphi)}{4\pi} \le \frac{2\tilde{\mu}^*(\theta)}{\sin\theta}.$$

On the other hand, for $|\beta| \ge 1$,

$$\left|\frac{1}{z + z^{-1} - \beta - \beta^{-1}}\right| = \left|\frac{z}{(z-\beta)(z-\beta^{-1})}\right| \le \frac{|z|}{|\operatorname{Im} z|^2} = \frac{1}{r\sin^2(\theta)}$$

if $z = re^{i\theta}$, so (2.61) yields

$$\operatorname{Im} \sum_{j,\pm} \frac{\alpha(\beta_j^\pm)}{z + z^{-1} - \beta_j^\pm - (\beta_j^\pm)^{-1}} \le \frac{\sum_{j,\pm} \alpha(\beta_j^\pm)}{r\sin^2(\theta)} \le \frac{1}{r\sin^2(\theta)}.$$

□

Proof of Theorem 3.2. Let

$$f_1(\varphi) = \frac{2\tilde{\mu}^*(\varphi)}{\sin\varphi}, \qquad f_2(\varphi) = \frac{2}{\sin^2(\varphi)}.$$

For a.e. φ we have $\ln_+[\operatorname{Im} M(re^{i\varphi})/a] \to \ln_+[\operatorname{Im} M(e^{i\varphi})/a]$ by (2.64). By (3.11), for all $r \in (\frac{1}{2}, 1)$, $\ln_+[\operatorname{Im} M(re^{i\varphi})/a] \leq \ln_+[(f_1(\varphi) + f_2(\varphi))/a]$. Thus if we prove that for all $p < \infty$

$$\int \left| \ln_+ \left(\frac{f_1(\varphi) + f_2(\varphi)}{a} \right) \right|^p w(\varphi)\, d\varphi < \infty,$$

we obtain (3.7) by the dominated convergence theorem. Since

$$|\ln_+(x)|^p \leq C(p,q)|x|^q$$

for any $p < \infty$, $q > 0$, and suitable $C(p,q)$, and

$$|x+y|^q \leq 2^q|x|^q + 2^q|y|^q,$$

it suffices to find some $q > 0$ such that

$$\int (|f_1(\varphi)|^q + |f_2(\varphi)|^q)\, w(\varphi)\, d\varphi < \infty.$$

Since for $v^{-1} + t^{-1} = 1$,

$$\int |f_1(\varphi)|^q w(\varphi)\, d\varphi \leq \left(\int |f_1(\varphi)|^{qv}\, d\varphi \right)^{1/v} \left(\int |w(\varphi)|^t\, d\varphi \right)^{1/t}$$

and $w(\varphi) \in L^t$ for some $t > 1$ by (3.3), it suffices to find some $s > 0$ with

$$\int (|f_1(\varphi)|^s + |f_2(\varphi)|^s)\, d\varphi < \infty.$$

If $s < \frac{1}{2}$, then $\int |f_2(\varphi)|^s\, d\varphi < \infty$ and by Cauchy-Schwartz and (3.10),

$$\int |f_1(\varphi)|^s\, d\varphi \leq \left(\int |2\tilde{\mu}^*(\varphi)|^{2s}\, d\varphi \right)^{\frac{1}{2}} \left(\int |\sin\varphi|^{-2s}\, d\varphi \right)^{\frac{1}{2}} < \infty.$$

□

As a preliminary to the proof of Theorem 3.3, we need

Lemma 3.5. *Let* w *obey* (3.4)*. Let* $0 < \varphi_0 < \pi$ *and let* $\varphi_1, \varphi_2 \in [0, \pi]$ *obey*

$$\text{(a)} \qquad d(\varphi_1) \geq d(\varphi_0), \quad d(\varphi_2) \geq d(\varphi_0), \tag{3.12}$$

$$\text{(b)} \qquad |\varphi_1 - \varphi_2| \leq d(\varphi_0)^\beta. \tag{3.13}$$

Then for $C_3 \equiv C_2 e^{C_2}$*,*

$$\left| \frac{w(\varphi_1)}{w(\varphi_2)} - 1 \right| \leq C_3 |\varphi_1 - \varphi_2| \, d(\varphi_0)^{-\beta}. \tag{3.14}$$

Proof.

$$\left| \frac{w(\varphi_1)}{w(\varphi_2)} - 1 \right| = \left| \exp\biggl(\int_{\varphi_1}^{\varphi_2} \frac{w'(\eta)}{w(\eta)} \, d\eta \biggr) - 1 \right| \leq \bigl| \exp\bigl(C_2 |\varphi_2 - \varphi_1| \, d(\varphi_0)^{-\beta} \bigr) - 1 \bigr|$$

by (3.4) and (3.12). But $|e^x - 1| \leq e^{|x|} |x|$, so by (3.13),

$$\left| \frac{w(\varphi_1)}{w(\varphi_2)} - 1 \right| \leq C_2 e^{C_2} |\varphi_1 - \varphi_2| \, d(\varphi_0)^{-\beta}.$$

□

We will also need the following pair of lemmas:

Lemma 3.6. *Let* $0 < \eta < \theta < \pi - \eta$ *and*

$$N_r(\theta, \eta) \equiv \int_{\theta - \eta}^{\theta + \eta} D_r(\theta, \varphi) \, \frac{d\varphi}{2\pi}.$$

Then

$$0 \leq 1 - N_r(\theta, \eta) \leq \frac{4(1 - r)}{r \sin^2(\eta)}. \tag{3.15}$$

Proof. We have

$$1 = \int_0^{2\pi} P_r(\theta, \varphi) \, \frac{d\varphi}{2\pi},$$

so since $D_r \leq P_r$, we obtain $N_r \leq 1$. Also, by (2.69),

$$1 - N_r(\theta, \eta) \leq \frac{2}{2\pi} \int_{\substack{\varphi \in [0,2\pi] \\ |\theta - \varphi| \geq \eta}} P_r(\theta, \varphi)\, d\varphi.$$

If $|\theta - \varphi| \geq \eta$, then

$$P_r(\theta, \varphi) = \frac{1 - r^2}{(1-r)^2 + 4r \sin^2[\frac{1}{2}(\theta - \varphi)]} \leq \frac{2(1-r)}{4r \sin^2(\eta/2)} \leq \frac{2(1-r)}{r \sin^2(\eta)}$$

and (3.15) is immediate. □

Lemma 3.7. *There is $c > 0$ such that for $\theta \in [0, \pi]$ and $r \in (\frac{1}{2}, 1)$,*

$$\operatorname{Im} M(re^{i\theta}) \geq c(r^{-1} - r) \sin \theta. \tag{3.16}$$

Proof. In terms of m, for $\varepsilon > 0$ and $E \in \mathbb{R}$,

$$\operatorname{Im}[-m(E - i\varepsilon)] \geq \int_{-2}^{2} \frac{\varepsilon\, d\nu(x)}{(E-x)^2 + \varepsilon^2}. \tag{3.17}$$

Now if $z = re^{i\theta}$, then

$$M(z) = -m(E - i\varepsilon)$$

with $z + z^{-1} = E - i\varepsilon$, or $E = (r + r^{-1}) \cos \theta$ and $\varepsilon = (r^{-1} - r) \sin \theta$. If $r > \frac{1}{2}$, then $|E| \leq 3$, $|\varepsilon| \leq 2$, and in (3.17), $|x| \leq 2$. Thus by (3.17),

$$\operatorname{Im} M(z) \geq \frac{\varepsilon}{29} \int_{-2}^{2} d\nu(x) = \frac{\nu([-2,2])}{29}\, \varepsilon,$$

which is (3.16). □

Proof of Theorem 3.3. Since $\ln_-$ is a decreasing function, to get upper bounds on $\ln_-[\operatorname{Im} M(re^{i\theta})/a]$, we can use a lower bound on $\operatorname{Im} M$. The elementary bound

$$\ln_-(ab) \leq \ln_-(a) + \ln_-(b) \tag{3.18}$$

will be useful.

As already noted, Fatou's lemma implies that the lim inf of the left side of (3.8) is bounded from below by the right side, so it suffices to prove that

$$\limsup_{r\uparrow 1} \int_0^\pi \ln_-\biggl(\frac{\operatorname{Im} M(re^{i\theta})}{a}\biggr) w(\theta)\,d\theta \le \int_0^\pi \ln_-\biggl(\frac{\operatorname{Im} M(e^{i\theta})}{a}\biggr) w(\theta)\,d\theta. \tag{3.19}$$

Pick γ and κ so that $0 < \max\{\beta, 1\}\gamma < \kappa < \frac{1}{2}$, and let $\theta_0(r) \equiv (1-r)^\gamma$ and $\eta(r) \equiv (1-r)^\kappa$. We will bound $\operatorname{Im} M(re^{i\theta})$ from below for $d(\theta) \le \theta_0(r)$ using (3.16), and for $d(\theta) \ge \theta_0(r)$ we will use the Poisson integral for the region $|\theta - \varphi| \le \eta(r)$.

By (3.16) and (3.3), using

$$\int_0^{\theta_0} \ln_-(\sin\theta)\theta^{-1+\alpha}\,d\theta = O\bigl(\theta_0^\alpha \ln_- \theta_0\bigr)$$

as $\theta_0 \to 0$, we have

$$\int_{d(\theta)\le\theta_0(r)} \ln_-\biggl(\frac{\operatorname{Im} M(re^{i\theta})}{a}\biggr) w(\theta)\,d\theta \le C_\alpha \theta_0^\alpha(r)\bigl[\tilde C_a + \ln_-(r^{-1}-r) + \ln_-(\theta_0(r))\bigr]$$

which goes to zero as $r \uparrow 1$ for any a. So suppose $d(\theta) > \theta_0(r)$. By (2.71), (2.73), and $D_r \ge 0$,

$$\begin{aligned}\operatorname{Im} M(re^{i\theta}) &\ge \int_{\theta-\eta(r)}^{\theta+\eta(r)} D_r(\theta,\varphi) \operatorname{Im} M(e^{i\varphi})\,\frac{d\varphi}{2\pi} \\ &= N_r(\theta,\eta) \int_{\theta-\eta(r)}^{\theta+\eta(r)} \frac{D_r(\theta,\varphi)}{2\pi N_r(\theta,\eta)} \operatorname{Im} M(e^{i\varphi})\,d\varphi,\end{aligned} \tag{3.20}$$

where we dropped the pole terms and the contribution of μ_{sing} in (2.71).

For later purposes, note that for $d(\theta) > \theta_0(r)$, (3.15) implies

$$0 \le 1 - N_r(\theta,\eta) \le C(1-r)^{1-2\kappa} \tag{3.21}$$

which goes to zero as $r \uparrow 1$ since $\kappa < \frac{1}{2}$. Using (3.20) and (3.18), we bound $\ln_-[\operatorname{Im} M(re^{i\theta})/a]$ as two $\ln_-$'s. Since $\ln_-$ is convex and $D_r(\theta,\varphi)[2\pi N_r(\theta,\eta)]^{-1}\,d\varphi$ restricted to $(\theta-\eta, \theta+\eta)$ is a probability measure, we can use Jensen's inequality to see that

$$
\begin{aligned}
w(\theta)\ln_-&\biggl(\frac{\operatorname{Im} M(re^{i\theta})}{a}\biggr) \\
&\le w(\theta)\ln_-\bigl[N_r(\theta,\eta)\bigr] + \int_{\theta-\eta(r)}^{\theta+\eta(r)} \frac{w(\theta)}{w(\varphi)}\,\frac{D_r(\theta,\varphi)}{N_r(\theta,\eta)}\,w(\varphi)\ln_-\biggl(\frac{\operatorname{Im} M(e^{i\varphi})}{a}\biggr)\frac{d\varphi}{2\pi}.
\end{aligned}
\tag{3.22}
$$

In the first term (for the θ's with $d(\theta) > \theta_0(r)$), N_r obeys (3.21), so as $r \uparrow 1$,

$$
\int_{d(\theta)>\theta_0(r)} w(\theta)\ln_-\bigl[N_r(\theta,\eta)\bigr]\,d\theta = O\bigl((1-r)^{1-2\kappa}\bigr) \to 0. \tag{3.23}
$$

In the second term, note that for the θ's in question, $N_r(\theta,\eta)^{-1} - 1 = O((1-r)^{1-2\kappa})$ and by (3.14), $w(\theta)/w(\varphi) - 1 = O(\eta(r)\theta_0^{-\beta}(r)) = O((1-r)^{\kappa-\beta\gamma})$. Since $D_r(\theta,\varphi) \le P_r(\theta,\varphi)$, we thus have

$$
\begin{aligned}
\int_{d(\theta)>\theta_0} &\ln_-\biggl(\frac{\operatorname{Im} M(re^{i\theta})}{a}\biggr)w(\theta)\,d\theta \\
&\le O\bigl((1-r)^{1-2\kappa}\bigr) + \bigl[1 + O\bigl((1-r)^{1-2\kappa}\bigr)\bigr]\bigl[1 + O\bigl((1-r)^{\kappa-\beta\gamma}\bigr)\bigr] \\
&\qquad \int_{d(\theta)>\theta_0}\int_{|\varphi-\theta|\le\eta} P_r(\theta,\varphi)w(\varphi)\ln_-\biggl(\frac{\operatorname{Im} M(e^{i\varphi})}{a}\biggr)\,d\varphi\,\frac{d\theta}{2\pi}.
\end{aligned}
\tag{3.24}
$$

Since the integrand is positive, we can extend it to $\{(\theta,\varphi) \mid \theta \in [0,2\pi], \varphi \in [0,\pi]\}$ and do the θ integration first, using $\int P_r(\theta,\varphi)d\theta/2\pi = 1$. We obtain

$$
\int_0^\pi \ln_-\biggl(\frac{\operatorname{Im} M(re^{i\theta})}{a}\biggr)w(\theta)\,d\theta \le o(1) + \bigl[1 + o(1)\bigr]\int_0^\pi \ln_-\biggl(\frac{\operatorname{Im} M(e^{i\theta})}{a}\biggr)w(\theta)\,d\theta.
$$

Take $r \uparrow 1$ and (3.19) follows. □

This concludes the proof of Theorem 3.1. By going through the proof, one easily sees that

Theorem 3.8. *Theorem 3.1 remains true if in* (3.1) *and* (3.6), $\ln[\operatorname{Im} M(re^{i\varphi})]$ *is replaced by* $\ln[g(r)\sin\varphi + \operatorname{Im} M(re^{i\varphi})]$ *where* $g(r) \ge 0$ *and* $g(r) \to 0$ *as* $r \uparrow 1$.

Proof. In the $\ln_+$ bounds, we get an extra $[\sup_{\frac{1}{2}<r<1} g(r)]\sin\theta$ in $f_2(\theta)$. Since we still have pointwise convergence, we easily get the analog of Theorem 3.2. In the proof of Theorem 3.3, Fatou is unchanged since $g(r) \to 0$, and since

$$\ln_- \big[g(r)\sin\varphi + \operatorname{Im} M(re^{i\varphi})\big] \le \ln_- \big[\operatorname{Im} M(re^{i\varphi})\big],$$

the lim sup bound has an unchanged proof as well. □

3.2 The Step-by-Step Sum Rules

Before we state the step-by-step sum rules, we need to define several quantities. By Lemma 2.8, if f is even or odd and monotone on $[2,\infty)$ with $f(2)=0$, then

$$\delta_n(f,J) \equiv \sum_{\pm}\sum_{j=1}^{\infty} \big[f(E_j^\pm(J)) - f(E_j^\pm(J^{(n)}))\big] \tag{3.25}$$

exists and is finite. If $\beta_j^\pm$ is defined by $E_j^\pm = \beta_j^\pm + (\beta_j^\pm)^{-1}$ and $|\beta_j| \ge 1$, we let

$$X_\ell^{(n)}(J) \equiv \delta_n(f,J), \qquad f(E) \equiv \begin{cases} \ln|\beta| & \ell = 0, \\ -\frac{1}{\ell}[\beta^\ell - \beta^{-\ell}] & \ell \ge 1. \end{cases} \tag{3.26}$$

In addition, we will need

$$\zeta_\ell^{(n)}(J) \equiv \begin{cases} -\sum_{j=1}^n \ln(a_j) & \ell = 0, \\ \frac{2}{\ell}\lim_{m\to\infty}\big[\operatorname{Tr}\big(T_\ell(\frac{1}{2}J_{m;F})\big) - \operatorname{Tr}\big(T_\ell(\frac{1}{2}J^{(n)}_{m-n;F})\big)\big] & \ell \ge 1, \end{cases} \tag{3.27}$$

where $J_{m;F}$ is the finite matrix formed from the first m rows and columns of J, and T_ℓ is the ℓ^{th} Chebyshev polynomial of the first kind defined in (2.10). By Lemma 3.31 (applied to $J, J^{(1)}, \dots, J^{(n-1)}$ and added together), the limit in (3.27) exists and the expression inside the limit is independent of m once $m > \ell + n$. Note that by (2.12),

$$\zeta_1^{(n)}(J) = \sum_{j=1}^n b_j, \tag{3.28}$$

$$\zeta_2^{(n)}(J) = \sum_{j=1}^{n} \tfrac{1}{2}\bigl[b_j^2 + (a_j^2 - 1)\bigr]. \tag{3.29}$$

By construction (with $J^{(0)} \equiv J$),

$$X_\ell^{(n)}(J) = \sum_{j=0}^{n-1} X_\ell^{(1)}(J^{(j)}) \tag{3.30}$$

and

$$\zeta_\ell^{(n)}(J) = \sum_{j=0}^{n-1} \zeta_\ell^{(1)}(J^{(j)}). \tag{3.31}$$

Finally, $M(\bar{z}) = \overline{M(z)}$, (2.63), and (2.29)/(2.30)/(2.32) imply

$$Z(J) = \frac{1}{4\pi} \int_0^{2\pi} \ln\biggl(\frac{\sin\theta}{\operatorname{Im} M(e^{i\theta}; J)}\biggr)\, d\theta, \tag{3.32}$$

and for $\ell \geq 1$,

$$Z_\ell^{\pm}(J) = \frac{1}{4\pi} \int_0^{2\pi} \ln\biggl(\frac{\sin\theta}{\operatorname{Im} M(e^{i\theta}; J)}\biggr) (1 \pm \cos(\ell\theta))\, d\theta, \tag{3.33}$$

$$Y_\ell(J) = -\frac{1}{2\pi} \int_0^{2\pi} \ln\biggl(\frac{\sin\theta}{\operatorname{Im} M(e^{i\theta}; J)}\biggr) \cos(\ell\theta)\, d\theta. \tag{3.34}$$

Our main goal in this section is to prove the next three theorems.

Theorem 3.9 (Step-by-Step Sum Rules). *Let J be a BW matrix. Then $Z(J) < \infty$ if and only if $Z(J^{(1)}) < \infty$. If $Z(J) < \infty$, then for $\ell \geq 1$ we have*

$$Z(J) = -\ln(a_1) + X_0^{(1)}(J) + Z(J^{(1)}), \tag{3.35}$$

$$Y_\ell(J) = \zeta_\ell^{(1)}(J) + X_\ell^{(1)}(J) + Y_\ell(J^{(1)}). \tag{3.36}$$

Remarks. 1. By iteration and (3.30)/(3.31), we obtain $Z(J) < \infty$ if and only if $Z(J^{(n)}) < \infty$, and

$$Z(J) = -\sum_{j=1}^{n} \ln(a_j) + X_0^{(n)}(J) + Z(J^{(n)}), \tag{3.37}$$

$$Y_\ell(J) = \zeta_\ell^{(n)}(J) + X_\ell^{(n)}(J) + Y_\ell(J^{(n)}). \tag{3.38}$$

2. We call (3.35)–(3.38) the step-by-step Case sum rules.

Theorem 3.10 (One-Sided Step-by-Step Sum Rules). *Let J be a BW matrix. Then $Z_1^\pm(J) < \infty$ if and only if $Z_1^\pm(J^{(1)}) < \infty$. If $Z_1^\pm(J) < \infty$, then for $\ell = 1, 3, 5, \dots$ we have*

$$Z_\ell^\pm(J) = -\ln(a_1) \mp \tfrac{1}{2}\,\zeta_\ell^{(1)}(J) + X_0^{(1)}(J) \mp \tfrac{1}{2}\,X_\ell^{(1)}(J) + Z_\ell^\pm(J^{(1)}). \tag{3.39}$$

Remark. Theorem 3.10 is intended to be two statements: one with all the upper signs used and one with all the lower signs used.

Theorem 3.11 (Quasi-Step-by-Step Sum Rules). *Let J be a BW matrix. Then $Z_2^-(J) < \infty$ if and only if $Z_2^-(J^{(1)}) < \infty$. If $Z_2^-(J) < \infty$, then for $\ell = 2, 4, 6, \dots$ we have*

$$Z_\ell^-(J) = -\ln(a_1) + \tfrac{1}{2}\,\zeta_\ell^{(1)}(J) + X_0^{(1)}(J) + \tfrac{1}{2}\,X_\ell^{(1)}(J) + Z_\ell^-(J^{(1)}). \tag{3.40}$$

Remarks. 1. Since $Z(J) < \infty$ implies $Z_1^+(J)$ and $Z_1^-(J) < \infty$, and $Z_1^+(J)$ or $Z_1^-(J) < \infty$ imply $Z_2^-(J) < \infty$, we have additional sum rules in various cases.

2. In [14], Laptev et al. prove sum rules for $Z_\ell^-(J)$ where $\ell = 4, 6, 8, \dots$. One can develop step-by-step sum rules in this case and use them to streamline the proof of their rules as we streamline the proof of the Killip-Simon P_2 rule (our Z_2^- rule) in the next section. One only needs to repeat the proofs in the previous section with $d(\varphi)$ as in the remark after (3.4).

The step-by-step sum rules were introduced in Killip-Simon, who first consider $r < 1$ (in our language below), then take $n \to \infty$, and then, with some technical hurdles, $r \uparrow 1$. By first letting $r \uparrow 1$ with $n = 1$ (using results from the previous section), and then taking $n \to \infty$ (as in the next section), we can both simplify their proof and obtain additional results. The idea of using the imaginary part of (2.74) is taken from [13].

Proof of Theorem 3.9. Taking imaginary parts of both sides of (2.74) with $z = re^{i\theta}$ and $r < 1$ yields

$$\operatorname{Im} M(re^{i\theta}; J)\, |M(re^{i\theta}; J)|^{-2} = (r^{-1} - r)\sin\theta + a_1^2 \operatorname{Im} M(re^{i\theta}; J^{(1)}).$$

Taking ln's of both sides, we obtain

$$\ln\left(\frac{\sin\theta}{\operatorname{Im} M(re^{i\theta}; J)}\right) = t_1 + t_2 + t_3 \tag{3.41}$$

where

$$\begin{aligned} t_1 &= -2\ln|M(re^{i\theta}; J)|, \\ t_2 &= -2\ln a_1, \\ t_3 &= \ln\left(\frac{\sin\theta}{g(r)\sin\theta + \operatorname{Im} M(re^{i\theta}; J^{(1)})}\right) \end{aligned}$$

with

$$g(r) \equiv a_1^{-2}(r^{-1} - r).$$

Let

$$f_r(z) \equiv \frac{M(rz; J)}{rz}, \tag{3.42}$$

so $f_r(0) = 1$ (see (2.75)). Obviously, f_r is meromorphic in $\frac{1}{r}\mathbb{D}$. Inside the unit disk, f_r has poles at $\{(r\beta_j^{\pm}(J))^{-1} \mid j \text{ so that } |\beta_j^{\pm}(J)| > r^{-1}\}$ and it has zeros at $\{(r\beta_j^{\pm}(J^{(1)}))^{-1} \mid j \text{ so that } |\beta_j^{\pm}(J^{(1)})| > r^{-1}\}$. This is because the zeros of $M(z; J)$ are the poles of $M(z; J^{(1)})$ by (2.74). Thus, by Jensen's formula (3.91) for f_r:

$$\frac{1}{4\pi}\int_0^{2\pi} t_1\, d\theta = -\ln r + \sum_{|\beta_j^{\pm}(J)|>r^{-1}} \ln|r\beta_j^{\pm}(J)| - \sum_{|\beta_j^{\pm}(J^{(1)})|>r^{-1}} \ln|r\beta_j^{\pm}(J^{(1)})|.$$

By (2.26), the numbers of terms in the sums differ by at most 2, so that the $\ln(r)$'s cancel up to at most $2\ln(r) \to 0$ as $r \uparrow 1$. Thus as $r \uparrow 1$, (3.26) shows that

$$\frac{1}{4\pi}\int_0^{2\pi} (t_1 + t_2)\, d\theta \to -\ln(a_1) + X_0^{(1)}(J).$$

By Theorems 3.1 and 3.8 (with $w(\theta) \equiv 1$) and by (3.41),

$$\frac{1}{4\pi}\int_0^{2\pi} t_3\, d\theta \to Z(J^{(1)}),$$
$$\frac{1}{4\pi}\int_0^{2\pi} (t_1 + t_2 + t_3)\, d\theta \to Z(J).$$

Hence $Z(J) < \infty$ if and only if $Z(J^{(1)}) < \infty$, and if they are finite, (3.35) holds.

To obtain (3.36) for $\ell \geq 1$, we use the same method but with higher Jensen's formulae (3.92) for f_r. We first note that by (3.42) and (3.98), the ℓ^{th} Taylor coefficient of $\ln f_r(z)$ is $r^\ell \zeta_\ell^{(1)}(J)$. So by (3.92):

$$\begin{aligned}
r^\ell \zeta_\ell^{(1)}(J) =& \frac{1}{\pi}\int_0^{2\pi} \ln|f_r(e^{i\theta})| \cos(\ell\theta)\, d\theta - \sum_{|\beta_j^\pm(J^{(1)})| > r^{-1}} \frac{(r\beta_j^\pm(J^{(1)}))^\ell - (r\beta_j^\pm(J^{(1)}))^{-\ell}}{\ell} \\
&+ \sum_{|\beta_j^\pm(J)| > r^{-1}} \frac{(r\beta_j^\pm(J))^\ell - (r\beta_j^\pm(J))^{-\ell}}{\ell} \\
=& -\frac{1}{2\pi}\int_0^{2\pi} (t_1 + t_2)\cos(\ell\theta)\, d\theta \\
&+ \frac{r^\ell}{\ell}\Bigg\{ \sum_{|\beta_j^\pm(J)| > r^{-1}} \big[(\beta_j^\pm(J))^\ell - 1\big] - \sum_{|\beta_j^\pm(J^{(1)})| > r^{-1}} \big[(\beta_j^\pm(J^{(1)}))^\ell - 1\big] \Bigg\} \\
&- \frac{r^{-\ell}}{\ell}\Bigg\{ \sum_{|\beta_j^\pm(J)| > r^{-1}} \big[(\beta_j^\pm(J))^{-\ell} - 1\big] - \sum_{|\beta_j^\pm(J^{(1)})| > r^{-1}} \big[(\beta_j^\pm(J^{(1)}))^{-\ell} - 1\big] \Bigg\}.
\end{aligned}$$

Again, as $r \uparrow 1$, we obtain

$$\begin{aligned}
-\frac{1}{2\pi}\int_0^{2\pi} (t_1 + t_2)\cos(\ell\theta)\, d\theta \;\to\; & \zeta_\ell^{(1)}(J) - \sum_{j,\pm} \frac{(\beta_j^\pm(J))^\ell - (\beta_j^\pm(J))^{-\ell}}{\ell} \\
&+ \sum_{j,\pm} \frac{(r\beta_j^\pm(J^{(1)}))^\ell - (r\beta_j^\pm(J^{(1)}))^{-\ell}}{\ell} \\
&= \zeta_\ell^{(1)}(J) + X_\ell^{(1)}(J).
\end{aligned}$$

By $Z(J) < \infty$, the L^1 convergence in Theorems 3.1 and 3.8, and by (3.41),

$$-\frac{1}{2\pi}\int_0^{2\pi} t_3 \cos(\ell\theta)\, d\theta \to Y_\ell(J^{(1)}),$$
$$-\frac{1}{2\pi}\int_0^{2\pi} (t_1 + t_2 + t_3)\cos(\ell\theta)\, d\theta \to Y_\ell(J),$$

proving (3.36). □

Proofs of Theorems 3.10 and 3.11. These are the same as the above proof, but now the weight $w(\theta)$ is either $1 \pm \cos(\theta)$ or $1 - \cos(2\theta)$, and that weight obeys (3.3) and (3.4). □

Corollary 3.12. *Let J be a BW matrix. If $J - \tilde{J}$ is finite rank, then J is Szegő (resp. Szegő at ± 2) if and only if $\tilde{J}$ is.*

Proof. For some n, $J^{(n)} = \tilde{J}^{(n)}$, so this is immediate from Theorems 3.9 and 3.10. □

Given this result, a natural question arises:

Conjecture 3.13. Let J be a BW matrix. If $J - \tilde{J}$ is trace class, then J is Szegő (resp. Szegő at ± 2) if and only if $\tilde{J}$ is. It is possible this conjecture is only generally true if $J - J_0$ is only assumed compact or is only assumed Hilbert-Schmidt.

This conjecture for $J = J_0$ is Nevai's conjecture recently proven by Killip-Simon. Ideas in this work would prove this conjecture if one can prove a result of the following form. Let $J - \tilde{J}$ be a finite rank operator so that by Lemma 2.8,

$$\delta(J, \tilde{J}) \equiv \lim_{N\to\infty} \sum_{\pm} \sum_{j=1}^{N} \left(\sqrt{|E_j^{\pm}(J)| - 2} - \sqrt{|E_j^{\pm}(\tilde{J})| - 2} \right)$$

exists and is finite. The conjecture would be provable by the methods of this work (by using the step-by-step sum rule to remove the first n pieces of J and then replacing them with the first n pieces of $\tilde{J}$) if one had a bound of the form

$$|\delta(J, \tilde{J})| \leq (\text{const.})\text{Tr}(|J - \tilde{J}|). \tag{3.43}$$

This is because $|\beta| - 1 = O(\sqrt{|E| - 2})$ shows that $X_0^{(n)}(J) - X_0^{(n)}(\tilde{J})$ is comparable to $\delta(J, \tilde{J})$.

Inequality (3.43) holds for $J = J_0$ by Theorem 2.3. There are counterexamples that show (3.43) does not hold for a universal constant c. However, in these examples, $\|J\| \to \infty$ as $c \to \infty$. Thus it could be that (3.43) holds with c only depending on J for some class of J's. If it held with a bound depending only on $\|J\|$, the conjecture would hold in general. If J was required in J_0+ Hilbert-Schmidt, we would get the conjecture for such J's.

For later reference we write down the step-by-step Z, $Z_1^{\pm}$, and Z_2^- sum rules (iterated (3.35) and (3.39)) explicitely. We define

$$\xi^{\pm}(E) \equiv \ln|\beta| \pm \tfrac{1}{2}(\beta - \beta^{-1}), \tag{3.44}$$

$$F(E) \equiv \tfrac{1}{4}\big[\beta^2 - \beta^{-2} - \ln(\beta^4)\big], \tag{3.45}$$

$$G(a) \equiv \tfrac{1}{2}\big[a^2 - 1 - \ln(a^2)\big], \tag{3.46}$$

with $E = \beta + \beta^{-1}$ and $|\beta| \geq 1$. We then have

$$Z(J) = -\sum_{j=1}^{n} \ln(a_j) + \sum_{j,\pm} \Big[\ln\big|\beta_j^{\pm}(J)\big| - \ln\big|\beta_j^{\pm}(J^{(n)})\big|\Big] + Z(J^{(n)}), \tag{3.47}$$

$$Z_1^+(J) = -\sum_{j=1}^{n} \big[\ln(a_j) + \tfrac{1}{2}b_j\big] + \sum_{j,\pm} \Big[\xi^+\big(E_j^{\pm}(J)\big) - \xi^+\big(E_j^{\pm}(J^{(n)})\big)\Big] + Z_1^+(J^{(n)}), \tag{3.48}$$

$$Z_1^-(J) = -\sum_{j=1}^{n} \big[\ln(a_j) - \tfrac{1}{2}b_j\big] + \sum_{j,\pm} \Big[\xi^-\big(E_j^{\pm}(J)\big) - \xi^-\big(E_j^{\pm}(J^{(n)})\big)\Big] + Z_1^-(J^{(n)}), \tag{3.49}$$

$$Z_2^-(J) = \sum_{j=1}^{n} \big[G(a_j) + \tfrac{1}{4}b_j^2\big] - \sum_{j,\pm} \Big[F\big(E_j^{\pm}(J)\big) - F\big(E_j^{\pm}(J^{(n)})\big)\Big] + Z_2^-(J^{(n)}). \tag{3.50}$$

3.3 The Z, $Z_1^{\pm}$, and Z_2^{-} Sum Rules

Our goal here is to prove that "full size" sum rules of Case type hold under certain hypotheses. Of interest on their own, these considerations also somewhat simplify the proof of the P_2 sum rule in Section 8 of [13], and considerably simplify the proof of the C_0 sum rule for trace class $J - J_0$ in Section 9 of [13]. Throughout, J will be a BW matrix. Our three main tools are lower semi-continuity of the Z's in J, their boundedness from below, and the step-by-step sum rules. We use lower semi-continuity of the Z's in two ways — we approximate J with J_n, and J_0 with $J^{(n)}$ (the latter when $J - J_0$ is compact). As we shall see, these and the step-by-step sum rules will yield the two opposite inequalities in the "full size" sum rules.

Motivated by (3.47)–(3.50), we introduce the following quantities:

$$\bar{A}_0(J) \equiv \limsup_{n\to\infty}\Big(-\sum_{j=1}^{n} \ln(a_j)\Big), \tag{3.51}$$

$$\underline{A}_0(J) \equiv \liminf_{n\to\infty}\Big(-\sum_{j=1}^{n} \ln(a_j)\Big),$$

$$\bar{A}_1^{\pm}(J) \equiv \limsup_{n\to\infty}\Big(-\sum_{j=1}^{n} \big(a_j - 1 \pm \tfrac{1}{2}b_j\big)\Big), \tag{3.52}$$

$$\underline{A}_1^{\pm}(J) \equiv \liminf_{n\to\infty}\Big(-\sum_{j=1}^{n} \big(a_j - 1 \pm \tfrac{1}{2}b_j\big)\Big),$$

$$A_2(J) \equiv \sum_{j=1}^{\infty} \big[G(a_j) + \tfrac{1}{4}b_j^2\big], \tag{3.53}$$

where $G(a)$ is from (3.46). Note that $G(a) \geq 0$ because $\ln(a^2) \leq 2a - 2$, and $G(a) \sim (a-1)^2$ for $a \sim 1$. Since $G(a) \geq 0$, the sum in (3.53) exists (but may be $+\infty$). Since $G(a) = O((a-1)^2)$, it follows that $A_2(J)$ is finite if and only if $J - J_0$ is Hilbert-Schmidt.

In (3.52), we use $a_j - 1$ in place of $\ln(a_j)$, which appears in (3.48). The reason for this is that we will mainly be interested in the $Z_1^{\pm}$ sum rules when $J - J_0$ is Hilbert-Schmidt, in which case $\{a_j - 1\} \in \ell^2$ and so $\sum|\ln(a_j) - (a_j - 1)| < \infty$. Notice also that in the case of a discrete Schrödinger operator (i.e., $a_n \equiv 1$), $\bar{A}_0(J) = \underline{A}_0(J) = 0$.

Next, we introduce some functions of the eigenvalues:

$$\mathcal{E}_0(J) \equiv \sum_{j,\pm} \ln|\beta_j^\pm|, \tag{3.54}$$

$$\mathcal{E}_1^\pm(J) \equiv \sum_{j} \sqrt{|E_j^\pm| - 2}\,, \tag{3.55}$$

$$\mathcal{E}_2(J) \equiv \sum_{j,\pm} F(E_j^\pm), \tag{3.56}$$

where $F(E)$ is from (3.45). In (3.54) and (3.56), we sum over $+$ and $-$. In (3.55), we define $\mathcal{E}_1^+$ and $\mathcal{E}_1^-$ with only the $+$ or only the $-$ terms. Note that F is even, increasing on $[2,\infty)$, $F(2)=0$, and $F(E) \sim \frac{2}{3}(|E|-2)^{3/2}$ for $|E| \sim 2$. Hence $\mathcal{E}_2(J) < \infty$ if and only if

$$\sum_{j,\pm} (|E_j^\pm| - 2)^{3/2} < \infty.$$

Also, since $|\beta| - 1 = O(\sqrt{|E|-2}\,)$, we have that $\mathcal{E}_0(J) < \infty$ if and only if

$$\sum_{j,\pm} \sqrt{|E_j^\pm| - 2} < \infty. \tag{3.57}$$

We will need the following basis-dependent notion:

Definition. Let B be a bounded operator on $\ell^2(\mathbb{Z}^+)$. We say that B has a *conditional trace* if

$$\lim_{\ell\to\infty} \sum_{j=1}^{\ell} \langle \delta_j, B\delta_j \rangle \equiv \text{c-Tr}(B) \tag{3.58}$$

exists and is finite.

Remark. If B is not trace class, this object is not unitarily invariant.

Our goal in this section is to prove the following three theorems whose proof is deferred until after all the statements.

Theorem 3.14. *Let J be a BW matrix. Consider the four statements:*

(i) $\bar{A}_0(J) > -\infty$,

(ii) $\underline{A}_0(J) < \infty$,

(iii) $Z(J) < \infty$,

(iv) $\mathcal{E}_0(J) < \infty$.

Then

(a) (ii) + (iv) $\Rightarrow$ (iii) + (i),

(b) (i) + (iii) $\Rightarrow$ (iv) + (ii),

(c) (iii) $\Rightarrow \bar{A}_0(J) < \infty$,

(d) (iv) $\Rightarrow \underline{A}_0(J) > -\infty$.

Thus (iii) + (iv) $\Rightarrow$ (i) + (ii). *In particular, if* $\underline{A}_0(J) = \bar{A}_0(J)$, *that is, the limit exists, then the finiteness of any two of* $Z(J)$, $\mathcal{E}_0(J)$, *and* $\bar{A}_0(J)$ *implies the finiteness of the third.*

If all four conditions hold and $J - J_0$ *is compact, then*

(e) *The limit*

$$\lim_{n\to\infty}\left(-\sum_{j=1}^{n}\ln(a_j)\right) \equiv A_0(J) \tag{3.59}$$

exists and is finite, and the Z *sum rule holds:*

$$Z(J) = A_0(J) + \mathcal{E}_0(J). \tag{3.60}$$

(f) *For each* $\ell = 1, 2, \dots,$

$$-\sum_{j,\pm} \tfrac{1}{\ell}[\beta_j^{\pm}(J)^{\ell} - \beta_j^{\pm}(J)^{-\ell}] \equiv X_\ell^{(\infty)}(J) \tag{3.61}$$

converges absolutely and equals $\lim_{n\to\infty} X_\ell^{(n)}(J)$.

(g) *For each* $\ell = 1, 2, \dots,$

$$B_\ell(J) = \frac{2}{\ell}\left[T_\ell\left(\frac{J}{2}\right) - T_\ell\left(\frac{J_0}{2}\right)\right] \tag{3.62}$$

has a conditional trace and

$$\text{c-Tr}(B_\ell(J)) = \lim_{n\to\infty} \zeta_\ell^{(n)}(J). \tag{3.63}$$

For example, for $\ell = 1$ *we have that* $\sum_{j=1}^{n} b_j$ *converges to a finite limit.*

(h) *The* Y_ℓ *sum rules hold:*

$$Y_\ell(J) = \text{c-Tr}(B_\ell(J)) + X_\ell^{(\infty)}(J) \tag{3.64}$$

where Y_ℓ *is given by* (3.34), $X_\ell^{(\infty)}$ *by* (3.61), *and* $\text{c-Tr}(B_\ell(J))$ *by* (3.58), (3.62), *and* (3.63).

Remarks. 1. In a sense, this is the main result of this chapter.

2. We will give examples later where $\bar{A}_0(J) = \underline{A}_0(J)$ and one of the conditions (i)/(ii), (iii), (iv) holds but the other two fail.

3. By Lemma 3.29, for ℓ odd, $T_\ell(J_0/2)$ vanishes on-diagonal, and for ℓ even, $T_\ell(J_0/2)$ eventually vanishes on-diagonal and $\text{c-Tr}(T_\ell(J_0/2)) = -\frac{1}{2}$. Thus (g) says $\text{c-Tr}(T_\ell(J/2))$ exists and the sum rule (3.64) can replace $\text{c-Tr}(B_\ell(J))$ by $\frac{2}{\ell}\text{c-Tr}(T_\ell(J/2))$ plus a constant (zero if ℓ is odd and $\frac{1}{\ell}$ if ℓ is even).

Corollary 3.15. *Let* $J - J_0$ *be compact. If* $Z(J) < \infty$, *then* $-\sum_{j=1}^{n} \ln(a_j)$ *either converges or diverges to* $-\infty$.

Remarks. 1. We will give an example later in which $Z(J) < \infty$, and $\lim_{n\to\infty}(-\sum_{j=1}^{n} \ln(a_j)) = -\infty$.

2. In other words, if $J - J_0$ is compact and $\bar{A}_0(J) \neq \underline{A}_0(J)$, then $Z(J) = \infty$.

3. Similarly, if $J - J_0$ is compact and $\mathcal{E}_0(J) < \infty$, then the limit exists and is finite or $+\infty$.

Proof. If $Z(J) < \infty$ and $\bar{A}_0(J) > -\infty$, then by Theorem 3.14(b), all four conditions hold, and so by (e), the limit exists. On the other hand, if $\bar{A}_0(J) = -\infty$, then $\bar{A}_0(J) = \underline{A}_0(J) = -\infty$. □

Corollary 3.16. *If* $J - J_0$ *is trace class, then* $Z(J) < \infty$, $\mathcal{E}_0(J) < \infty$, *and the sum rules* (3.60) *and* (3.64) *hold.*

Remark. This is a result of Killip-Simon [13]. Our proof that $Z(J) < \infty$ is essentially the same as theirs, but our proof of the sum rules is much easier.

Proof. Since $J - J_0$ is trace class, it is compact. Clearly, $\bar{A}_0(J) = \underline{A}_0(J)$, and is neither ∞ nor $-\infty$ since $a_j > 0$ and $\sum |a_j - 1| < \infty$ imply $\sum |\ln(a_j)| < \infty$. By Theorem 2.3 and (3.57), $\mathcal{E}_0(J) < \infty$. The sum rules then hold by (a), (e), and (h) of Theorem 3.14. □

The following result is a "one-sided" analogue of (a)-(d) of Theorem 3.14 for $J - J_0$ Hilbert-Schmidt:

Theorem 3.17. *Suppose $J - J_0$ is Hilbert-Schmidt. Then*
(i) $\underline{A}_1^{\pm}(J) < \infty$ *and* $\mathcal{E}_1^{\pm}(J) < \infty$ *implies* $Z_1^{\pm}(J) < \infty$,
(ii) $\bar{A}_1^{\pm}(J) > -\infty$ *and* $Z_1^{\pm}(J) < \infty$ *implies* $\mathcal{E}_1^{\pm}(J) < \infty$,
(iii) $Z_1^{\pm}(J) < \infty$ *implies* $\bar{A}_1^{\pm}(J) < \infty$,
(iv) $\mathcal{E}_1^{\pm}(J) < \infty$ *implies* $\underline{A}_1^{\pm}(J) > -\infty$.

Remarks. 1. Each of (i)–(iv) is intended as two statements.

2. In Section 3.5, we will explore (iii), which is the most striking of these results since its contrapositive gives very general conditions under which the Szegő condition fails.

3. The Hilbert-Schmidt condition in (i) and (iv) can be replaced by the somewhat weaker condition

$$\sum_{j,\pm} (|E_j^{\pm}| - 2)^{3/2} < \infty. \tag{3.65}$$

That is true for (ii) and (iii) also, but by (3.66) below, (3.65) plus $Z_1^{\pm}(J) < \infty$ implies $J - J_0$ is Hilbert-Schmidt.

Theorem 3.18. *Let J be a BW matrix. Then the Z_2^- sum rule holds:*

$$Z_2^-(J) + \mathcal{E}_2(J) = A_2(J). \tag{3.66}$$

Remarks. 1. This is, of course, the P_2 sum rule of Killip-Simon [13]. Our proof that $Z_2^-(J) + \mathcal{E}_2(J) \leq A_2(J)$ is identical to that in [13], but our proof of the opposite inequality is somewhat streamlined.

2. As in [13], the values $+\infty$ are allowed in (3.66).

Proof of Theorem 3.14. We let J_n and $J^{(n)}$ be as in (2.18) and (2.20). Then (3.47) for J_n (noting $(J_n)^{(n)} = J_0$ and $Z(J_0) = 0$) reads

$$Z(J_n) = -\sum_{j=1}^{n} \ln(a_j) + \sum_{j,\pm} \ln|\beta_j^{\pm}(J_n)|. \tag{3.67}$$

Lemma 2.7 implies that the eigenvalue sum converges to $\mathcal{E}_0(J)$ if $J - J_0$ is compact. More generally, the sum is bounded above by $\mathcal{E}_0(J) + c_0$ where $c_0 \equiv 0$ if $J - J_0$ is compact and

$$c_0 \equiv \ln|\beta_1^+(J) + 2| + \ln|\beta_1^-(J) - 2| \tag{3.68}$$

otherwise. Moreover, by Theorem 2.13, $Z(J) \leq \liminf Z(J_n)$. Thus we have

$$Z(J) \leq \underline{A}_0(J) + \mathcal{E}_0(J) + c_0. \tag{3.69}$$

Thus far, the proof is directly from [13]. On the other hand, by (3.37), we have

$$Z(J) \geq \bar{A}_0(J) + \liminf_{n\to\infty} X_0^{(n)}(J) + \liminf_{n\to\infty} Z(J^{(n)}). \tag{3.70}$$

By Lemma 2.8, $\lim X_0^{(n)}(J) = \mathcal{E}_0(J)$. Moreover, by Theorem 2.13, $Z(J^{(n)}) \geq -\frac{1}{2}\ln(2)$, and if $J - J_0$ is compact, that is, $J^{(n)} \to J_0$, then $0 = Z(J_0) \leq \liminf Z(J^{(n)})$. Therefore, (3.70) implies that

$$Z(J) \geq \bar{A}_0(J) + \mathcal{E}_0(J) - c \tag{3.71}$$

where

$$c \equiv 0 \text{ if } J - J_0 \text{ is compact}, \qquad c \equiv \tfrac{1}{2}\ln(2) \text{ in general}.$$

With these preliminaries out of the way the rest of the proof is straightforward:

<u>Proof of (d).</u> (iv) and (3.69) imply that

$$\bar{A}_0(J) \geq \underline{A}_0(J) \geq Z(J) - \mathcal{E}_0(J) - c_0 > -\infty. \tag{3.72}$$

Proof of (a). (3.69) shows $Z(J) < \infty$, and (d) shows that (i) holds.

Proof of (c). By (3.71) and $\mathcal{E}_0(J) \geq 0$,

$$Z(J) \geq \bar{A}_0(J) - c,$$

so $Z(J) < \infty$ implies $\bar{A}_0(J) < \infty$.

Proof of (b). Since $\bar{A}_0(J) > -\infty$ and $c < \infty$, (3.71) plus $Z(J) < \infty$ implies $\mathcal{E}_0(J) < \infty$. Clearly, (c) shows that (ii) holds.

Note that (iii), (iv), and (3.71) imply that

$$\underline{A}_0(J) \leq \bar{A}_0(J) \leq Z(J) - \mathcal{E}_0(J) + \tfrac{1}{2}\ln(2) < \infty. \tag{3.73}$$

Thus we have shown more than merely (iii) + (iv) $\Rightarrow$ (i) + (ii), namely, (iii) + (iv) imply by (3.72) and (3.73)

$$-\infty < \bar{A}_0(J) \leq \underline{A}_0(J) + \tfrac{1}{2}\ln(2) + c_0 < \infty.$$

With c_0 as in (3.68). We can say more if $J - J_0$ is compact:

Proof of (e). (3.73) is now replaced by

$$\underline{A}_0(J) \leq \bar{A}_0(J) \leq Z(J) - \mathcal{E}_0(J)$$

since we can take $c = 0$ in (3.71). This plus (3.72) with $c_0 = 0$ implies $\bar{A}_0(J) = \underline{A}_0(J)$ and (3.60).

Proof of (f), (g), (h). We have the sum rules (3.37), (3.38). By Theorem 2.13, $Z_\ell^{\pm}(J) = Z(J) \mp \frac{1}{2}Y_\ell(J)$ is lower semi-continous in J. Since $\|J^{(n)} - J_0\| \to 0$, we have

$$\liminf_{n\to\infty} \left[Z(J^{(n)}) \mp \tfrac{1}{2}Y_\ell(J^{(n)})\right] \geq Z_\ell^{\mp}(J_0) = 0. \tag{3.74}$$

On the other hand, since $Z(J^{(n)}) < \infty$ and $\mathcal{E}_0(J^{(n)}) \leq \mathcal{E}_0(J) < \infty$, $J^{(n)}$ obeys the sum rule (3.60). Since $-\sum_{j=1}^n \ln(a_j)$ converges conditionally,

$$\lim_{n\to\infty} A_0(J^{(n)}) = \lim_{n\to\infty}\biggl(-\sum_{j=n}^\infty \ln(a_j)\biggr) = 0.$$

Moreover, $\mathcal{E}_0(J^{(n)}) \to 0$ by Lemma 2.8 and by the fact that $\mathcal{E}_0(J) < \infty$, and we conclude that $Z(J^{(n)}) \to 0$. Thus (3.74) becomes

$$\limsup_{n\to\infty} Y_\ell(J^{(n)}) \leq 0, \qquad \liminf_{n\to\infty} Y_\ell(J^{(n)}) \geq 0,$$

or

$$\lim_{n\to\infty} Y_\ell(J^{(n)}) = 0. \tag{3.75}$$

By Lemma 2.8, $\lim_n X_\ell^{(n)}(J) = X_\ell^{(\infty)}(J)$, with $X_\ell^{(\infty)}(J)$ from (3.61). Since $\mathcal{E}_0(J) < \infty$ implies $\sum_{j,\pm}(|\beta_j^\pm| - 1) < \infty$, we have that the sum defining $X_\ell^{(\infty)}(J)$ is absolutely convergent. This proves (f).

By this fact, (3.38), and (3.75), $\lim_n \zeta_\ell^{(n)}(J)$ exists, is finite, and obeys the sum rule

$$Y_\ell(J) = \lim_{n\to\infty} \zeta_\ell^{(n)}(J) + X_\ell^{(\infty)}(J).$$

Hence (h) will follow from (g), and we are left with showing (3.63). But by (3.27), the existence of $\lim_n \zeta_\ell^{(n)}(J)$ is precisely the existence of the conditional trace of $B_\ell(J)$, and they are equal. Indeed, if $m > 2\ell + n$, then for $k \geq \ell$,

$$\begin{aligned}\bigl(T_\ell(\tfrac12 J_{m-n;F}^{(n)})\bigr)_{k,k} &= \bigl(T_\ell(\tfrac12 J_{m;F})\bigr)_{k+n,k+n}, \\ \bigl(T_\ell(\tfrac12 J_0)\bigr)_{k,k} &= 0\end{aligned}$$

by the argument in the proof of Lemma 3.29 below, and for $k < \ell$,

$$\bigl(T_\ell(\tfrac12 J_{m-n;F}^{(n)})\bigr)_{k,k} \to \bigl(T_\ell(\tfrac12 J_0)\bigr)_{k,k}$$

as $n \to \infty$ (and $m > 2\ell + n$) by compactness of $J - J_0$. This proves (3.63). $\square$

Proof of Theorem 3.18. By (2.47), $Z_2^-(J^{(n)}) \geq 0$ for all $J^{(n)}$. Thus, following the proofs of (3.69) and (3.71), but using (3.50) in place of (3.47),

$$Z_2^-(J) + \mathcal{E}_2(J) \leq A_2(J)$$

and

$$Z_2^-(J) + \mathcal{E}_2(J) \geq A_2(J),$$

which yields the Z_2^- sum rule (3.66). In the above, we use the fact that in place of $Z(J) \geq -\frac{1}{2}\ln(2)$ one has $Z_2^-(J) \geq 0$ (and so $c = 0$), and the fact that $A_2(J) < \infty$ implies $J - J_0$ is compact (and so always $A_2(J) + c_0 = A_2(J)$). □

Proof of Theorem 3.17. Let $\xi^{\pm}(E)$ be as in (3.44) and consider $g(\beta) \equiv \xi^-(E)$ in the region $\beta \geq 1$. Then

$$g'(\beta) = \beta^{-1} - \tfrac{1}{2} - \tfrac{1}{2}\beta^{-2} = -\tfrac{1}{2}\beta^{-2}(\beta - 1)^2,$$

so g is analytic near $\beta = 1$ and $g(1) = g'(1) = g''(1) = 0$, that is, $g(\beta) = O((\beta - 1)^3)$. On the other hand, $\xi^+(E) = g(\beta) + \beta - \beta^{-1} = \beta - \beta^{-1} + O((\beta - 1)^3)$. Since $\beta + \beta^{-1} = E$ means $\beta - \beta^{-1} = \sqrt{E^2 - 4} = 2\sqrt{E - 2} + O(|E - 2|^{3/2})$ and $\beta - 1 = O(\sqrt{E - 2})$, we conclude that

$$E > 2 \Rightarrow \begin{cases} \xi^-(E) = O(|E - 2|^{3/2}), \\ \xi^+(E) = 2\sqrt{|E| - 2} + O(|E - 2|^{3/2}), \end{cases} \tag{3.76}$$

while in the same way

$$E < -2 \Rightarrow \begin{cases} \xi^-(E) = 2\sqrt{|E| - 2} + O(|E + 2|^{3/2}), \\ \xi^+(E) = O(|E + 2|^{3/2}). \end{cases} \tag{3.77}$$

It follows that

$$\sum_{j,\pm} \xi^+\big(E_j^\pm\big) = 2\mathcal{E}_1^+(J) + O(\|J-J_0\|_2),$$
$$\sum_{j,\pm} \xi^-\big(E_j^\pm\big) = 2\mathcal{E}_1^-(J) + O(\|J-J_0\|_2),$$

since Theorem 2.3 implies $\sum_{j,\pm}(|E_j^\pm|-2)^{3/2} \le c_{3/2}\|J-J_0\|_2$. Thus for some $c<\infty$ we have

$$Z_1^\pm(J) \le \underline{A}_1^\pm(J) + 2\mathcal{E}_1^\pm(J) + c\|J-J_0\|_2 \tag{3.78}$$

by writing the sum rule (3.48)/(3.49) for J_n (with $Z_1^\pm((J_n)^{(n)})=0$), taking limits, and using Lemma 2.7 and $Z_1^\pm(J) \le \liminf Z_1^\pm(J_n)$. Theorem 2.13 says $Z_1^\pm(J^{(n)}) \ge -\kappa$, and so by (3.48)/(3.49) and Lemma 2.8,

$$Z_1^\pm(J) \ge \bar{A}_1^\pm(J) + 2\mathcal{E}_1^\pm(J) - c\|J-J_0\|_2 - \kappa. \tag{3.79}$$

With these preliminaries, the proof is straightforward:

Proof of (i), (iv). Immediate from (3.78) and $Z_1^\pm(J) \ge -\kappa$.

Proof of (ii), (iii). Immediate from (3.79) and $\mathcal{E}_1^\pm(J) \ge 0$. □

Remark. (i)–(iv) of Theorem 3.17 are exactly (a)–(d) of Theorem 3.14 for the $Z_1^\pm$ sum rules. One therefore expects a version of (e) of that theorem to hold as well. Indeed, a modification of the above proof yields for $J-J_0$ Hilbert-Schmidt that if $\mathcal{E}_1^+(J)$, $Z_1^+(J)$, $\bar{A}_1^+(J)$ are finite, then

$$Z_1^+(J) = -\sum_{n=1}^\infty \big[\ln(a_n) + \tfrac{1}{2}b_n\big] + \sum_{j,\pm}\big[\ln|\beta_j^\pm| + \tfrac{1}{2}(\beta_j^\pm - (\beta_j^\pm)^{-1})\big],$$

and if $\mathcal{E}_1^-(J)$, $Z_1^-(J)$, $\bar{A}_1^-(J)$ are finite, then

$$Z_1^-(J) = -\sum_{n=1}^\infty \big[\ln(a_n) - \tfrac{1}{2}b_n\big] + \sum_{j,\pm}\big[\ln|\beta_j^\pm| - \tfrac{1}{2}(\beta_j^\pm - (\beta_j^\pm)^{-1})\big].$$

3.4 Shohat's Theorem with an Eigenvalue Estimate

Shohat [28] translated Szegő's theory from the unit circle to the real line and was able to identify all Jacobi matrices which lead to measures with no mass points outside $[-2, 2]$ and have $Z(J) < \infty$. The strongest result of this type, so far, is the following theorem from Killip-Simon [13, Theorem 4′] (the methods of Nevai [18] can prove the same result):

Theorem 3.19. *Consider the statements*

(i) $\underline{A}_0(J) < \infty$,

(ii) $Z(J) < \infty$,

(iii) $\sum_{n=1}^{\infty} \left[(a_n - 1)^2 + b_n^2\right] < \infty$,

(iv) $\underline{A}_0(J) = \bar{A}_0(J)$ *and is finite,*

(v) $\lim_{N\to\infty} \sum_{n=1}^{N} b_n$ *exists and is finite.*

If $\sigma(J) \subseteq [-2, 2]$, *then we have*

$$\text{(i)} \Longleftrightarrow \text{(ii)},$$

and either one implies (iii), (iv), *and* (v).

We can prove the following extension of this result ($\equiv$ Theorem 1.2):

Theorem 3.20. *Theorem 3.19 remains true if the assumption* $\sigma(J) \subseteq [-2, 2]$ *is replaced by* $\sigma_{\text{ess}}(J) \subseteq [-2, 2]$ *and* $\mathcal{E}_0(J) < \infty$.

Remarks. 1. Gončar [11], Nevai [18], and Nikishin [21] extended Shohat-type theorems to allow finitely many bound states outside $[-2, 2]$.

2. Peherstorfer-Yuditskii [22] recently proved that (ii) and $\mathcal{E}_0(J) < \infty$ implies (iv) and additional results on polynomial asymptotics.

Proof. Let us first suppose that $\sigma_{\text{ess}}(J) = [-2, 2]$, so that J is a BW matrix. By Theorem 3.14(a), (i) of this theorem plus $\mathcal{E}_0(J) < \infty$ implies (ii) of this theorem. By Theorem 3.14(c), (ii) of this theorem implies (i) of this theorem.

If either holds, then (iv) follows from (e) of Theorem 3.14 and (v) from the $\ell = 1$ case of (g) of Theorem 3.14. Finally, (iii) follows from Theorem 3.18 if we note that $\mathcal{E}_0(J) < \infty$ implies $\mathcal{E}_2(J) < \infty$, that $Z(J) < \infty$ implies $Z_2^-(J) < \infty$, and that $G(a) = O((a-1)^2)$.

If we only have a priori that $\sigma_{\mathrm{ess}}(J) \subseteq [-2,2]$, we proceed as follows. If $Z(J) < \infty$, then $\sigma_{\mathrm{ac}}(J) \supseteq [-2,2]$, so in fact $\sigma_{\mathrm{ess}}(J) = [-2,2]$. If $\underline{A}_0(J) < \infty$, we look closely at the proof of Theorem 3.14(a). Inequality (3.69) does not require $\sigma_{\mathrm{ess}}(J) = [-2,2]$, but only that $\sigma_{\mathrm{ess}}(J) \subseteq [-2,2]$. Thus, $\underline{A}_0(J) < \infty$ implies $Z(J) < \infty$ if $\mathcal{E}_0(J) < \infty$. $\square$

There is an interesting way of rephrasing this. Let γ_n be the leading coefficient of the orthogonal polynomial P_n. Then by (2.7),

$$\gamma_n = (a_1 a_2 \dots a_n)^{-1}. \tag{3.80}$$

Thus

$$\underline{A}_0(J) = \liminf_{n\to\infty} \ln(\gamma_n) \tag{3.81}$$

and

$$\bar{A}_0(J) = \limsup_{n\to\infty} \ln(\gamma_n). \tag{3.82}$$

Corollary 3.21. *Suppose $\sigma_{\mathrm{ess}}(J) \subseteq [-2,2]$ and $\mathcal{E}_0(J) < \infty$. Then $Z(J) < \infty$ (i.e., the Szegő condition holds) if and only if γ_n is bounded from above (and in that case, it is also bounded away from 0; indeed, $\lim_{n\to\infty} \gamma_n$ exists and is in $(0,\infty)$).*

Remark. Actually, $\limsup \gamma_n < \infty$ is not needed; $\liminf \gamma_n < \infty$ is enough.

Proof. By (3.81), γ_n bounded above implies $\underline{A}_0(J) < \infty$, and thus $Z(J) < \infty$. Conversely, $Z(J) < \infty$ implies $-\infty < \underline{A}_0(J) = \bar{A}_0(J) < \infty$. So by (3.80), it implies γ_n is bounded above and below. $\square$

In the case of orthogonal polynomials on the unit circle, Szegő's theorem says $Z < \infty$ if and only if κ_n is bounded if and only if $\sum_{j=1}^\infty |\alpha_j|^2 < \infty$, where κ_n is the leading coefficient of the orthogonal polynomial φ_n, and α_j are the Verblunsky (a.k.a. Geronimus, a.k.a. reflection) coefficients. In the real line case, if one drops the a priori requirement that $\mathcal{E}_0(J) < \infty$, it can happen that γ_n is bounded but $Z(J) = \infty$. For example, if $a_n \equiv 1$ and $b_n = n^{-1}$, then $Z(J)$ cannot be finite. For, as $J - J_0$ is Hilbert-Schmidt, Theorem 3.17(iii) is applicable and $\bar{A}_1^-(J) = \infty$ implies $Z(J) = \infty$.

But the other direction always holds:

Theorem 3.22. *Let J be a BW matrix with $Z(J) < \infty$ (i.e., the Szegő condition holds). Then γ_n is bounded. Moreover, if $J - J_0$ is compact, then $\lim_{n\to\infty} \gamma_n$ exists.*

Remarks. 1. The examples of the next section show that $Z(J) < \infty$ is consistent with $\lim \gamma_n = 0$.

2. This result — even without a compactness hypothesis — is known. For γ_n is monotone decreasing in the measure (see, e.g., Nevai [19]) and so one can reduce this to the case $\sigma(J) \subseteq [-2, 2]$.

Proof. By Theorem 3.14(c), $Z(J) < \infty$ implies $\bar{A}_0(J) < \infty$ which, by (3.82), implies γ_n is bounded. If $J - J_0$ is compact, then Corollary 3.15 implies that $\lim \gamma_n = \exp(\lim -\sum_{j=1}^n \ln(a_j))$ exists but can be zero. □

Here is another interesting application of Theorem 3.20:

Theorem 3.23. *Suppose $b_n \geq 0$ and*

$$\sum_{n=1}^{\infty} |a_n - 1| < \infty. \tag{3.83}$$

Then $\mathcal{E}_0(J) < \infty$ if and only if $\sum_{n=1}^\infty b_n < \infty$.

Proof. If $\sum_{n=1}^\infty b_n < \infty$, then $\mathcal{E}_0(J) < \infty$ by (3.83) and Theorem 2.3. On the other hand, if $\mathcal{E}_0(J) < \infty$, (3.83) implies $\underline{A}_0(J) < \infty$, so by Theorem 3.20, $\sum_{n=1}^N b_n$ is convergent. Since $b_n \geq 0$, $\sum_{n=1}^\infty b_n < \infty$. □

3.5 Necessary Conditions for $Z(J) < \infty$

One necessary condition for the Szegő condition to hold is Corollary 3.15. In this section we will provide others. These will yield one part of Askey's conjecture.

Theorem 3.24. *Suppose*

$$\sum_{n=1}^{\infty} \left[(a_n - 1)^2 + b_n^2\right] < \infty, \tag{3.84}$$

and

$$\limsup_{N\to\infty} \left(-\sum_{n=1}^{N} \left(a_n - 1 \pm \tfrac{1}{2} b_n\right) \right) = \infty \tag{3.85}$$

for either plus or minus. Then the Szegő condition fails at ± 2.

Remark. This proves Theorem 1.3.

Proof. (3.85) implies that $\bar{A}_1^{\pm}(J) = \infty$, so by Theorem 3.17(iii), $Z_1^{\pm}(J) = \infty$. □

Here is a related result:

Theorem 3.25. *Let* J *be a BW matrix. If*

$$\limsup_{N\to\infty} \left(-\sum_{n=1}^{N} \left[\ln(a_n) + p\, b_n\right] \right) = \infty \tag{3.86}$$

for some $|p| < \frac{1}{2}$, *then the Szegő condition fails.*

Remark. If (3.84) holds, assumption (3.86) is slightly stronger than (3.85), but we do not need (3.84) here. This also shows why $\ln(a_n)$ replaces $a_n - 1$ in (3.86).

Proof. Note that one can prove a step-by-step sum rule and a version of Theorem 3.14 for the weight $w_p(\theta) \equiv 1 + 2p\cos\theta$ just as we did it for the weight $w_0(\theta) = 1$. Here $Z(J)$ is replaced by the Szegő-type integral with the weight $w_p(\theta)$, $\bar{A}_0(J)$ by the lim sup in (3.86), and $\mathcal{E}_0(J)$ by $\sum_{j,\pm} \xi_p(E_j^{\pm})$, where

$$\xi_p(E) \equiv \left(\tfrac{1}{2} + p\right)\xi^+(E) + \left(\tfrac{1}{2} - p\right)\xi^-(E).$$

We have $\xi_p(E) \sim (1+2p)\sqrt{|E|-2}$ if $E \sim 2$ and $\xi_p(E) \sim (1-2p)\sqrt{|E|-2}$ if $E \sim -2$ (see (3.76) and (3.77)). In particular, $|2p| < 1$ gives $\sum_{j,\pm} \xi_p(E_j^\pm) > -\infty$. It follows that (c) of this modified Theorem 3.14 holds. This, (3.86), and $0 \le w_p(\theta) \le 2$ imply $Z(J) = \infty$. □

These considerations yield another interesting result:

Theorem 3.26. *Let* $|p| < \frac{1}{2}$ *and* $|q| < \frac{1}{2}$.

(i) *If*

$$\limsup_{N\to\infty}\biggl(-\sum_{n=1}^{N}\bigl[\ln(a_n) + p\,b_n\bigr]\biggr) > -\infty \tag{3.87}$$

and

$$\liminf_{N\to\infty}\biggl(-\sum_{n=1}^{N}\bigl[\ln(a_n) + q\,b_n\bigr]\biggr) = -\infty, \tag{3.88}$$

then $Z(J) = \infty$.

(ii) *If*

$$\limsup_{N\to\infty}\biggl(-\sum_{n=1}^{N}\bigl[\ln(a_n) + p\,b_n\bigr]\biggr) = \infty$$

and

$$\liminf_{N\to\infty}\biggl(-\sum_{n=1}^{N}\bigl[\ln(a_n) + q\,b_n\bigr]\biggr) < \infty,$$

then $\mathcal{E}_0(J) = \infty$.

Remark. In particular, if $a_n \equiv 1$, $b_n \ge 0$, and $\sum_{n=1}^\infty b_n = \infty$, we have $Z(J) = \infty$ and $\mathcal{E}_0(J) = \infty$. On the other hand, if instead $\sum_{n=1}^\infty b_n < \infty$, then $Z(J) < \infty$ and $\mathcal{E}_0(J) < \infty$ by Theorems 3.23 and 3.14(a).

Proof. Consider Theorem 3.14 for the weight w_p and its corresponding Szegő-type integral in place of $Z(J)$. Since w_p is bounded away from 0 and ∞, the integral is finite if only if $Z(J) < \infty$. By the computed asymptotics of $\xi_p(E)$ at ± 2, the corresponding $\mathcal{E}$-sum is finite if and only if $\sum_{j,\pm} \sqrt{|E_j^\pm| - 2} < \infty$, which holds if and only if $\mathcal{E}_0(J) < \infty$. The same is true for the weight w_q.

If $Z(J) < \infty$, then by using (b) of Theorem 3.14 for w_p and (3.87), one obtains $\mathcal{E}_0(J) < \infty$. But then (d) of Theorem 3.14 for w_q contradicts (3.88). This proves (i).

The proof of (ii) is similar, using (a) and (c) of this modified Theorem 3.14. □

Corollary 3.27. *If*

$$a_n \equiv 1 + \frac{\alpha}{n} + e_a(n), \qquad\qquad b_n \equiv \frac{\beta}{n} + e_b(n)$$

with

$$\lim_{n\to\infty} n\big(|e_a(n)| + |e_b(n)|\big) = 0 \tag{3.89}$$

and $2\alpha \pm \beta < 0$*, then the Szegő condition fails at* ± 2*.*

Remarks. 1. This is intended as separate results for $+$ and for $-$.

2. All we need is

$$\lim_{n\to\infty} (\ln N)^{-1} \sum_{n=1}^{N} \big(|e_a(n)| + |e_b(n)|\big) = 0$$

instead of (3.89). In particular, trace class errors can be accommodated.

3. This settles the $2\alpha < |\beta|$ case of Askey's conjecture. The complementary region $2\alpha \geq |\beta|$ will be treated in the next chapter.

Proof. We use Theorem 3.24. If (3.89) holds, then

$$\sum_{n=1}^{N} \big(a_n - 1 \pm \tfrac{1}{2} b_n\big) = (\alpha \pm \tfrac{1}{2}\beta) \ln N + o(\ln N),$$

so (3.85) holds if $2\alpha \pm \beta < 0$. □

We can use these examples to illustrate the limits of Theorem 3.14:

(1) If $a_n = 1$, $b_n = \frac{1}{n}$, then $Z(J) = \infty$ (by Corollary 3.27) while $\bar{A}_0(J) = \underline{A}_0(J) < \infty$. Thus $\mathcal{E}_0(J) = \infty$.

(2) If $a_n = 1 - \frac{1}{n}$, $b_n = 0$, then $Z(J) = \infty$ (by Corollary 3.27) and $\bar{A}_0(J) = \underline{A}_0(J) = \infty$, but $\mathcal{E}_0(J) < \infty$ since J has no spectrum outside $[-2, 2]$.

(3) If $a_n = 1 + \frac{1}{n}$, $b_n = 0$, then $Z(J) < \infty$ (by Theorem 1.4, proved in Section 4.3) while $\bar{A}_0(J) = \underline{A}_0(J) = -\infty$. Thus $\mathcal{E}_0(J) = \infty$.

Finally, we note that Nevai's result that $a_n = 1 + (-1)^n\alpha/n + O(n^{-2})$ and $b_n = (-1)^n\beta/n + O(n^{-2})$ implies $Z(J) < \infty$ ([17]; see also [4]) shows that we can have $Z(J) < \infty$, $\mathcal{E}_0(J) < \infty$, and have the sums $\sum a_n$ and/or $\sum b_n$ be only conditionally and not absolutely convergent.

3.6 Appendix to Chapter 3

In this appendix we collect auxiliary results which we have used in the present chapter. The first result are *Jensen's formulae* for Taylor coefficients of logarithms of functions meromorphic in a neighborhood of $\bar{\mathbb{D}}$ (see, e.g., [13, Proposition 3.1]).

Lemma 3.28. *Let f be a function meromorphic in a neighborhood of $\bar{\mathbb{D}}$ with $f(0) \neq 0$ and*

$$\ln\left(\frac{f(z)}{f(0)}\right) = \sum_{\ell=1}^{\infty} \alpha_\ell z^\ell \tag{3.90}$$

for small $|z|$. If z_j are the zeros of f inside $\mathbb{D}$ and p_j the poles, then

$$\ln|f(0)| = \frac{1}{2\pi}\int_0^{2\pi} \ln|f(e^{i\theta})|d\theta + \sum_j \ln|z_j| - \sum_j \ln|p_j| \tag{3.91}$$

and

$$\mathrm{Re}(\alpha_\ell) = \frac{1}{\pi}\int_0^{2\pi} \ln|f(e^{i\theta})|\cos(\ell\theta)d\theta - \mathrm{Re}\sum_j \frac{z_j^{-\ell} - \bar{z}_j^{\ell}}{\ell} + \mathrm{Re}\sum_j \frac{p_j^{-\ell} - \bar{p}_j^{\ell}}{\ell}. \tag{3.92}$$

The next three lemmas are from [13]. The last of them, Lemma 3.31, computes the Taylor coefficients of $\ln(M(z)/z)$ using a method independent of Lemma 3.28. Our proof of higher order sum rules (3.36) rests on equating the outputs of these two lemmas.

Recall that the upper left-hand corner of a matrix A is $A_{0,0}$.

Lemma 3.29. *Let T_ℓ be as in* (2.10) *and let $n \geq \ell \geq 1$. Then*

$$\mathrm{Tr}\big[T_\ell(\tfrac{1}{2}J_{0,n;F})\big] = -\tfrac{1}{2}\big(1 + (-1)^\ell\big). \tag{3.93}$$

If ℓ is odd then both $T_\ell(\frac{1}{2}J_{0,n;F})$ and $T_\ell(\frac{1}{2}J_0)$ vanish on-diagonal. If ℓ is even, then $(T_\ell(\frac{1}{2}J_0))_{k,k} = 0$ for $k \geq \frac{\ell}{2}$, and

$$\big(T_\ell(\tfrac{1}{2}J_{0,n;F})\big)_{k,k} = \begin{cases} \big(T_\ell(\tfrac{1}{2}J_0)\big)_{k,k} & \text{if } 0 \leq k \leq \frac{\ell}{2}-1, \\ \big(T_\ell(\tfrac{1}{2}J_0)\big)_{n-1-k,n-1-k} & \text{if } n-\frac{\ell}{2} \leq k \leq n-1, \\ 0 & \text{otherwise.} \end{cases} \tag{3.94}$$

In particular, the sum of the diagonal elements of $T_\ell(\frac{1}{2}J_0)$ is $-\frac{1}{4}(1+(-1)^\ell)$.

Remark. The picture we are establishing for even ℓ is the following. If J_0 were a doubly infinite matrix with 0's and 1's (acting on $\ell^2(\mathbb{Z})$), then $T_\ell(\frac{1}{2}J_0)$ would vanish on-diagonal. Since J_0 has one end, this will affect the first $\frac{\ell}{2}$ diagonal terms. And, of course, $J_{0,n;F}$ has two ends.

Proof. First notice that by (2.19), the Chebyshev polynomial of the second kind $U_n(\frac{x}{2})$ from (2.11) is a multiple of the characteristic polynomial of $J_{0,n;F}$. This means that its zeros $y_j \equiv 2\cos(\frac{j\pi}{n+1})$ ($j = 1,\dots,n$) are the eigenvalues of $J_{0,n;F}$. By (2.10), $T_\ell(\frac{1}{2}y_j) = \cos(\frac{\ell j\pi}{n+1})$, and so

$$\operatorname{Tr}\big[T_\ell(\tfrac{1}{2}J_{0,n;F})\big] = \sum_{j=1}^{n} \cos(\tfrac{\ell j\pi}{n+1}) = -\tfrac{1}{2} - \tfrac{1}{2}(-1)^\ell + \tfrac{1}{2}\sum_{j=-n}^{n+1} \exp(i\tfrac{\ell j\pi}{n+1}).$$

The last sum is 0 because ℓ is not a multiple of $2(n+1)$. This proves (3.93).

Assume ℓ is odd. By (2.9) and induction, T_ℓ contains only odd powers of x. Since J_0 has non-zero terms only on places with odd sums of indices, J_0^m and $J_{0,n;F}^m$ vanish on-diagonal when m is odd. Hence so do $T_\ell(\frac{1}{2}J_0)$ and $T_\ell(\frac{1}{2}J_{0,n;F})$.

Now assume ℓ is even and consider J_0 and $J_{0,n;F}$ extended to act on $\ell^2(\mathbb{Z})$ by adding only zeros (so they become doubly infinite matrices). Notice that if A is a tridiagonal matrix, then $(A^m)_{k,j}$ only depends on elements of A with distance at most $m-1$ from the position (k,j) (in the metric $|k_1-k_2|+|j_1-j_2|$). This means that

$$\big(T_\ell(\tfrac{1}{2}J_{0,n;F})\big)_{k,k} = \big(T_\ell(\tfrac{1}{2}J_0)\big)_{k,k}$$

for $k < n - \frac{\ell}{2}$. But it also means that if $\ell \le n-1$, then

$$\mathrm{Tr}\big[T_\ell(\tfrac{1}{2}J_{0,n;F})\big] - \mathrm{Tr}\big[T_\ell(\tfrac{1}{2}J_{0,n-1;F})\big] = \big(T_\ell(\tfrac{1}{2}J_{0,n;F})\big)_{k,k}$$

for any $k \in [\frac{\ell}{2}, n-1-\frac{\ell}{2}]$. Hence, by (3.93) for n and $n-1$, this element must be 0 for any such k. Since each $J^m_{0,n;F}$ must have a symmetric diagonal, (3.94) follows. $\square$

Lemma 3.30. *For any fixed $\lambda \in \mathbb{R}$ and small z,*

$$\ln\left(1 - \frac{\lambda}{z+z^{-1}}\right) = \sum_{\ell=1}^{\infty} \tfrac{2}{\ell}\big[T_\ell(0) - T_\ell(\tfrac{1}{2}\lambda)\big] z^\ell. \tag{3.95}$$

Proof. We use the generating function

$$g(x,z) \equiv \sum_{\ell=1}^{\infty} T_\ell(x)\frac{z^\ell}{\ell} = -\tfrac{1}{2}\ln(1-2xz+z^2). \tag{3.96}$$

Hence, with $2x = \lambda$,

$$\ln\left(1 - \frac{2x}{z+z^{-1}}\right) = 2\big[g(0,z) - g(x,z)\big] = \sum_{\ell=1}^{\infty} \tfrac{2}{\ell}\big[T_\ell(0) - T_\ell(x)\big] z^\ell.$$

Eq. (3.96) is well known (see, e.g., [36, eq. (4.7.25)] or [13]) and can be proved as follows. First consider $x = \cos\theta \in (-1,1)$ and $|z| < 1$. Then

$$\begin{aligned}
\frac{\partial g}{\partial z}(\cos\theta, z) &= \frac{1}{z}\sum_{\ell=1}^{\infty}\cos(\ell\theta) z^\ell \\
&= \frac{1}{2z}\left(-2 + \sum_{\ell=0}^{\infty}\Big[\big(ze^{i\theta}\big)^\ell + \big(ze^{-i\theta}\big)^\ell\Big]\right) \\
&= \frac{1}{2z}\left(-2 + \frac{1}{1-ze^{i\theta}} + \frac{1}{1-ze^{-i\theta}}\right) \\
&= \frac{\cos\theta - z}{1 - 2z\cos\theta + z^2} \\
&= -\frac{1}{2}\frac{\partial}{\partial z}\ln(1 - 2z\cos\theta + z^2).
\end{aligned}$$

Since (3.96) obviously holds for $z = 0$, it holds for $|x| < 1$ and $|z| < 1$. The coefficient at z^ℓ of both sides of (3.96) is clearly an ℓ^{th} degree polynomial in x, so the polynomials must coincide and the equation holds for any fixed x and all small z. $\square$

Using this lemma, we will now compute the Taylor coefficients of $\ln(M(z)/z)$ in terms of J.

Lemma 3.31. *For $\ell \geq 1$,*

$$\zeta_\ell^{(1)}(J) \equiv \tfrac{2}{\ell} \lim_{m\to\infty} \Big[\mathrm{Tr}\Big(T_\ell\big(\tfrac{1}{2}J_{m;F}\big)\Big) - \mathrm{Tr}\Big(T_\ell\big(\tfrac{1}{2}J^{(1)}_{m-1;F}\big)\Big)\Big] \tag{3.97}$$

exists, and for small z,

$$\ln\left(\frac{M(z)}{z}\right) = \sum_{\ell=1}^{\infty} \zeta_\ell^{(1)}(J) z^\ell. \tag{3.98}$$

Proof. First notice that by the argument in the proof of Lemma 3.29, the difference of traces in (3.97) is constant once $m > \frac{\ell}{2}$, so $\zeta_\ell^{(1)}(J)$ exists.

If we consider $J_{m;F}$ as an operator on $\ell^2(\mathbb{Z}^+)$ (extended by zeros to a semi-infinite matrix), then $J_{m;F} \to J$ elementwise as $m \to \infty$. Hence the spectral measures of $J_{m;F}$ converge weakly to ν, and so do the M-functions (at any fixed $z \in \mathbb{D}$). We let $\zeta \equiv z + z^{-1}$, so that $z\zeta = 1 + z^2$. By (2.50), (2.58), and Cramer's rule,

$$f_m(z) \equiv \frac{M(z; J_{m;F})}{z} = \frac{1}{z}\frac{\det(\zeta - J^{(1)}_{m-1;F})}{\det(\zeta - J_{m;F})} = \frac{1}{1+z^2}\frac{\det(1 - \zeta^{-1}J^{(1)}_{m-1;F})}{\det(1 - \zeta^{-1}J_{m;F})},$$

where the last equality holds because the numerator matrix has order one less than the denominator matrix. By the above argument, for any $z \in \mathbb{D}$ we have

$$f_m(z) \to f(z) \equiv \frac{M(z;J)}{z}.$$

Next we notice that if λ_j are the eigenvalues of a matrix A, then $\ln\det(A) = \sum \ln(\lambda_j)$. Hence, by Lemma 3.30, with $K_\ell(x) \equiv \frac{2}{\ell}[T_\ell(0) - T_\ell(\frac{x}{2})]$ and $|z|$ small,

$$\ln f_m(z) = -\ln(1+z^2) + \sum_{\ell=1}^{\infty} \Big[\mathrm{Tr}\big(K_\ell(J^{(1)}_{m-1;F})\big) - \mathrm{Tr}\big(K_\ell(J_{m;F})\big)\Big] z^\ell$$

$$= -\ln(1+z^2) - \sum_{k=1}^{\infty} \frac{z^{2k}}{k}(-1)^k + \sum_{\ell=1}^{\infty} \frac{2}{\ell}\Big[\mathrm{Tr}\big(T_\ell(\tfrac{1}{2}J_{m;F})\big) - \mathrm{Tr}\big(T_\ell(J^{(1)}_{m-1;F})\big)\Big] z^\ell,$$

where the first sum appears because with $0_{n\times n}$ the zero $n \times n$ matrix,

$$\frac{2z^\ell}{\ell}\Big[\mathrm{Tr}\big(T_\ell\big(0_{(m-1)\times(m-1)}\big)\big) - \mathrm{Tr}\big(T_\ell\big(0_{m\times m}\big)\big)\Big] = \frac{2z^\ell}{\ell} T_\ell(0),$$

and $T_{2k+1}(0) = 0$ and $T_{2k}(0) = (-1)^k$ by (2.10). Since

$$\sum_{k=1}^{\infty} \frac{z^{2k}}{k}(-1)^k = -\ln(1+z^2),$$

the ℓ^{th} Taylor coefficient of $\ln f_m(z)$ converges to $\zeta_\ell^{(1)}(J)$ as $m \to \infty$. But $\ln f_m(z) \to \ln f(z)$ for all z in a neighborhood of 0, so $\zeta_\ell^{(1)}(J)$ must be the ℓ^{th} Taylor coefficient of $\ln f(z)$. □

Chapter 4

Szegő Jacobi Matrices

The contents of the first four sections of this chapter follow, often verbatim, the contents of [42] although, of course, we change numbering to be appropriate. Our goal is to derive sufficient conditions for $Z(J) < \infty$, which will yield the $2\alpha \geq |\beta|$ case of Askey's conjecture. We let $a_+ \equiv \max\{a, 0\}$ and $a_- \equiv \max\{-a, 0\}$. Our main result is

Theorem 4.1. *Let*

$$a_n \equiv c_n + O(n^{-1-\varepsilon}) \qquad b_n \equiv d_n + O(n^{-1-\varepsilon}) \tag{4.1}$$

for some $\varepsilon > 0$*, where* $c_n \geq 1 + \frac{|d_n|}{2}$ *for* $n > N$*,* $\lim_{n\to\infty} c_n = 1$ *and*

$$\sum_{n=1}^{\infty} n \left[c_{n+1}^2 - c_n^2 + \frac{c_{n+1}}{2}|d_{n+2} - d_{n+1}| + \frac{c_n}{2}|d_{n+1} - d_n| \right]_+ < \infty \tag{4.2}$$

Then the matrix J*, given by* (1.1)*, satisfies the Szegő condition.*

Remarks. 1. The notation $n > N$ means that $c_n \geq 1 + \frac{|d_n|}{2}$ is required for all but finitely many n.

2. Notice that the sum in (4.2) cannot be simplified. We cannot replace the last two terms by $c_n|d_{n+1} - d_n|$ because we take positive parts of the summands in (4.2).

3. In particular, one can take $c_n \equiv 1 + \alpha/n$ and $d_n \equiv \beta/n$ with $2\alpha \geq |\beta|$. This settles the $2\alpha \geq |\beta|$ case of Askey's conjecture.

We will prove this theorem in two steps. The first one is an extension of a result in [8], and shows that J is Szegő whenever a_n, b_n satisfy the conditions for c_n, d_n in Theorem 4.1.

The second step lets us add $O(n^{-1-\varepsilon})$ errors to such a_n, b_n. Our tools here are the sum rules, in particular, the step-by-step Z sum rule (3.47). By Corollary 3.12, the Szegő condition is stable under finite rank perturbations. We will be able to pass to certain infinite rank perturbations of J by representing them as limits of finite rank perturbations and using (2.48). To do this, we will need to control the change of the $E_j^{\pm}$'s under these perturbations, in order to estimate the eigenvalue sum in (3.47) (or, more precisely, in (4.22) below).

In Section 4.1 we prove an extension of the abovementioned result from [8]. Section 4.2 provides the desired control of movement of eigenvalues under perturbations. In Section 4.3 we use these tools to prove Theorem 4.1 and related results (including Theorem 1.4). In Section 4.4 we complete the picture outlined in Chapter 1 by providing sufficient conditions for $Z_1^{\pm}(J) < \infty$.

4.1 On an Argument of Dombrowski-Nevai

In this section we will improve a result of Dombrowski-Nevai [8]. We will closely follow their presentation and introduce an additional twist which will yield this improvement. The notation here is slightly different from [8] because their b_n's start with $n = 0$ and their "free" a_n's are $\frac{1}{2}$. We define

$$S_n(x) \equiv a_1^2 + \sum_{j=1}^{n} \Big[(a_{j+1}^2 - a_j^2)P_j^2(x) + a_j(b_{j+1} - b_j)P_j(x)P_{j-1}(x)\Big] \tag{4.3}$$

for $n \geq 0$. Notice that the S_n obey the obvious recurrence relation

$$S_n(x) = S_{n-1}(x) + (a_{n+1}^2 - a_n^2)P_n^2(x) + a_n(b_{n+1} - b_n)P_n(x)P_{n-1}(x). \tag{4.4}$$

Using this and (2.5), one proves by induction the following formula from [7]:

$$S_n(x) = a_{n+1}^2\left[P_{n+1}^2(x) - \frac{x-b_{n+1}}{a_{n+1}}P_{n+1}(x)P_n(x) + P_n^2(x)\right]. \tag{4.5}$$

The results in [8] are based on (4.4) and (4.5). Our simple but essential improvement is the introduction of a function closely related to S_n, but satisfying a recurrence relation which is more suitable for the purposes of this argument. We define

$$R_n(x) \equiv S_n(x) + \frac{a_{n+1}}{2}|b_{n+2} - b_{n+1}|P_n^2(x), \tag{4.6}$$

so that we have

$$\begin{aligned} R_n(x) = R_{n-1}(x) &+ (a_{n+1}^2 - a_n^2)P_n^2(x) + a_n(b_{n+1} - b_n)P_n(x)P_{n-1}(x) \\ &+ \frac{a_{n+1}}{2}|b_{n+2} - b_{n+1}|P_n^2(x) - \frac{a_n}{2}|b_{n+1} - b_n|P_{n-1}^2(x). \end{aligned}$$

The importance of this relation lies in the fact that it implies the crucial inequality

$$R_n(x) \le R_{n-1}(x) + \left[a_{n+1}^2 - a_n^2 + \frac{a_{n+1}}{2}|b_{n+2} - b_{n+1}| + \frac{a_n}{2}|b_{n+1} - b_n|\right]P_n^2(x) \tag{4.7}$$

by writing $|P_n(x)P_{n-1}(x)| \le \frac{1}{2}\big(P_n^2(x) + P_{n-1}^2(x)\big)$. Hence, our choice of R_n eliminated the unpleasant cross term in (4.4).

Now we are ready to apply the argument from [8], but to R_n in place of S_n. We define

$$\delta_n \equiv \left[a_{n+1}^2 - a_n^2 + \frac{a_{n+1}}{2}|b_{n+2} - b_{n+1}| + \frac{a_n}{2}|b_{n+1} - b_n|\right]_+. \tag{4.8}$$

Lemma 4.2. *If $a_n \ge 1 + \frac{|b_n|}{2}$ for $n > N$, then for $n > N$*

$$P_n^2(x) \le \frac{4}{4-x^2}R_{n-1}(x), \qquad |x| < 2, \tag{4.9}$$

$$\max_{|x|\le 2} P_n^2(x) \le (n+1)^2 \max_{|x|\le 2} R_{n-1}(x), \tag{4.10}$$

$$0 \le R_n(x) \le \exp\left(\frac{4\delta_n}{4-x^2}\right)R_{n-1}(x), \qquad |x| < 2, \tag{4.11}$$

$$\max_{|x|\leq 2} R_n(x) \leq e^{(n+1)^2\delta_n} \max_{|x|\leq 2} R_{n-1}(x). \tag{4.12}$$

Proof. From (4.5),

$$S_{n-1}(x) = a_n^2\left[P_{n-1}(x) - \frac{x-b_n}{2a_n}P_n(x)\right]^2 + \frac{1}{4}\left[4a_n^2 - (x-b_n)^2\right]P_n^2(x).$$

The assumption $2a_n \geq 2 + |b_n|$ implies $4a_n^2 - (x-b_n)^2 \geq 4 - x^2$ for $|x| \leq 2$, and (4.6) implies $R_{n-1}(x) \geq S_{n-1}(x)$. This proves (4.9). Inequality (4.10) follows from (4.9) and Lemma 4.23, and (4.11)/(4.12) from (4.7), (4.8), and (4.9)/(4.10). □

In [8], similar statements are proved for S_n. The important difference is that the proofs use (4.4) rather than (4.7), and therefore involve $\delta_n' = [a_{n+1}^2 - a_n^2]_+ + a_n|b_{n+1} - b_n|$. This is a serious drawback because the condition $\sum n\delta_n < \infty$ will play a central role in our considerations. If, for example, $a_n = 1 + \alpha/n$ and $b_n = \beta/n$, then $\sum n\delta_n' < \infty$ only if $\alpha \geq 0$ and $\beta = 0$ (cf. the result from [8] mentioned in Chapter 1), but $\sum n\delta_n < \infty$ whenever $2\alpha \geq |\beta|$. This is because in δ_n (and not in δ_n') the contribution of the positive $|b_{n+1} - b_n|$ terms can be canceled by a decrease in a_n. Therefore R_n can sometimes be a better object to look at than S_n.

The next result relates R_n and $Z(J)$.

Lemma 4.3. *Suppose* $\lim_{n\to\infty} a_n = 1$, $\lim_{n\to\infty} b_n = 0$, *and*

$$\sum_{n=1}^{\infty} \big(|a_{n+1} - a_n| + |b_{n+1} - b_n|\big) < \infty. \tag{4.13}$$

Then $\nu'(x)$ *is continuous in* $(-2, 2)$ *and for* $x \in (-2, 2)$,

$$\lim_{n\to\infty} R_n(x) = \frac{\sqrt{4-x^2}}{2\pi\nu'(x)}. \tag{4.14}$$

Remark. The right-hand side appears in (2.28) and so one can use (4.14) and Fatou's lemma to obtain upper bounds on $Z(J)$ in terms of the R_n's (see the proof of Theorem 4.6).

Proof. Theorem 4.25 shows continuity of $\nu'(x)$ and that for any $x \in (-2, 2)$,

$$\lim_{n\to\infty} \left[P_{n+1}^2(x) - xP_{n+1}(x)P_n(x) + P_n^2(x)\right] = \frac{\sqrt{4-x^2}}{2\pi\nu'(x)}.$$

Then (4.5), (4.6), boundedness of $\{P_n(x)\}_n$ (Theorem 4.25), $a_n \to 1$, and $b_n \to 0$ imply that this limit is the same as $\lim_n R_n(x)$. □

In the light of the discussion preceding Lemma 4.3, the following will be useful.

Lemma 4.4. *If* $\inf\{a_n\} > 0$ *and* $\sum_n \delta_n < \infty$, *then* (4.13) *holds.*

Proof. We have $0 \le [a_{n+1}^2 - a_n^2]_+ \le \delta_n$, hence $\sum[a_{n+1}^2 - a_n^2]_+ < \infty$. By telescoping $\sum[a_{n+1}^2 - a_n^2]_- \le a_1^2 + \sum[a_{n+1}^2 - a_n^2]_+ < \infty$ and so $\sum|a_{n+1}^2 - a_n^2| < \infty$. Since $\inf\{a_n\} > 0$, it follows that $\sum|a_{n+1} - a_n| < \infty$. Also, since

$$0 \le \frac{a_{n+1}}{2}|b_{n+2} - b_{n+1}| + \frac{a_n}{2}|b_{n+1} - b_n| \le \delta_n + |a_{n+1}^2 - a_n^2|$$

and a_n are bounded away from zero, $\sum|b_{n+1} - b_n| < \infty$. □

These lemmas have the same consequences as in [8], but with δ_n in place of δ_n'. Thus we can prove the following two results.

Theorem 4.5. *Suppose* $a_n \ge 1 + \frac{|b_n|}{2}$ *for* $n > N$, $\lim_{n\to\infty} a_n = 1$, *and*

$$\sum_{n=1}^{\infty} n^2 \left[a_{n+1}^2 - a_n^2 + \frac{a_{n+1}}{2}|b_{n+2} - b_{n+1}| + \frac{a_n}{2}|b_{n+1} - b_n|\right]_+ < \infty.$$

Then there is $c > 0$ *such that for* $x \in (-2, 2)$,

$$\nu'(x) \ge c\sqrt{4-x^2}.$$

Remarks. 1. In particular, the corresponding matrix J is Szegő.

2. Notice that the above conditions are satisfied for $a_n \downarrow 1$, $b_n \equiv 0$, as pointed out in [8].

Proof. By (4.8) and (4.12), we have for all $|x| \leq 2$ and $n > N$

$$R_n(x) \leq \exp\left(\sum_{j=N}^{\infty}(j+1)^2\delta_j\right) \max_{|x|\leq 2} R_N(x) \equiv \frac{1}{2\pi c} < \infty.$$

Lemmas 4.4 and 4.3 finish the proof. □

The main result of this section is

Theorem 4.6. *Suppose* $a_n \geq 1 + \frac{|b_n|}{2}$ *for* $n > N$, $\lim_{n\to\infty} a_n = 1$, *and*

$$\sum_{n=1}^{\infty} n\left[a_{n+1}^2 - a_n^2 + \frac{a_{n+1}}{2}|b_{n+2} - b_{n+1}| + \frac{a_n}{2}|b_{n+1} - b_n|\right]_+ < \infty.$$

Then $Z(J) < \infty$.

Remark. This is Theorem 4.1 without the $O(n^{-1-\varepsilon})$ errors.

Proof. Once again, we closely follow [8]. By Lemmas 4.4, 4.3, and Fatou's lemma

$$Z(J) \leq \lim_{\varepsilon\downarrow 0}\left(\liminf_{n\to\infty} \frac{1}{2\pi}\int_{-2+\varepsilon}^{2-\varepsilon} \ln_+(R_n(x))\,\frac{dx}{\sqrt{4-x^2}}\right),$$

and so it is sufficient to prove

$$\int_0^{2-n^{-2}} \ln_+(R_n(x))\,\frac{dx}{\sqrt{2-x}} + \int_{-2+n^{-2}}^{0} \ln_+(R_n(x))\,\frac{dx}{\sqrt{2+x}} \leq C$$

for some $C < \infty$. Let us consider the first integral, which we denote I_n (the other can be treated similarly).

By (4.11) and (4.12), for $n > N$

$$\begin{aligned}
I_n \leq& I_{n-1} + 2\delta_n \int_0^{2-\frac{1}{(n-1)^2}} \frac{dx}{(2-x)^{\frac{3}{2}}} + \ln_+\left[\max_{|x|\leq 2} R_n(x)\right]\int_{2-\frac{1}{(n-1)^2}}^{2-\frac{1}{n^2}} \frac{dx}{\sqrt{2-x}} \\
=& I_{n-1} + 2\delta_n(2n-2-\sqrt{2}) + \left(\frac{2}{n-1} - \frac{2}{n}\right)\ln_+\left[\max_{|x|\leq 2} R_n(x)\right] \\
\leq& I_{n-1} + 4n\delta_n + \frac{2}{n-1}\ln_+\left[\max_{|x|\leq 2} R_{n-1}(x)\right] + \frac{2(n+1)^2\delta_n}{n-1} - \frac{2}{n}\ln_+\left[\max_{|x|\leq 2} R_n(x)\right]
\end{aligned}$$

$$\leq I_{n-1} + 13n\delta_n + \frac{2}{n-1}\ln_+\left[\max_{|x|\leq 2} R_{n-1}(x)\right] - \frac{2}{n}\ln_+\left[\max_{|x|\leq 2} R_n(x)\right]$$

because $\ln_+(xy) \leq \ln_+(x) + \ln_+(y)$. Iterating this we obtain

$$I_n \leq I_N + 13\sum_{j=N+1}^{n} j\delta_j + \frac{2}{N}\ln_+\left[\max_{|x|\leq 2} R_N(x)\right] \leq 13\sum_{n=1}^{\infty} n\delta_n + 5\ln_+\left[\max_{|x|\leq 2} R_N(x)\right] \equiv \frac{C}{2}$$

as desired. □

For further reference we make the following

Definition. We call a pair of sequences $\{a_n, b_n\}_{n=1}^{\infty}$ *admissible*, if $a_n \geq 1 + \frac{|b_n|}{2}$ for $n > N$, $\lim_{n\to\infty} a_n = 1$, and

$$\sum_{n=1}^{\infty} n\left[a_{n+1}^2 - a_n^2 + \frac{a_{n+1}}{2}|b_{n+2} - b_{n+1}| + \frac{a_n}{2}|b_{n+1} - b_n|\right]_+ < \infty.$$

Hence, if $\{a_n, b_n\}$ is admissible, then J is Szegő. We make some useful observations.

Lemma 4.7. *Suppose $\{a_n, b_n\}$ is admissible and $\{e_n, f_n\}$ is such that $2e_n \geq |f_n|$ for $n > N$, $e_n \to 0$, and $\sum n\big(|e_{n+1} - e_n| + |f_{n+1} - f_n|\big) < \infty$. Then $\{a_n + e_n, b_n + f_n\}$ is also admissible.*

Proof. We only need to show the last condition for admissibility. If

$$\begin{aligned}\varepsilon_n \equiv (a_{n+1} + e_{n+1})^2 - (a_n + e_n)^2 &+ \frac{a_{n+1} + e_{n+1}}{2}|b_{n+2} + f_{n+2} - b_{n+1} - f_{n+1}| \\ &+ \frac{a_n + e_n}{2}|b_{n+1} + f_{n+1} - b_n - f_n|,\end{aligned}$$

then we want $\sum n[\varepsilon_n]_+ < \infty$. Notice that

$$\begin{aligned}\varepsilon_n \leq \delta_n + 2a_{n+1}|e_{n+1} - e_n| + 2|a_{n+1} - a_n||e_n| + |e_{n+1} + e_n||e_{n+1} - e_n| \\ + \frac{a_{n+1} + e_{n+1}}{2}|f_{n+2} - f_{n+1}| + \frac{a_n + e_n}{2}|f_{n+1} - f_n|\end{aligned}$$

$$+\frac{e_{n+1}}{2}|b_{n+2}-b_{n+1}|+\frac{e_n}{2}|b_{n+1}-b_n|,$$

and so we only need to prove $\sum nX_n < \infty$ for X_n being any of the above terms. If X_n is δ_n or one of the terms containing $|e_{n+1}-e_n|$ or $|f_{n+1}-f_n|$, then this is obvious. For the remaining three terms the same will hold by Lemma 4.4 if $\{ne_n\}_n$ is bounded. But $\sum n|e_{n+1}-e_n| < \infty$ and $e_n \to 0$ imply $ne_n \le \sum_{m=n}^{\infty} n|e_{m+1}-e_m| \to 0$ as $n \to \infty$. □

Lemma 4.8. *Suppose $\{a_n, b_n\}$ is admissible and $e_n \downarrow 0$ is such that $\{ne_n|a_{n+1}-a_n|\}$ or $\{ne_n|b_{n+2}-b_{n+1}|\}$ is bounded. Then $\{a_n+e_n, b_n\}$ is also admissible.*

Proof. If

$$\varepsilon_n \equiv (a_{n+1}+e_{n+1})^2-(a_n+e_n)^2+\frac{a_{n+1}+e_{n+1}}{2}|b_{n+2}-b_{n+1}|+\frac{a_n+e_n}{2}|b_{n+1}-b_n|,$$

then by $e_{n+1} \le e_n$,

$$\begin{aligned}\varepsilon_n \le &\delta_n+2a_{n+1}e_{n+1}-2a_ne_n+e_{n+1}^2-e_n^2+\frac{e_{n+1}}{2}|b_{n+2}-b_{n+1}|+\frac{e_n}{2}|b_{n+1}-b_n| \\ \le &\delta_n+e_n\big(2(a_{n+1}-a_n)+\tfrac{1}{2}|b_{n+2}-b_{n+1}|+\tfrac{1}{2}|b_{n+1}-b_n|\big) \\ \le &\delta_n+\frac{2e_n}{a_{n+1}+a_n}\left(\delta_n+\frac{|a_n-a_{n+1}|}{4}|b_{n+2}-b_{n+1}|+\frac{|a_{n+1}-a_n|}{4}|b_{n+1}-b_n|\right),\end{aligned}$$

and so $\sum n[\varepsilon_n]_+ < \infty$ by the hypotheses and Lemma 4.4. □

We conclude this section with an interesting corollary. It shows that there are many Jacobi matrices which are Szegő, but one cannot pass to the “full size” sum rule (3.60) because $\bar{A}_0(J) = -\infty$ and $\mathcal{E}_0(J) = \infty$.

Corollary 4.9. *Let $\{a_n, b_n\}$ be admissible and let $\tilde{J}$ be a matrix with $\tilde{a}_n \equiv a_n + c/n$ and $\tilde{b}_n \equiv b_n$ for some $c > 0$. Then $Z(\tilde{J}) < \infty$ but $\bar{A}_0(\tilde{J}) = -\infty$ and $\mathcal{E}_0(\tilde{J}) = \infty$.*

Proof. $Z(\tilde{J}) < \infty$ by Lemma 4.8, and Theorem 3.14(c) shows $\bar{A}_0(J) < \infty$. Since $a_n \to 1$ and $\sum \frac{c}{n} = \infty$, we obtain $\bar{A}_0(\tilde{J}) = -\infty$. By Theorem 3.14(d), this implies $\mathcal{E}_0(\tilde{J}) = \infty$. □

4.2 Control of Change of Eigenvalues under Perturbations

In this section we will prove results on the behavior of eigenvalues under certain finite rank perturbations of the a_n's and b_n's. Namely, we will show that these perturbations decrease E_j^+ and increase E_j^- for all but finitely many j. This, of course, means that we will not consider arbitrary perturbations. Indeed, in all the perturbations we can treat, the a_n's cannot increase. Immediately a question arises, how is this compatible with the possibility of $a_n > c_n$ in Theorem 4.1. The answer is in Lemma 4.8. Before doing a general $O(n^{-1-\varepsilon})$ perturbation of c_n, d_n, we will increase the c_n's by $Cn^{-1-\varepsilon}$ for some large C, so that the assumptions of Theorem 4.1 will stay valid and the new c_n will be larger than a_n. Then we will use results from this section. For details see the proof of Theorem 4.1 in the next section.

For $j \geq 1$ and $n \geq 0$ we define

$$p_n(\pm j) \equiv \frac{P_n(E_j^\pm)}{\left(\sum_{m=0}^\infty P_m^2(E_j^\pm)\right)^{1/2}}.$$

Hence $p(\pm j) \equiv \{p_n(\pm j)\}_{n=-1}^\infty$ with $p_{-1}(\pm j) \equiv 0$ is the normalized Dirichlet eigenfunction of J for energy $E_j^\pm$. Naturally, $p(\pm j)$ satisfies the same recurrence relation as $P(E_j^\pm)$, and so for $n \geq 0$,

$$p_{n+1}(\pm j) = \frac{E_j^\pm - b_{n+1}}{a_{n+1}} p_n(\pm j) - \frac{a_n}{a_{n+1}} p_{n-1}(\pm j). \tag{4.15}$$

In what follows, we will use a well-known result from first order eigenvalue perturbation theory (see, e.g., [38, p.151]):

Lemma 4.10. *Let $J(t) \equiv J + tA$ for $t \in (-\varepsilon, \varepsilon)$ where J and A are bounded self-adjoint operators on a Hilbert space. Assume that $J(0)$ has a simple isolated eigenvalue $E(0) \notin \sigma_{\text{ess}}(J(0))$ and let $\varphi(0)$ be the corresponding normalized eigenfunction. Then there are analytic functions $E(t)$, $\varphi(t)$ defined on some interval $(-\varepsilon', \varepsilon')$ such* *that $E(t)$ is a simple isolated eigenvalue of $J(t)$ with normalized eigenfunction $\varphi(t)$, and we have $\frac{\partial}{\partial t}E(t) = \langle \varphi(t), A\varphi(t)\rangle$.*

In the case of Jacobi matrices, all eigenvalues outside $[-2, 2]$ are simple. Hence if $J(t) \equiv J + tA$ with A bounded self-adjoint matrix, then

$$\tfrac{\partial}{\partial t}E_j^{\pm}(t) = \langle p(\pm j; t), Ap(\pm j; t)\rangle \tag{4.16}$$

as long as $E_j^{\pm}(t)$ stays outside $[-2, 2]$.

We have $E_j^{\pm} = \pm 2$ whenever J has fewer than j positive/negative bound states. Then, of course, (4.16) does not apply when $E_j^{\pm}(t) = \pm 2$, but we at least have continuity of $E_j^{\pm}(t)$ in t by norm-continuity of $J(t)$.

Here is the main idea of this section. Fix n and take A to be the matrix with $A_{n-1,n} = A_{n,n-1} = -1$ and all other entries zero (the upper left-hand corner of A being $A_{0,0}$). Then increasing t corresponds to decreasing a_n. We have

$$\tfrac{\partial}{\partial t}E_j^{\pm}(t) = -2p_n(\pm j; t)p_{n-1}(\pm j; t).$$

Let us take $j = 1$. Then by Theorem 2.2(i),(iii) we know that $\operatorname{sgn}(p_n(1; t)) = \operatorname{sgn}(p_{n-1}(1; t))$ and $\operatorname{sgn}(p_n(-1; t)) = -\operatorname{sgn}(p_{n-1}(-1; t))$ for $n \geq 1$. Hence E_1^+ will decrease and E_1^- will increase when we decrease a_n. This is exactly what we want.

Unfortunately, it is not always the case for other eigenvalues. Indeed, let us consider a positive eigenvalue E_j^+. By Theorem 2.2(i), $p(j)$ changes sign $j-1$ times, and so E_j^+ will grow when we decrease the corresponding a_n's. However, if $E_j^+ \sim 2$, $a_n \sim 1$, and $b_n \sim 0$, then by (4.15), $p_{n+1}(j) \sim 2p_n(j) - p_{n-1}(j)$, that is, $p(j)$ is (locally) close to a linear function of n. Therefore, if $\operatorname{sgn}(p_n(j)) = -\operatorname{sgn}(p_{n-1}(j))$, then $\operatorname{sgn}(p_m(j)) = \operatorname{sgn}(p_{m-1}(j))$ for $m \neq n$ but close to n. Hence, a suitable decrease of a_n along with some neighboring a_m's should still result into a decrease of E_j^+. This is the content of the present section.

Definition. Let $\delta > 0$. We say that $\tilde{J}$ *δ-minorates* J, if $|E_j^{\pm}(\tilde{J})| \leq |E_j^{\pm}(J)|$ whenever $|E_j^{\pm}(J)| < 2 + \delta$.

Remarks. 1. This is well defined because $E_j^{\pm} = \pm 2$ whenever J has less than j positive/negative bound states.

2. Notice that for fixed δ this relation is transitive.

Lemma 4.11. *There exists $\delta > 0$ such that the following is true. If for some J we have $|a_m - 1| < \delta$ and $|b_m| < \delta$ for $m \in \{n, n+1, n+2\}$, and $\tilde{J}$ is obtained from J by decreasing a_n by $c > 0$ and a_{n+2} by $d > 0$ so that $|a_n - c - 1| < \delta$, $|a_{n+2} - d - 1| < \delta$, and $c/d \in [\frac{1}{13}, 13]$, then $\tilde{J}$ δ-minorates J.*

Remark. That is, decreasing both a_n and a_{n+2} results into a decrease of all but finitely many $|E_j^{\pm}|$. The same trick applied to a_n and a_{n+1} fails.

Proof. Let $q \equiv c/d$. Let $E \equiv E_j^+$ and $p_n \equiv p_n(+j)$ with $2 < E_j^+ < 2 + \delta$. Then by (4.15),

$$\begin{aligned} p_{n+1} =& 2p_n - p_{n-1} + \frac{E - 2a_{n+1} - b_{n+1}}{1 + (a_{n+1} - 1)} p_n + \frac{a_{n+1} - a_n}{1 + (a_n - 1)} p_{n-1} \\ =& 2p_n - p_{n-1} + O(\delta)(|p_n| + |p_{n-1}|) \end{aligned} \tag{4.17}$$

with $|O(\delta)| \leq C\delta$ for some universal constant $C < \infty$ and all small δ. Similarly we obtain by iterating (4.15),

$$p_{n+2} = 3p_n - 2p_{n-1} + O(\delta)(|p_n| + |p_{n-1}|). \tag{4.18}$$

Let now $J(t) \equiv J + tA$ where A is such that $A_{n-1,n} = A_{n,n-1} = -q$, $A_{n+1,n+2} = A_{n+2,n+1} = -1$ and all other entries are 0. Then obviously $E_j^{\pm}(0) = E_j^{\pm}$ and $\tilde{J} = J(d)$. By (4.16),

$$\tfrac{\partial}{\partial t} E_j^+(0) = \langle p, Ap \rangle = -2(q p_n p_{n-1} + p_{n+2} p_{n+1}).$$

By (4.17) and (4.18),

$$q p_n p_{n-1} + p_{n+2} p_{n+1} = 6p_n^2 - (7 - q) p_n p_{n-1} + 2p_{n-1}^2 + O(\delta)(p_n^2 + p_{n-1}^2). \tag{4.19}$$

Since $6 \cdot 2 - \left(\frac{7-q}{2}\right)^2 > 0$ for $q \in (7-4\sqrt{3}, 7+4\sqrt{3}) \supset [\frac{1}{13}, 13]$, it follows that

$$6p_n^2 - (7-q)p_n p_{n-1} + 2p_{n-1}^2 > \delta_0(p_n^2 + p_{n-1}^2)$$

for some small δ_0 and all $q \in [\frac{1}{13}, 13]$. So if we choose δ such that $|O(\delta)| \le \delta_0$, then $\frac{\partial}{\partial t}E_j^+(0) < 0$.

This argument obviously applies to all $t \in [0, d]$, not only to $t = 0$, as long as $E_j^+(t) > 2$. This is because for each such t, $J(t)$ satisfies the conditions of this lemma. Hence $E_j^+(t)$ can only decrease with t (and so stays smaller than $2+\delta$). Also, no new bound states can appear. Indeed, if $E_j^+(t_1) = 2$ and $E_j^+(t_2) > 2$ for some $t_2 > t_1$, then $E_j^+(t)$ would have to have a discontinuity in $[t_1, t_2]$, because by the above argument it has to decrease whenever it is larger than 2.

A similar argument applies to $E_j^-(0) > -2-\delta$, with $p_{n+1} \sim -2p_n - p_{n-1}$ and $p_{n+2} \sim 3p_n + 2p_{n-1}$ in place of (4.17) and (4.18), and shows that such E_j^- increases with t. The result follows. □

As mentioned earlier, same trick with a_{n+1} in place of a_{n+2} does not work. Indeed, in (4.19) we would have $2p_n^2 - (1-q)p_n p_{n-1} + O(\delta)(p_n^2 + p_{n-1}^2)$, which cannot be guaranteed to be positive for any $\delta > 0$. However, we can replace a_{n+2} by a_{n+k} for $k \ge 2$, and the lemma stays valid for some smaller $\delta = \delta(k) > 0$ and $c/d \in [(4k^2-3)^{-1}, 4k^2-3]$ (we use that $p_{n+k} \sim (k+1)p_n - kp_{n-1}$ for E_j^+). Of course, the bounds on $|a_m - 1|$ and $|b_m|$ have to hold for all $m \in \{n, \dots, n+k\}$.

Before we start perturbing the b_n's, let us state one more result with the same flavor.

Lemma 4.12. *There exists $\delta > 0$ such that the following is true. If for some J we have $|a_m - 1| < \delta$ and $|b_m| < \delta$ for $m \in \{n, n+1, n+2\}$, and $\tilde{J}$ is obtained from J by decreasing a_n, a_{n+1}, and a_{n+2} by $c > 0$ so that $|a_m - c - 1| < \delta$ for $m \in \{n, n+1, n+2\}$, then $\tilde{J}$ δ-minorates J.*

Remark. Again, the result can be extended to decreasing $a_n, \dots, a_{n+k}$ (for $k \ge 2$) by $c > 0$, with a smaller $\delta = \delta(k) > 0$.

Proof. An argument as above gives for $A_{n-1,n} = A_{n,n-1} = A_{n,n+1} = A_{n+1,n} = A_{n+1,n+2} = A_{n+2,n+1} = -1$ that

$$\begin{aligned}\tfrac{\partial}{\partial t}E_j^+(0) &= -2(p_{n-1}p_n + p_n p_{n+1} + p_{n+1}p_{n+2}) \\ &= -2\big(8p_n^2 - 7p_n p_{n-1} + 2p_{n-1}^2 + O(\delta)(p_n^2 + p_{n-1}^2)\big)\end{aligned}$$

which is negative for small enough δ, since $8 \cdot 2 - (\frac{7}{2})^2 > 0$. The rest of the previous proof applies. □

Our next aim is to allow perturbations of the b_n's as well. If one decreases b_n, it is obvious that all E_j^+ decrease, but all E_j^- decrease as well. Hence, perturbing the b_n's alone will not move "in" all bound states. To ensure that, we have to counter the undesired movement of $E_j^\pm$ by decreasing a_n's.

Lemma 4.13. *There exists $\delta > 0$ such that the following is true. If for some J we have $|a_m - 1| < \delta$ and $|b_m| < \delta$ for $m \in \{n, n+1, n+2\}$, and $\tilde{J}$ is obtained from J by decreasing a_n and a_{n+2} by $c > 0$ and changing b_n by $d \in [-\frac{c}{2}, \frac{c}{2}]$ so that $|a_n - c - 1| < \delta$, $|a_{n+2} - c - 1| < \delta$, and $|b_n + d| < \delta$, then $\tilde{J}$ δ-minorates J.*

Proof. This time we have $A_{n-1,n} = A_{n,n-1} = A_{n+1,n+2} = A_{n+2,n+1} = -1$ and $A_{n-1,n-1} = q \equiv d/c$. We obtain

$$\begin{aligned}\tfrac{\partial}{\partial t}E_j^+(0) &= -2(p_{n-1}p_n + p_{n+1}p_{n+2}) + qp_{n-1}^2 \\ &= -2\big(6p_n^2 - 6p_n p_{n-1} + (2 - \tfrac{q}{2})p_{n-1}^2 + O(\delta)(p_n^2 + p_{n-1}^2)\big),\end{aligned}$$

which is negative for small enough δ if $q < 1$ (i.e., if $6(2 - \frac{q}{2}) - (\frac{6}{2})^2 > 0$). A similar argument for E_j^- requires $q > -1$, so there is a $\delta > 0$ which works for all $q \in [-\frac{1}{2}, \frac{1}{2}]$. □

4.3 Sufficient Conditions for $Z(J) < \infty$

We will now outline an argument which shows how to use (3.47) to prove stability of the Szegő condition under certain trace class perturbations. A hint of this appears in Section 3.2 as a commentary to Conjecture 3.13.

Let $\tilde{J}$ be a trace class perturbation of a matrix J such that $Z(J) < \infty$. That is,

$$\sum_n \big(|\tilde{a}_n - a_n| + |\tilde{b}_n - b_n|\big) < \infty. \tag{4.20}$$

Let $\tilde{J}_n$ be the matrix which we obtain from J by replacing a_j, b_j by $\tilde{a}_j, \tilde{b}_j$ for $j = 1, \dots, n$. Notice that this is different from (2.18), but we still have $\tilde{J}_n \to \tilde{J}$ (elementwise and also in norm). Now by applying (3.47) to both $\tilde{J}_n$ and J and subtracting, we obtain

$$Z(\tilde{J}_n) = Z(J) - \sum_{j=1}^{n} \big[\ln(\tilde{a}_j) - \ln(a_j)\big] + \sum_{j,\pm} \Big[\ln|\beta_j^\pm(\tilde{J}_n)| - \ln|\beta_j^\pm(J)|\Big]. \tag{4.21}$$

From (2.48) we know that $Z(\tilde{J}) \le \liminf Z(\tilde{J}_n)$. So by taking $n \to \infty$,

$$Z(\tilde{J}) \le Z(J) + \sum_{j=1}^{\infty} |\ln(\tilde{a}_j) - \ln(a_j)| + \liminf_{n\to\infty} \sum_{j,\pm} \Big[\ln|\beta_j^\pm(\tilde{J}_n)| - \ln|\beta_j^\pm(J)|\Big]. \tag{4.22}$$

If $\inf_j\{\tilde{a}_j, a_j\} > 0$, then the first sum is finite by (4.20). Hence, if we could show that the lim inf is smaller than $+\infty$, we would prove $Z(\tilde{J}) < \infty$. Notice that this is true if for some $\delta > 0$ each $\tilde{J}_n$ δ-minorates J, because then $|\beta_j^\pm(\tilde{J}_n)| \le |\beta_j^\pm(J)|$ whenever $|E_j^\pm(J)| < 2 + \delta$ and the remaining $|\beta_j^\pm(\tilde{J}_n)|$ are bounded. This is where results from the previous section enter the picture.

Unfortunately, we cannot treat general trace class perturbations at this moment. The reason is the necessity of using Lemma 4.8, as described in Section 4.2. It also needs to be said that in what follows, the "partial perturbations" $\tilde{J}_n$ will be slightly different from those above. They will differ in some matrix elements, but they will still converge to $\tilde{J}$ and so (4.22) will stay valid.

Let us now apply the above argument. We start with

Lemma 4.14. *Let J be Szegő with $a_n \to 1$, $b_n \to 0$, and let $e_n \downarrow 0$, $e_n < a_n$, $\sum_n e_n < \infty$. Then the matrix $\tilde{J}$ with $\tilde{a}_n \equiv a_n - e_n$ and $\tilde{b}_n \equiv b_n$ is also Szegő.*

Proof. Let $\delta \equiv \min\{\delta(2), \delta(3), \delta(4)\} > 0$ where $\delta(k)$ are as in the remark after Lemma 4.12 (that is, good for decreasing 3, 4, and 5 consecutive a_n's). Let N be such that for $j \geq N$ we have $|a_j - 1| < \delta$, $|\tilde{a}_j - 1| < \delta$, and $|b_j| < \delta$. For $n \geq N+1$ let $\tilde{J}_n$ be such that $b_j(\tilde{J}_n) \equiv b_j$ and

$$a_j(\tilde{J}_n) \equiv \begin{cases} \tilde{a}_j & j \leq N-1, \\ \tilde{a}_j + e_{n+1} & N \leq j \leq n, \\ a_j & j \geq n+1. \end{cases}$$

Then $\tilde{J}_{N+1}$ is Szegő because it is a finite rank perturbation of J.

Let $n \geq N+2$. Notice that $\tilde{J}_n$ is obtained from $\tilde{J}_{n-1}$ by decreasing $a_j(\tilde{J}_{n-1})$ by $c \equiv e_n - e_{n+1}$ for $j = N, \dots, n$. This can be accomplished by successive decreases of 3, 4, or 5 neighboring a_j's by c, as in Lemma 4.12 (and the remark after it). It follows that $\tilde{J}_n$ δ-minorates $\tilde{J}_{n-1}$, and so by induction $\tilde{J}_n$ δ-minorates $\tilde{J}_{N+1}$. Then by (4.21) (with $\delta < \frac{1}{2}$),

$$Z(\tilde{J}_n) \leq Z(\tilde{J}_{N+1}) + 2\sum_{j=N}^{\infty} e_j + K\ln(M) < \infty,$$

where K is the number of eigenvalues of $\tilde{J}_{N+1}$ outside of $(-2-\delta, 2+\delta)$ and $M \equiv 3\sup_j\{a_j, |b_j|\} \geq \|\tilde{J}_n\|$. So $Z(\tilde{J}_n)$ are uniformly bounded and since $\tilde{J}_n \to \tilde{J}$, (2.48) implies $Z(\tilde{J}) < \infty$. □

Corollary 4.15. *Suppose $\{a_n, b_n\}$ is admissible and $\{e_n, f_n\}$ is such that $e_n \to 0$, $f_n \to 0$, $e_n > -a_n$, and $\sum n\big(|e_{n+1} - e_n| + |f_{n+1} - f_n|\big) < \infty$. Then the matrix $\tilde{J}$ with $\tilde{a}_n \equiv a_n + e_n$, $\tilde{b}_n \equiv b_n + f_n$ is Szegő.*

Remark. This is Lemma 4.7 with the condition $2e_n \geq |f_n|$ removed.

Proof. Let us define $\bar{e}_n \equiv \sum_{j=n}^{\infty} |e_{j+1} - e_j|$ and similarly for f_n. Notice that $\bar{e}_n \geq |e_n|$, $\bar{e}_n \downarrow 0$, and

$$\sum_{n=1}^{\infty} \bar{e}_n \leq \sum_{n=1}^{\infty} n|e_{n+1} - e_n| < \infty.$$

Then if $\tilde{e}_n \equiv e_n + \bar{e}_n + \bar{f}_n$, we have $2\tilde{e}_n \geq |f_n|$, and so $\{a_n + \tilde{e}_n, b_n + f_n\}$ is admissible by Lemma 4.7. By Lemma 4.14, the result follows. □

We are now ready to prove Theorem 4.1.

Proof of Theorem 4.1. Our strategy is as outlined at the beginning of Section 4.2 and this section. We let

$$C \equiv \sup_n \left\{ n^{1+\varepsilon}|\tilde{a}_n - a_n|,\, n^{1+\varepsilon}|\tilde{b}_n - b_n| \right\} < \infty, \tag{4.23}$$

and increase a_n by $6Cn^{-1-\varepsilon}$ (we call these again a_n). Then by Lemma 4.8 (or by Lemma 4.7), $\{a_n, b_n\}$ (with the new a_n) is also admissible. Thus, the new J is Szegő and we now have

$$\begin{aligned} a_n - \tilde{a}_n &\in [5Cn^{-1-\varepsilon}, 7Cn^{-1-\varepsilon}], \\ b_n - \tilde{b}_n &\in [-Cn^{-1-\varepsilon}, Cn^{-1-\varepsilon}]. \end{aligned} \tag{4.24}$$

Let δ be such that both Lemmas 4.11 and 4.13 are valid. Let N be such that for $j \geq N$ we have $|a_j - 1| < \delta$, $|\tilde{a}_j - 1| < \delta$, $|b_j| < \delta$, and $|\tilde{b}_j| < \delta$. We let $\tilde{J}_{N-1}$ be such that

$$a_j(\tilde{J}_{N-1}) \equiv \begin{cases} \tilde{a}_j & j \leq N-1, \\ a_j & j \geq N, \end{cases}$$

and similarly for $b_j(\tilde{J}_{N-1})$. Then $\tilde{J}_{N-1}$ is Szegő because it is a finite rank perturbation of J.

We construct $\tilde{J}_N$ from $\tilde{J}_{N-1}$ in two steps. First we decrease a_N, a_{N+2} by $2|b_N - \tilde{b}_N|$ and change b_N to $\tilde{b}_N$. Then we decrease a_N by $a_N - \tilde{a}_N$ and a_{N+2} by $(a_N - \tilde{a}_N)/13$ (in terms of the new a_N). Both perturbations are δ-minorating by Lemmas 4.11 and 4.13, and the obtained matrix $\tilde{J}_N$ agrees with $\tilde{J}$ in first N couples $a_j(\tilde{J}_N)$, $b_j(\tilde{J}_N)$. The others are the same as in J, a possible exception being $a_{N+2}(\tilde{J}_N)$, for which we only know

$$a_{N+2}(\tilde{J}_N) - \tilde{a}_{N+2} \in [2C(N+2)^{-1-\varepsilon}, 7C(N+2)^{-1-\varepsilon}] \tag{4.25}$$

(if N is chosen so that $(2+\frac{7}{13})N^{-1-\varepsilon} \le 3(N+2)^{-1-\varepsilon}$).

Now we apply the same procedure to inductively construct $\tilde{J}_n$ from $\tilde{J}_{n-1}$ for $n \ge N+1$. Each $\tilde{J}_n$ will agree with $\tilde{J}$ up to index n, and other elements will be the same as in J, possibly except of $a_{n+1}(\tilde{J}_n)$ and $a_{n+2}(\tilde{J}_n)$. For these we will have (4.25) (with $n+1$ and $n+2$ in place of $N+2$), which is just enough so that we can change b_{n+1} to $\tilde{b}_{n+1}$ when passing to $\tilde{J}_{n+1}$ by the same method. Since $\tilde{J}_n$ δ-minorates $\tilde{J}_{n-1}$, we obtain by induction that each $\tilde{J}_n$ δ-minorates $\tilde{J}_{N-1}$.

Again, we have by (4.21) (with $\delta < \frac{1}{2}$),

$$Z(\tilde{J}_n) \le Z(\tilde{J}_{N-1}) + 14C \sum_{j=N}^{\infty} j^{-1-\varepsilon} + K \ln(M) < \infty$$

with K and M as in the proof of Lemma 4.14. Since $\tilde{J}_n \to \tilde{J}$, the result follows. □

For a sequence e_n we define $\partial e_n \equiv e_{n+1} - e_n$ and $\partial^2 e_n \equiv \partial(\partial e_n) = e_{n+2} - 2e_{n+1} + e_n$. Using results in this section and those in Section 3.5, we can prove the following:

Theorem 4.16. *Let*

$$a_n \equiv 1 + \alpha e_n + O(n^{-1-\varepsilon}), \qquad b_n \equiv \beta e_n + O(n^{-1-\varepsilon})$$

with $e_n \downarrow 0$, $\sum_n e_n = \infty$, $\sum_n n[\partial^2 e_n]_- < \infty$, *and* $\varepsilon > 0$. *Then* $Z(J) < \infty$ *if and only if* $2\alpha \ge |\beta|$.

Remark. Notice that the last condition on e_n is satisfied whenever e_n is eventually a convex sequence. In particular, $e_n = n^{-\gamma}$ with $0 < \gamma \le 1$ is included, proving Theorem 1.4.

Proof. First consider $\alpha < 0$. Then

$$-\sum_{n=1}^{N} \ln(a_n) = \sum_{n=1}^{N} \big[|\alpha| e_n + O(e_n^2) + O(n^{-1-\varepsilon})\big] \to \infty$$

as $N \to \infty$, and so $Z(J) = \infty$ by Corollary 3.15.

Next assume $0 \le 2\alpha < |\beta|$. If we take $|p| < \frac{1}{2}$ such that $\alpha < -p\beta$, then

$$-\sum_{n=1}^{N} \big[\ln(a_n) + pb_n\big] = \sum_{n=1}^{N} \big[(-\alpha - p\beta)e_n + O(e_n^2) + O(n^{-1-\varepsilon})\big] \to \infty$$

by the hypotheses. Also, since $-\alpha + p\beta \le p\beta < -\alpha \le 0$,

$$-\sum_{n=1}^{N} \big[\ln(a_n) - pb_n\big] = \sum_{n=1}^{N} \big[(-\alpha + p\beta)e_n + O(e_n^2) + O(n^{-1-\varepsilon})\big] \to -\infty.$$

Theorem 3.26(i) then gives $Z(J) = \infty$.

Finally, assume $2\alpha \ge |\beta|$. Note that $\partial e_n \le 0$. We let $c_n \equiv 1 + \alpha e_n$ and $d_n \equiv \beta e_n$. Then the square bracket in (4.2) equals

$$\begin{aligned}
&2\alpha \partial e_n + \alpha^2(e_{n+1} + e_n)\partial e_n - |\beta| \frac{1 + \alpha e_{n+1}}{2} \partial e_{n+1} - |\beta| \frac{1 + \alpha e_n}{2} \partial e_n \\
&\quad = \left[2\alpha + \alpha^2(e_{n+1} + e_n) - |\beta| \frac{1 + \alpha e_{n+1}}{2} - |\beta| \frac{1 + \alpha e_n}{2}\right] \partial e_n - |\beta| \frac{1 + \alpha e_{n+1}}{2} \partial^2 e_n \\
&\quad = (2\alpha - |\beta|) \frac{2 + \alpha(e_{n+1} + e_n)}{2} \partial e_n - |\beta| \frac{1 + \alpha e_{n+1}}{2} \partial^2 e_n \\
&\quad \le |\beta| \frac{1 + \alpha e_{n+1}}{2} [\partial^2 e_n]_-
\end{aligned}$$

since $\partial e_n \le 0$ and $1 + \alpha e_{n+1} > 0$. Hence, (4.2) holds by $\sum_n n[\partial^2 e_n]_- < \infty$ (i.e., $\{c_n, d_n\}$ is admissible). Theorem 4.1 finishes the proof. $\square$

Corollary 4.17. *Let $2\alpha \ge |\beta|$, $e_n \downarrow 0$, $\gamma > 0$, $\varepsilon > 0$, and*

$$a_n \equiv 1 + \frac{\alpha}{n^\gamma} + e_n + O(n^{-1-\varepsilon}), \qquad b_n \equiv \frac{\beta}{n^\gamma} + O(n^{-1-\varepsilon}).$$

Then $Z(J) < \infty$.

Remarks. In these cases, $-\sum_{n=1}^{N}\ln(a_n)$ diverges to $-\infty$. This is only consistent with (3.69) because $\mathcal{E}_0(J)=\infty$, that is, the eigenvalue sum diverges and the two infinities cancel.

Proof. By the remark after Theorem 4.16 and by the proof, $\{1+\alpha n^{-\gamma},\beta n^{-\gamma}\}$ is admissible if $2\alpha\geq|\beta|$. By Lemma 4.8, $\{1+\alpha n^{-\gamma}+e_n,\beta n^{-\gamma}\}$ is admissible. Then use Theorem 4.1. □

A natural question here is what happens if we allow errors more general than just $O(n^{-1-\varepsilon})$, but still small compared to the leading term of the perturbation. As for the $Z(J)=\infty$ result in Theorem 4.16, it certainly holds for such errors, as can be seen from the arguments in the proof.

On the other hand, the stability of $Z(J)<\infty$ is unclear. One can easily see that we need strong hypotheses at $2\alpha=|\beta|$, the boundary of the "Szegő" region. For example, if $a_n=1+\alpha n^{-1}-(n\ln(n))^{-1}$ and $b_n=2\alpha n^{-1}$, then the Szegő condition fails (at -2), as follows from Theorem 3.24. Hence, in this case one cannot expect more than trace class errors to preserve the Szegő condition. Inside the "Szegő" region the situation might be different, but at the present time we are not able to treat even trace class errors for $2\alpha\geq|\beta|$ (see Conjecture 3.13).

Let us now return to considering perturbations of a single a_n. As noted in Section 4.2, decreasing it can only guarantee decrease of $|E_1^{\pm}|$. However, if we know that J has *no* bound states, then this is sufficient to conclude that no new bound states can appear when decreasing a_n.

Theorem 4.18. *Assume that J with $a_n\to 1$, $b_n\to 0$ has only finitely many bound states, and let $\tilde{J}$ have $\tilde{a}_n\leq a_n$ and $\tilde{b}_n=b_n$ with $\tilde{a}_n\to 1$. Then $Z(\tilde{J})<\infty$ if and only if $Z(J)<\infty$ and $\sum_n(a_n-\tilde{a}_n)<\infty$. In any case, $\tilde{J}$ also has only finitely many bound states.*

Proof. We only need to prove this theorem for J with no bound states. For by Theorem 2.2(i),(ii), J has finitely many of them if and only if $J^{(n)}$ has none for large enough n — one only needs to choose n to be larger than the last crossing of zero of some eigenfunction for energy 2 and the last non-crossing of zero of an eigenfunction for -2. And by (3.47), J is Szegő if and only if $J^{(n)}$ is.

So let us assume that J has no bound states. Then by the above discussion, $\tilde{J}$ has none as well. Indeed, if we let $\tilde{J}_n$ have $a_j(\tilde{J}_n) \equiv \tilde{a}_j$ for $j = 1, \dots, n$ and all other entries same as J, then $\tilde{J}_n$ is created from $\tilde{J}_{n-1}$ by decreasing a_n. Since $\tilde{J}_{n-1}$ has no bound states, the same must be true for $\tilde{J}_n$. Since $\tilde{J}_n \to \tilde{J}$ in norm, $\tilde{J}$ also has no bound states.

If $Z(J) < \infty$ and $\sum(a_n - \tilde{a}_n) < \infty$, then $Z(\tilde{J}) < \infty$ by (4.22). No bound states and Theorem 3.14(d) imply $\bar{A}_0(J) > -\infty$. So if $\sum(a_n - \tilde{a}_n) = \infty$, we obtain $\bar{A}_0(\tilde{J}) = \infty$, and then $Z(\tilde{J}) = \infty$ by Theorem 3.14(c). Finally, if $Z(J) = \infty$, then no bound states and Theorem 3.14(a) give $\bar{A}_0(J) = \infty$. This implies $\bar{A}_0(\tilde{J}) = \infty$ and so again $Z(\tilde{J}) = \infty$. □

Since Theorem 3.14 does not distinguish between no bound states and $\mathcal{E}_0(J) < \infty$, we can extend the above result to that case, but we need to restrict it to δ-minorating perturbations of the a_n's only (e.g., decreasing a_n by $e_n \downarrow 0$). If $\mathcal{E}_0(J) = \infty$, then such a result cannot be generally true. For example, if $a_n \equiv 1 + \alpha/n$ and $b_n \equiv \beta/n$ with $2\alpha > |\beta|$, then decreasing α by $\alpha - |\beta|/2$ results into a non-summable change of the a_n's, but the matrix stays Szegő.

4.4 One-Sided Szegő Conditions

In this section we will discuss Jacobi matrices which are Szegő at 2 or -2. That is, such that $Z_1^+(J) < \infty$ or $Z_1^-(J) < \infty$. One might say that a better definition would be to call J Szegő at ± 2 if the Szegő integral converges at ± 2, without any conditions on the rate of divergence at ∓ 2. We cannot object to this, but note that in the case $J = J_0$+Hilbert-Schmidt (i.e., $J - J_0 \in \mathfrak{I}_2$), which we will consider here, these two definitions coincide. Indeed, for such J we know from Theorem 3.18 that

$$Z_2^-(J) < \infty. \tag{4.26}$$

That, of course, means that $Z(J)$ can only diverge at ± 2, and it diverges at ± 2 if and only if $Z_1^{\pm}(J) = \infty$ (since the weight in $Z_1^{\pm}$ has the same decay at ∓ 2 as the one in Z_2^{-}).

Hence we will use the sum rules (3.48) and (3.49) in this section. Just as with $Z(J)$, the infinite sums are always absolutely convergent and (3.48), (3.49) hold even if $Z_1^{\pm}(J) = \infty$. This shows that the one-sided Szegő conditions are also stable under finite rank perturbations.

Actually, we will only consider the Szegő condition at 2 and use only (3.48). The reason for this is the spectral symmetry discussed in Section 2.2. Therefore, our results for 2 will immediately translate into similar results for -2.

As in the previous section, the main tool for handling trace class perturbations will be the following inequality, which we obtain from (3.48) just as we obtained (4.22) from (3.47) (with the same $\tilde{J}_n$). With $\xi^+(E)$ from (3.44) we have

$$\begin{aligned} Z_1^+(\tilde{J}) \le Z_1^+(J) &+ \sum_{j=1}^{\infty} |\ln(\tilde{a}_j) - \ln(a_j)| + \tfrac{1}{2} \sum_{j=1}^{\infty} |\tilde{b}_j - b_j|, \\ &+ \liminf_{n\to\infty} \sum_{j,\pm} \Big[\xi^+\big(E_j^{\pm}(\tilde{J}_n)\big) - \xi^+\big(E_j^{\pm}(J)\big)\Big]. \end{aligned} \tag{4.27}$$

A direct computation shows that $\xi^+(E)$ is increasing and positive on $[2,\infty)$, and increasing and negative on $(-\infty,-2]$. This means that the last sum in (4.27) will be negative whenever $E_j^+(\tilde{J}_n) \le E_j^+(J)$ and $E_j^-(\tilde{J}_n) \le E_j^-(J)$ for all j. In particular, if $\tilde{a}_j = a_j$ and $\tilde{b}_j \le b_j$ for all j.

Theorem 4.19. *Suppose $J - J_0$ is compact.*

(i) *If J is Szegő at 2, and $\tilde{J}$ has $\tilde{a}_n = a_n$, $\tilde{b}_n \le b_n$ with $\sum_n (b_n - \tilde{b}_n) < \infty$, then $\tilde{J}$ is also Szegő at 2.*

(ii) *If J is Szegő at -2, and $\tilde{J}$ has $\tilde{a}_n = a_n$, $\tilde{b}_n \ge b_n$ with $\sum_n (\tilde{b}_n - b_n) < \infty$, then $\tilde{J}$ is also Szegő at -2.*

(iii) *Let $\hat{J}$ have $\hat{a}_n = a_n$, $\hat{b}_n \ge b_n$ with $\sum_n (\hat{b}_n - b_n) < \infty$, and let both $J, \hat{J}$ be Szegő. If $\tilde{J}$ has $\tilde{a}_n = a_n$ and $b_n \le \tilde{b}_n \le \hat{b}_n$, then $\tilde{J}$ is also Szegő.*

Proof. (i) follows from the discussion above, (ii) from (i) by symmetry, and (iii) from

(i) and (ii) and the fact that J is Szegő if and only if it is Szegő at both ± 2. $\square$

When perturbing the a_n's as in Section 4.2, we have to be careful with negative bound states. Indeed, decreasing all $|E_j^{\pm}|$ does not necessarily make the last sum in (4.27) negative because $\xi^+(E)$ increases on $(-\infty, -2]$. This problem can be overcome if the contribution of the $E_j^-(J)$'s to that sum is finite. Since for $E \sim -2$ we have $\xi^+(E) = O(|E+2|^{3/2})$ by (3.77), this means that we need

$$\sum_j |E_j^-(J) + 2|^{3/2} < \infty. \tag{4.28}$$

Then the lim inf in (4.27) will be bounded from above as long as every change $\tilde{J}_{n-1} \to \tilde{J}_n$ decreases all $E_j^+ \in (2, 2+\delta)$, irrespective of what happens to E_j^- (because $\xi^+(E_j^-(\tilde{J}_n)) \leq 0$). By Theorem 3.18, (4.28) holds whenever $J - J_0 \in \mathfrak{I}_2$.

But before we can use this idea to handle certain trace class perturbations as in Section 4.3, we first need to find some a_n, b_n to be perturbed. Our aim is to treat the case $a_n = 1 + \alpha n^{-\gamma} + O(n^{-1-\varepsilon})$ and $b_n = \beta n^{-\gamma} + O(n^{-1-\varepsilon})$ with $2\alpha > \pm\beta$, and show that such J is Szegő at ∓ 2. Since we need $J - J_0 \in \mathfrak{I}_2$, we will consider $\gamma > \frac{1}{2}$. To prove the next result, we will return to the methods of Section 4.1.

Lemma 4.20. *Suppose $a_n \to 1$, $b_n \to 0$.*

(i) *Let $\{a_n\}$ be eventually strictly monotone and*

$$\frac{a_n - a_{n-1}}{a_{n+1} - a_n} \to 1, \qquad \frac{b_{n+1} - b_n}{a_{n+1} - a_n} \to \omega \tag{4.29}$$

with ω finite. If eventually

$$\omega \operatorname{sgn}(a_{n+1} - a_n) < -2 \operatorname{sgn}(a_{n+1} - a_n),$$

then there are $\delta > 0$, $c > 0$ such that $\nu'(x) \geq c\sqrt{4 - x^2}$ for $x \in (2-\delta, 2)$.

(ii) *Let $\{b_n\}$ be eventually strictly monotone and*

$$\frac{b_n - b_{n-1}}{b_{n+1} - b_n} \to 1, \qquad \frac{a_{n+1} - a_n}{b_{n+1} - b_n} \to \omega_1 \tag{4.30}$$

with ω_1 finite. If eventually

$$\omega_1 \operatorname{sgn}(b_{n+1}-b_n) < -\tfrac{1}{2} \operatorname{sgn}(b_{n+1}-b_n),$$

then there are $\delta > 0$, $c > 0$ such that $\nu'(x) \geq c\sqrt{4-x^2}$ for $x \in (2-\delta, 2)$.

Remarks. 1. (ii) is (i) with $\omega_1 = \omega^{-1}$. It handles the case $\omega = \pm\infty$.

2. In particular, such J is Szegő at 2 if $J - J_0 \in \mathfrak{I}_2$.

3. By symmetry, the same result holds for the Szegő condition at -2, with "< -2" and "$< -\frac{1}{2}$" replaced by "> 2" and "$< \frac{1}{2}$."

Proof. (i) First notice that (4.13) holds because a_n is (eventually) monotone, and either b_n is monotone (if $\omega \neq 0$) or $|b_{n+1}-b_n| \leq |a_{n+1}-a_n|$ (if $|\omega| < 1$). Hence, we can use Lemma 4.3. This time we will work with S_n instead of R_n, because it has a simpler recurrence relation (4.4). Notice that by the proof of Lemma 4.3, for every $|x| < 2$ we have $S_n(x) \to \sqrt{4-x^2}/2\pi\nu'(x)$ as $n \to \infty$. The result will follow if we prove that $S_n(x) \leq C$ for some $C < \infty$, all $x \in (2-\delta, 2)$, and all large n.

We will show this by proving that for some K and all large enough n we have $S_{n+K-1}(x) \leq S_{n-1}(x)$ for all $x \in (2-\delta, 2)$. That is, we will iterate (4.4) K times at once. Here $K \geq 3$ and $\delta > 0$ will be fixed, but they will not be specified until later.

We let n be large and such that for all $j \geq n$ we have $|a_j - 1| < \delta$ and $|b_j| < \delta$, and we take $x \in (2-\delta, 2)$. Then by (2.5) in the form (4.15) we obtain for $P_n \equiv P_n(x)$ and $k \in \{0, \ldots, K-1\}$

$$P_{n+k} = (k+1)P_n - kP_{n-1} + O(\delta)(|P_n| + |P_{n-1}|).$$

We also have

$$\begin{aligned} a_{n+k+1}^2 - a_{n+k}^2 =& (a_{n+k+1} - a_{n+k})(2 + o(1)), \\ a_{n+k}(b_{n+k+1} - b_{n+k}) =& (a_{n+k+1} - a_{n+k})(\omega + o(1)) \end{aligned}$$

with $o(1) = o(n^0)$ taken w.r.t. n. From these estimates we obtain

$$\begin{aligned} S_{n+k} - S_{n+k-1} &= (a_{n+k+1}^2 - a_{n+k}^2)P_{n+k}^2 + a_{n+k}(b_{n+k+1} - b_{n+k})P_{n+k}P_{n+k-1} \\ &= (a_{n+k+1} - a_{n+k})\Big\{ \big[(2+o(1))(k+1)^2 + (\omega + o(1))k(k+1)\big] P_n^2 \\ &\quad - \big[(2+o(1))2k(k+1) + (\omega + o(1))(2k^2-1)\big] P_n P_{n-1} \\ &\quad + \big[(2+o(1))k^2 + (\omega + o(1))k(k-1)\big] P_{n-1}^2 \\ &\quad + O(\delta)(P_n^2 + P_{n-1}^2)\Big\}, \end{aligned}$$

where the $O(\delta)$ also depends on K and ω (but not on x or n). Using the identities $\sum_{k=0}^{K-1} k^2 = K(2K^2 - 3K + 1)/6$, $\sum_{k=0}^{K-1} k = K(K-1)/2$, and $a_{n+k+1} - a_{n+k} = (a_{n+1} - a_n)(1 + o(1))$, we obtain for $K \geq 3$,

$$\begin{aligned} \frac{3}{K}\frac{S_{n+K-1} - S_{n-1}}{a_{n+1} - a_n} =& O(\delta)(P_n^2 + P_{n-1}^2) \\ &+ \big[2K^2 + 3K + 1 + \omega(K^2 - 1) + o(1)\big] P_n^2 \\ &- \big[4K^2 - 4 + \omega(2K^2 - 3K - 2) + o(1)\big] P_n P_{n-1} \\ &+ \big[2K^2 - 3K + 1 + \omega(K^2 - 3K + 2) + o(1)\big] P_{n-1}^2 \end{aligned}$$

where both $O(\delta)$ and $o(1)$ depend on K and ω. Let I, II, III denote the three square brackets in the above expression, without the $o(1)$ terms. If $I \cdot III - (II/2)^2 > 0$, then for small enough δ and large n (so that $O(\delta)$ and $o(1)$ are negligible) the above expression will have the same sign as I. We have $I \cdot III - (II/2)^2 > 0$ whenever

$$\omega \notin [c_1(K), c_2(K)] \equiv \left[-2 - \frac{6 + 2\sqrt{3}\sqrt{K^2-1}}{K^2 - 4}, -2 - \frac{6 - 2\sqrt{3}\sqrt{K^2-1}}{K^2 - 4}\right].$$

Also, $I > 0$ when $\omega > d(K) \equiv -(2K^2 + 3K + 1)/(K^2 - 1)$, and $I < 0$ when $\omega < d(K)$. Since $c_1(K), c_2(K), d(K) \to -2$ as $K \to \infty$, and by the above,

$$\operatorname{sgn}(S_{n+K-1} - S_{n-1}) = \operatorname{sgn}(a_{n+1} - a_n)\operatorname{sgn}(I),$$

one only needs to take K large so that $\omega > \max\{c_2(K), d(K)\}$ (if $\operatorname{sgn}(a_{n+1} - a_n) = -1$)

or $\omega < \min\{c_1(K), d(K)\}$ (if $\operatorname{sgn}(a_{n+1} - a_n) = 1$). Then for small enough δ and all large n one obtains $\operatorname{sgn}(S_{n+K-1}(x) - S_{n-1}(x)) = -1$ whenever $x \in (2-\delta, 2)$. The result follows.

(ii) The proof is as in (i), but with the role of $a_{n+1} - a_n$ played by $b_{n+1} - b_n$. We obtain $I = \omega_1(2K^2+3K+1)+K^2-1$ and $\operatorname{sgn}(S_{n+K-1} - S_{n-1}) = \operatorname{sgn}(b_{n+1} - b_n)\operatorname{sgn}(I)$ whenever

$$\omega_1 \notin \left[-\frac{1}{2} - \frac{\sqrt{3}}{2\sqrt{K^2-1}}, -\frac{1}{2} + \frac{\sqrt{3}}{2\sqrt{K^2-1}}\right].$$

□

Now we are ready to introduce errors and state the main result of this section.

Theorem 4.21. *Suppose $\tilde{J}$ has*

$$\tilde{a}_n \equiv a_n + O(n^{-1-\varepsilon}), \qquad \tilde{b}_n \equiv b_n + O(n^{-1-\varepsilon})$$

with $\sum_{n=1}^{\infty} \left[(a_n-1)^2 + b_n^2\right] < \infty$ and $\varepsilon > 0$.

(i) *Assume a_n, b_n satisfy (4.29) and $n^{2+\varepsilon}|a_{n+1} - a_n| \to \infty$. If eventually*

$$\omega \operatorname{sgn}(a_{n+1} - a_n) < -2 \operatorname{sgn}(a_{n+1} - a_n),$$

then $\tilde{J}$ is Szegő at 2. If eventually

$$\omega \operatorname{sgn}(a_{n+1} - a_n) > 2 \operatorname{sgn}(a_{n+1} - a_n),$$

then $\tilde{J}$ is Szegő at -2.

(ii) *Assume a_n, b_n satisfy (4.30) and $n^{2+\varepsilon}|b_{n+1} - b_n| \to \infty$. If eventually*

$$\omega_1 \operatorname{sgn}(b_{n+1} - b_n) < -\tfrac{1}{2} \operatorname{sgn}(b_{n+1} - b_n),$$

then $\tilde{J}$ is Szegő at 2. If eventually

$$\omega_1 \operatorname{sgn}(b_{n+1} - b_n) < \tfrac{1}{2} \operatorname{sgn}(b_{n+1} - b_n),$$

then $\tilde{J}$ is Szegő at -2.

Remark. Notice that if $\sup\{n^{2+\varepsilon}|a_{n+1}-a_n|\}<\infty$, then $|a_n-1|\lesssim n^{-1-\varepsilon}$ and since (in (i)) ω is finite, we also have $|b_n|\lesssim n^{-1-\varepsilon}$. Hence, $J-J_0$ is trace class and so Szegő by Corollary 3.16.

Proof. (i) We follow the proof of Theorem 4.1. First we increase a_n by $6Cn^{-1-\varepsilon}$ with C from (4.23). We have

$$\frac{a_n+\frac{6C}{n^{1+\varepsilon}}-a_{n-1}-\frac{6C}{(n-1)^{1+\varepsilon}}}{a_{n+1}+\frac{6C}{(n+1)^{1+\varepsilon}}-a_n-\frac{6C}{n^{1+\varepsilon}}}-\frac{a_n-a_{n-1}}{a_{n+1}-a_n}=\frac{O(1)}{n^{2+\varepsilon}(a_{n+1}-a_n)+O(1)}\to 0.$$

So if we call $a_n+6Cn^{-1-\varepsilon}$ again a_n, we still have $(a_n-a_{n-1})/(a_{n+1}-a_n)\to 1$. Similarly, $(b_{n+1}-b_n)/(a_{n+1}-a_n)\to\omega$. And, of course, $\{a_n\}$ has the same type of monotonicity as before, by the assumption $n^{2+\varepsilon}|a_{n+1}-a_n|\to\infty$. We call the matrix with these new a_n, b_n again J. By hypothesis $J-J_0\in\mathfrak{I}_2$, so J is Szegő at 2 by Lemma 4.20(i) and (4.26).

Now we consider the same $\tilde{J}_n$ as in the proof of Theorem 4.1. The first of them is $\tilde{J}_{N-1}$ and it is Szegő at 2 because it is a finite rank perturbation of J. Each next $\tilde{J}_n$ will δ-minorate $\tilde{J}_{n-1}$. That proves that in (4.27) (with $\tilde{J}_{N-1}$ in place of J) the sum involving E_j^+ will be bounded above by $K\xi^+(M)$ with K and M as in Lemma 4.14. The sum with E_j^- will be bounded above by $c=\sum_j[-\xi^+(E_j^-(\tilde{J}_{N-1}))]$, and this is finite by (3.77) and (4.28) (which holds because $\tilde{J}_{N-1}-J_0\in\mathfrak{I}_2$). So the $\liminf$ in (4.27) cannot be $+\infty$ and the result follows.

(ii) The proof is identical. □

Corollary 4.22. *Let $\gamma>\frac{1}{2}$, $\varepsilon>0$, and*

$$a_n\equiv 1+\frac{\alpha}{n^\gamma}+O(n^{-1-\varepsilon}),\qquad\qquad b_n\equiv\frac{\beta}{n^\gamma}+O(n^{-1-\varepsilon}).\tag{4.31}$$

If $2\alpha>\pm\beta$, then J is Szegő at ∓ 2.

Proof. If $\gamma>1$, then $Z(J)<\infty$ by Corollary 3.16, and so $Z_1^{\pm}(J)<\infty$. If $\gamma\in(\frac{1}{2},1]$, then use Theorem 4.21(i) (if $\alpha\neq 0$) or (ii) (if $\alpha=0$) with a_n, b_n in that theorem being $1 + \alpha n^{-\gamma}$ and $\beta n^{-\gamma}$. □

As for other pairs (α, β) in (4.31), Theorem 3.17(iii) shows that if $2\alpha < \pm\beta$, then J cannot be Szegő at ∓ 2. Hence, the (α, β) plane is divided into four regions by the lines $2\alpha = \pm\beta$. Inside the right-hand region J is Szegő, inside the top and bottom regions J is Szegő only at, respectively, 2 and -2, and inside the left-hand region J is Szegő neither at 2 nor at -2. On the borderlines the situation is as follows. If $2\alpha = \pm\beta$ and $\alpha \geq 0$, then Corollary 4.17 shows that J is Szegő, and so Szegő at both 2 and -2. If $2\alpha = \pm\beta$ and $\alpha < 0$, then J cannot be Szegő at ± 2 by Theorem 3.17(iii). It is possible that such J is Szegő at ∓ 2.

By this, the picture from Chapter 1 is justified.

4.5 Appendix to Chapter 4

In this appendix we prove auxiliary results which we used in the present chapter. The following lemma from [16] was applied in the proof of Lemma 4.2:

Lemma 4.23. *If $Q(x)$ is a polynomial of degree at most $n-1$ and for $|x| \leq 2$,*

$$\sqrt{4 - x^2}\, |Q(x)| \leq 1, \tag{4.32}$$

then for $|x| \leq 2$,

$$|Q(x)| \leq \frac{n}{2}.$$

In the proof we will need the *Gauss-Jacobi quadrature* for the Chebyshev polynomials of the first kind:

Lemma 4.24. *Let $x_j \equiv \cos\big((2j-1)\pi/2n\big)$ with $j = 1, \ldots, n$ be the roots of the Chebyshev polynomial of the first kind $T_n(x)$. If $Q(x)$ is a polynomial of degree at most $n-1$, then*

$$Q(2x) = \sum_{j=1}^{n} \frac{(-1)^{j-1}}{n} \sqrt{1 - x_j^2}\, Q(2x_j) \frac{T_n(x)}{x - x_j}. \tag{4.33}$$

Proof. By (2.10), $T_n(x) = \cos(n \arccos(x))$ for $|x| \le 1$. Since x_j is a root of $T_n(x)$, the right-hand side of (4.33) (denoted $\tilde{Q}(2x)$) is a polynomial of degree at most $n-1$. Obviously $\lim_{x \to x_j} T_n(x)/(x - x_j) = T_n'(x_j)$. Moreover,

$$T_n'(x) = [\cos(n \arccos(x))]' = \frac{n \sin(n \arccos(x))}{\sqrt{1 - x^2}}, \tag{4.34}$$

and so

$$T_n'(x_j) = \frac{(-1)^{j-1} n}{\sqrt{1 - x_j^2}}.$$

Since for $j = 1, \ldots, n$,

$$\tilde{Q}(2x_j) = \frac{(-1)^{j-1}}{n} \sqrt{1 - x_j^2}\, Q(2x_j) T_n'(x_j) = Q(2x_j),$$

and both Q and $\tilde{Q}$ are of degree $n-1$, they must coincide. □

Proof of Lemma 4.23. Let x_j be as in Lemma 4.24. First assume $2x_n \le x \le 2x_1$. Then

$$|Q(x)| \le \left(4 - x_1^2\right)^{-\frac{1}{2}} = \left(4 - 4\cos^2\left(\tfrac{\pi}{2n}\right)\right)^{-\frac{1}{2}} = \frac{1}{2\sin\left(\frac{\pi}{2n}\right)} \le \frac{n}{2}$$

because $|x_1| = |x_n|$ and $\sin(\frac{\pi}{2n}) \ge \frac{1}{n}$.

Now let $x > 2x_1$ (the case $x < 2x_n$ is identical) and put $y \equiv \frac{x}{2}$. By (4.32) and (4.33),

$$|Q(x)| = |Q(2y)| \le \frac{|T_n(y)|}{2n} \sum_{j=1}^{n} \left| \frac{1}{y - x_j} \right| = \frac{1}{2n} \left| \sum_{j=1}^{n} \frac{T_n(y)}{y - x_j} \right|$$

because $y > x_j$ for all j. Now since x_j are precisely the roots of $T_n(y)$, the last sum is just $T_n'(y)$. We have

$$|T_n'(y)| = n \left| \frac{\sin n\theta}{\sin \theta} \right| \le n^2$$

by (4.34) with $y = \cos\theta$ and induction on n. Hence $|Q(x)| \le \frac{n^2}{2n} = \frac{n}{2}$. □

The following result from [15] was used in the proof of Lemma 4.3:

Theorem 4.25. *Suppose* $\lim_{n\to\infty} a_n = 1$, $\lim_{n\to\infty} b_n = 0$, *and*

$$\sum_{n=1}^{\infty} \big(|a_{n+1} - a_n| + |b_{n+1} - b_n|\big) < \infty. \tag{4.35}$$

Then the spectral measure of J is purely absolutely continuous in $(-2, 2)$ with continuous density $\nu'(x) > 0$. Moreover, for any energy $x \in (-2, 2)$, all eigenfunctions are bounded and

$$\lim_{n\to\infty} \big[P_{n+1}^2(x) - xP_{n+1}(x)P_n(x) + P_n^2(x)\big] = \frac{\sqrt{4 - x^2}}{2\pi\nu'(x)}. \tag{4.36}$$

Remarks. 1. In [15], $a_n \to \frac{1}{2}$ and the limit is $2\sqrt{1 - x^2}/\pi\nu'(x)$.

2. With slightly more effort one can show that the m-function is continuous on $\mathbb{C}^+ \cup (-2, 2)$.

3. Results relating density of the absolutely continuous part of the spectral measure and asymptotics of the solutions of difference (or differential) equations, under the assumption of finite variation of the potential, go back to Weidmann [40, 41].

Proof. We start with showing the existence of WKB asymptotics for energies in $(-2, 2)$, as in [31]. We fix $x \in (-2, 2)$ and define $\omega_n \equiv (x - b_n)/2a_n$. We let $\tilde{I} \subset (-1, 1)$ be a closed interval containing $\frac{x}{2}$ in its interior and consider n_0 such that $\omega_n \in \tilde{I}$ for all $n \geq n_0$. Then we have

$$|\omega_{n+1} - \omega_n| \leq \frac{|x| + |b_n|}{2a_n a_{n+1}}|a_{n+1} - a_n| + \frac{1}{2a_{n+1}}|b_{n+1} - b_n|. \tag{4.37}$$

Next we define

$$u_n^{\pm} = e^{\pm i \sum_{n_0}^{n} \arccos(\omega_j)} \tag{4.38}$$

for $n \geq n_0$. Then

$$a_{n+1}u_{n+1}^{\pm} + (b_{n+1} - x)u_n^{\pm} + a_n u_{n-1}^{\pm} = c_n^{\pm} u_n^{\pm} \tag{4.39}$$

with

$$\begin{aligned} c_n^{\pm} =& a_{n+1} e^{\pm i \arccos(\omega_{n+1})} + a_n e^{\mp i \arccos(\omega_n)} + b_{n+1} - x \\ =& \frac{b_{n+1} - b_n}{2} \pm i\Big(a_{n+1}\sqrt{1-\omega_{n+1}^2} - a_n\sqrt{1-\omega_n^2}\Big), \end{aligned}$$

since $\sin(\arccos(t)) = \sqrt{1-t^2}$. Hence

$$|c_n^{\pm}| \leq \frac{1}{2}|b_{n+1} - b_n| + |a_{n+1} - a_n| + a_n \frac{|\omega_{n+1} - \omega_n|}{\sqrt{1-\omega_n^2}} \leq C d_n$$

with $d_n \equiv |a_{n+1} - a_n| + |b_{n+1} - b_n|$, and $C < \infty$ depending on $\tilde{I}$. That is, $c_n^{\pm} \in \ell^1$.

We will also need the Wronskian of u^+ and u^- (which depends on n). We have

$$W_n(u^+, u^-) = a_n(u_n^+ u_{n-1}^- - u_{n-1}^+ u_n^-) = a_n(e^{i \arccos(\omega_n)} - e^{-i \arccos(\omega_n)})$$

and since $\omega_n \to \frac{x}{2}$,

$$\lim_{n\to\infty} W_n(u^+, u^-) = i\sqrt{4 - x^2}. \tag{4.40}$$

Now we turn to eigenfunctions φ_n for energy x. We will show that each of them asymptotically approaches a linear combination of u^+ and u^-. If

$$a_{n+1}\varphi_{n+1} + (b_{n+1} - x)\varphi_n + a_n\varphi_{n-1} = 0, \tag{4.41}$$

then we let α_n, β_n be such that

$$\begin{pmatrix} \varphi_n \\ \varphi_{n-1} \end{pmatrix} = \begin{pmatrix} u_n^+ & u_n^- \\ u_{n-1}^+ & u_{n-1}^- \end{pmatrix} \begin{pmatrix} \alpha_n \\ \beta_n \end{pmatrix}. \tag{4.42}$$

By (4.41),

$$\begin{pmatrix} u_{n+1}^+ & u_{n+1}^- \\ u_n^+ & u_n^- \end{pmatrix} \begin{pmatrix} \alpha_{n+1} \\ \beta_{n+1} \end{pmatrix} = \begin{pmatrix} \frac{x - b_{n+1}}{a_{n+1}} & -\frac{a_n}{a_{n+1}} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_n^+ & u_n^- \\ u_{n-1}^+ & u_{n-1}^- \end{pmatrix} \begin{pmatrix} \alpha_n \\ \beta_n \end{pmatrix}.$$

From this and (4.39),

$$\begin{pmatrix}\alpha_{n+1}\\ \beta_{n+1}\end{pmatrix} = \left[\mathrm{Id} + \frac{1}{W_{n+1}(u^+,u^-)}\begin{pmatrix}-c_n^+u_n^+u_n^- & -c_n^-u_n^-u_n^-\\ c_n^+u_n^+u_n^+ & c_n^-u_n^+u_n^-\end{pmatrix}\right]\begin{pmatrix}\alpha_n\\ \beta_n\end{pmatrix}$$
$$= (\mathrm{Id} + M_n)\begin{pmatrix}\alpha_n\\ \beta_n\end{pmatrix},$$

with

$$M_n \equiv \frac{1}{W_{n+1}(u^+,u^-)}\begin{pmatrix}-c_n^+ & -c_n^-(u_n^-)^2\\ c_n^+(u_n^+)^2 & c_n^-\end{pmatrix}$$

summable because $c_n^\pm \in \ell^1$. Hence for $D \equiv 2C/\sqrt{4-x^2}$ (so that $\|M_n\| \le Dd_n$ for large n) and $n \to \infty$,

$$\left\|\mathrm{Id} - \prod_n^\infty(\mathrm{Id} + M_j)\right\| \le e^{\sum_n^\infty \|M_j\|}\sum_n^\infty \|M_j\| \le e^{D\sum_n^\infty d_j}\, D\sum_n^\infty d_j \to 0. \tag{4.43}$$

It follows that $\alpha_n \to \alpha_\infty$ and $\beta_n \to \beta_\infty$. Then from $|u_n^\pm| = 1$ and (4.42) we have

$$\lim_{n\to\infty} |\varphi_n - (\alpha_\infty u_n^+ + \beta_\infty u_n^-)| = 0. \tag{4.44}$$

This proves boundedness of all eigenfunctions for energy x.

Before we proceed, we note that if we consider a closed interval of energies $I \subset (-2,2)$ instead of a single energy x, then n_0, C, and D can be chosen uniformly for $x \in I$, and (4.40), (4.43) also hold uniformly in x. Hence from now on we will consider all $x \in I$ with $I \subset (-2,2)$ an arbitrary closed interval.

Let us now prove the remaining claims for $J - J_0$ finite rank. For all small $\varepsilon \ge 0$ and $x \in I$ we let $\theta(x+i\varepsilon) \equiv \arccos(\frac{x+i\varepsilon}{2})$, taking the usual branch of arccos. Note that $\mathrm{Im}(\theta(x+i\varepsilon)) < 0$ for $\varepsilon > 0$. We define $u(x+i\varepsilon)$ to be the unique eigenfunction for energy $x+i\varepsilon$ such that $u_n(x+i\varepsilon) = e^{-i\theta(x+i\varepsilon)n}$ for large n. Then $u(x+i\varepsilon) \in \ell^2(\mathbb{Z}^+)$ for $\varepsilon > 0$ and so by (2.56),

$$m(x+i\varepsilon) = -\frac{u_0(x+i\varepsilon)}{u_{-1}(x+i\varepsilon)}.$$

Since $u_n(x+i\varepsilon)$ and $u_{n+1}(x+i\varepsilon)$ are obviously continuous up to $\varepsilon = 0$ for large n, by solving the eigenfunction equation backwards, so must be $u_{-1}(x+i\varepsilon)$ and $u_0(x+i\varepsilon)$. Also, $u_{-1}(x) \neq 0$, because $u_{-1}(x) = 0$ forces $u_0(x) \neq 0$, and then $u_n(x)/u_0(x)$ would be real for all n, which is a contradiction. In conclusion, $m(x+i\varepsilon)$ and each $u_n(x+i\varepsilon)$ are continuous in ε up to $\varepsilon = 0$. This shows that $\lim_{\varepsilon\downarrow 0} m(x+i\varepsilon)$ is finite and so there is no singular spectrum in $(-2,2)$ by Theorem 2.14. We define $m(x) \equiv m(x+i0) = \lim_{\varepsilon\downarrow 0} m(x+i\varepsilon)$.

Next we let $v_n(x) \equiv -u_n(x)/u_{-1}(x)$ so that $v_{-1}(x) = -1$ and $v_0(x) = m(x)$. Let $\eta(x) \equiv i|u_{-1}(x)|/u_{-1}(x)$ so that $|\eta(x)| = 1$ and $v_n(x) = i\eta(x)u_n(x)/|u_{-1}(x)|$. Since $v_n(x) - \overline{v_n(x)}$ is an eigenfunction for energy x with $v_{-1}(x) - \overline{v_{-1}(x)} = 0$ and $v_0(x) - \overline{v_0(x)} = 2i \operatorname{Im} m(x)$, the orthogonal polynomials clearly satisfy

$$P_n(x) = \frac{v_n(x) - \overline{v_n(x)}}{2i \operatorname{Im} m(x)}.$$

So for large n

$$P_n(x) = \frac{\eta(x)e^{-i\theta(x)n} + \overline{\eta(x)}e^{i\theta(x)n}}{2|u_{-1}(x)| \operatorname{Im} m(x)}. \tag{4.45}$$

Notice that $\operatorname{Im} m(x) = \operatorname{Im} v_0(x) \neq 0$ because otherwise $v_n(x)$ would be real for all n, which is a contradiction. Also notice that $J - J_0$ finite rank and (4.38) implies that $e^{-i\theta(x)n}/u_n^-(x)$ is constant in n for large n, and this constant has modulus 1. Similarly for $e^{i\theta(x)n}/u_n^+(x)$, and the two constants are complex conjugates of each other. It follows that if $P(x)$ plays the role of φ in (4.44), then

$$|\alpha_\infty(x)| = |\beta_\infty(x)| = \frac{1}{2|u_{-1}(x)| \operatorname{Im} m(x)}$$

and $\alpha_\infty(x) = \overline{\beta_\infty(x)}$. A direct computation, using (4.45) and $x = e^{i\theta(x)} + e^{-i\theta(x)}$, then gives for large n

$$P_{n+1}^2 - xP_{n+1}P_n + P_n^2 = |\alpha_\infty|^2\big(2 - e^{2i\theta} - e^{-2i\theta}\big) = |\alpha_\infty|^2(4 - x^2). \tag{4.46}$$

Looking at the Wronskian of v and $\bar{v}$ at $n = 0$ and at large n, we obtain

$$W(v, \overline{v}) = (-1)m - (-1)\overline{m} = -2i \operatorname{Im} m$$

and

$$W(v, \overline{v}) = \frac{1}{|u_{-1}|^2}\big(i\eta u_n \overline{i\eta u_{n-1}} - i\eta u_{n-1}\overline{i\eta u_n}\big) = \frac{2i \operatorname{Im}(u_n \overline{u_{n-1}})}{|u_{-1}|^2} = -i\frac{\sqrt{4-x^2}}{|u_{-1}|^2}.$$

By equating these we have

$$|\alpha_\infty(x)| = |\beta_\infty(x)| = \frac{1}{2|u_{-1}(x)| \operatorname{Im} m(x)} = \left[\frac{1}{2\sqrt{4-x^2} \operatorname{Im} m(x)}\right]^{\frac{1}{2}}. \tag{4.47}$$

Substituting this into (4.46) and using (2.54), we obtain (4.36) for a.e. x. By (4.46), $P_{n+1}^2(x) - xP_{n+1}(x)P_n(x) + P_n^2(x)$ is constant in n for large n, and it is obviously continuous on I for all n. So the density $\nu'(x)$ must be positive and continuous too. Since I was arbitrary, the result for finite rank $J - J_0$ follows. Notice that we have shown that in this case $\sqrt{4-x^2}/2\pi\nu'(x)$ is a polynomial, positive on $(-2, 2)$.

Now we return to general J. Let J_k be obtained from J by replacing a_n by 1 and b_n by 0 for $n > k$. Notice that n_0, C, D can be chosen uniformly for all $x \in I$ and all J_k. The functions $u_n^\pm$ will, of course, be k dependent, but $u_n^\pm(x; J_k) = u_n^\pm(x; J)$ whenever $n_0 \leq n \leq k$. Therefore also $\alpha_k(x; J_k) = \alpha_k(x; J)$. Moreover, obviously $|\alpha_\infty(x; J_k) - \alpha_k(x; J_k)| \to 0$ as $k \to \infty$ uniformly on I, and by (4.43) the same is true for $|\alpha_\infty(x; J) - \alpha_k(x; J)|$. Thus, $\alpha_\infty(x; J_k) \to \alpha_\infty(x; J)$ uniformly on I. The same holds for $\beta_\infty(x; J)$, and so $\alpha_\infty(x; J) = \overline{\beta_\infty(x; J)}$. This means that $\alpha_\infty(x; J) \neq 0$, because otherwise $P_n(x) \to 0$ by (4.44). Then, however, $W(P(x), \varphi(x)) = 0$ for any other eigenfunction $\varphi(x)$ (by (4.44), $\varphi_n(x)$ is bounded) and so $P_n(x) \equiv 0$, a contradiction. Therefore, $|\alpha_\infty(x; J)|$ must be bounded away from 0 and ∞ on I, because it is a uniform limit of continuous functions $|\alpha_k(x; J)|$, and hence continuous.

By the above, (4.47) for J_k, and (2.54), we have for $g_k(x) \equiv \nu'(x; J_k)$ and

$$g(x) \equiv \frac{1}{2\pi\sqrt{4-x^2}\,|\alpha_\infty(x;J)|^2} > 0,$$

that $g_k(x) \to g(x)$ uniformly on I. Since g_k are continuous, so is g. By Theorem 2.4 we know that $g_k(x)dx$ weakly converge to $d\nu(x)$ on I, so we must have $\nu'(x) = g(x)$ for $x \in I$, and $\nu_{\text{sing}}(I) = 0$. Since I was arbitrary, ν is purely a.c. in $(-2, 2)$ with positive continuous density. Finally, by (4.46) we have

$$\begin{aligned}
\lim_{k\to\infty} \left[P_{k+1}^2(x) - xP_{k+1}(x)P_k(x) + P_k^2(x)\right] &= \lim_{k\to\infty} |\alpha_\infty(x; J_{k+1})|^2(4-x^2) \\
&=|\alpha_\infty(x;J)|^2(4-x^2) \\
&=\frac{\sqrt{4-x^2}}{2\pi g(x)},
\end{aligned}$$

which is (4.36). The proof is complete. $\square$

Bibliography

[1] R. Askey and M. Ismail, *Recurrence relations, continued fractions, and orthogonal polynomials*, Mem. Amer. Math. Soc. **49** (1984).

[2] K. M. Case, *Orthogonal polynomials. II*, J. Math. Phys. **16** (1975), 1435–1440.

[3] J. Charris and M. E. H. Ismail, *On sieved orthogonal polynomials, V. Sieved Pollaczek polynomials*, SIAM J. Math. Anal. **18** (1987), 1177–1218.

[4] D. Damanik, D. Hundertmark, and B. Simon, *Bound states and the Szegő condition for Jacobi matrices and Schrödinger operators*, J. Funct. Anal., to appear.

[5] P. Deift and R. Killip, *On the absolutely continuous spectrum of one-dimensional Schrödinger operators with square summable potentials*, Comm. Math. Phys. **203** (1999), 341–347.

[6] S. A. Denisov, *On the coexistence of absolutely continuous and singular continuous components of the spectral measure for some Sturm-Liouville operators with square summable potentials*, J. Differential Equations, to appear.

[7] J. Dombrowski, *Tridiagonal matrix representations of cyclic self-adjoint operators II*, Pacific J. Math. **120** (1985), 47–53.

[8] J. Dombrowski and P. Nevai, *Orthogonal polynomials, measures and recurrence relations*, SIAM J. Math. Anal. **17** (1986), 752–759.

[9] A. Figotin and L. Pastur, *Spectra of random and almost-periodic operators*, Springer-Verlag, Berlin, 1992.

[10] H. Flaschka, *On the Toda lattice. II. Inverse-scattering solution*, Progr. Theoret. Phys. **51** (1974), 703–716.

[11] A. A. Gončar, *On convergence of Padé approximants for some classes of meromorphic functions*, Math. USSR Sb. **26** (1975), 555–575.

[12] D. Hundertmark and B. Simon, *Lieb-Thirring inequalities for Jacobi matrices*, J. Approx. Theory, to appear.

[13] R. Killip and B. Simon, *Sum rules for Jacobi matrices and their applications to spectral theory*, Ann. of Math., to appear.

[14] A. Laptev, S. Naboko, and O. Safronov, *On new relations between spectral properties of Jacobi matrices and their coefficients*, preprint.

[15] A. Máté and P. Nevai, *Orthogonal polynomials and absolutely continuous measures*, in Approximation Theory, IV, C.K. Chui et al., eds., Academic Press, New York, 1983, pp. 611–617.

[16] I. P. Natanson, *Constructive Function Theory*, Vol. 1, F. Ungar, New York, 1964.

[17] P. Nevai, *Orthogonal polynomials defined by a recurrence relation*, Trans. Amer. Math. Soc. **250** (1979), 369–384.

[18] P. Nevai, *Orthogonal polynomials*, Mem. Amer. Math. Soc. **18** (1979), no. 213, 185 pp.

[19] P. Nevai, *Géza Freud, orthogonal polynomials and Christoffel functions. A case study*, J. Approx. Theory **48** (1986), 3–167.

[20] P. Nevai, *Orthogonal polynomials, recurrences, Jacobi matrices, and measures*, in Progress in Approximation Theory (Tampa, FL, 1990), Springer Ser. Comput. Math., **19**, Springer, New York, 1992, pp.79–104.

[21] E. M. Nikishin, *Discrete Sturm-Liouville operators and some problems of function theory*, J. Sov. Math. **35** (1986), 2679–2744.

[22] F. Peherstorfer and P. Yuditskii, *Asymptotics of orthonormal polynomials in the presence of a denumerable set of mass points*, Proc. Amer. Math. Soc. **129** (2001), 3213–3220.

[23] F. Pollaczek, *Sur une généralisation des polynomes de Legendre*, C. R. Acad. Sci. Paris **228** (1949), 1363–1365.

[24] F. Pollaczek, *Systèmes de polynomes biorthogonaux qui généralisent les polynomes ultrasphériques*, C. R. Acad. Sci. Paris **228** (1949), 1998–2000.

[25] F. Pollaczek, *Sur une famille de polynômes orthogonaux qui contient les polynômes d'Hermite et de Laguerre comme cas limites*, C. R. Acad. Sci. Paris **230** (1950), 1563–1565.

[26] M. Reed and B. Simon, *Methods of Modern Mathematical Physics, IV. Analysis of Operators*, Academic Press, New York, 1978.

[27] W. Rudin, *Real and Complex Analysis*, 3rd edition, Mc-Graw Hill, New York, 1987.

[28] J. A. Shohat, *Théorie Générale des Polinomes Orthogonaux de Tchebichef*, Mémorial des Sciences Mathématiques, Vol. 66, Gauthier-Villars, Paris, 1934.

[29] B. Simon, *Trace Ideals and Their Applications*, London Mathematical Society Lecture Notes Series, 35, Cambridge University Press, Cambridge-New York, 1979.

[30] B. Simon, *Spectral analysis of rank one perturbations and applications*, CRM Proceedings and Lecture Notes **8** (J. Feldman, R. Froese, L. Rosen, eds.), pp. 109–149, Amer. Math. Soc., Providence, RI, 1995.

[31] B. Simon, *Bounded eigenfunctions and absolutely continuous spectra for one-dimensional Schrödinger operators*, Proc. Amer. Math. Soc. **124** (1996), 3361–3369.

[32] B. Simon, *The classical moment problem as a self-adjoint finite difference operator*, Adv. Math. **137** (1998), 82–203.

[33] B. Simon and A. Zlatoš, *Sum rules and the Szegő condition for orthogonal polynomials on the real line*, Comm. Math. Phys., to appear.

[34] G. Szegő, *Beiträge zur Theorie der Toeplitzschen Formen, I, II*, Math. Z. **6** (1920), 167–202; **9** (1921), 167–190.

[35] G. Szegő, *On certain special sets of orthogonal polynomials*, Proc. Amer. Math. Soc. **1** (1950), 731–737.

[36] G. Szegő, *Orthogonal Polynomials*, 4th edition. American Mathematical Society, Colloquium Publications, Vol. XXIII. American Mathematical Society, Providence, R.I., 1975.

[37] G. Teschl, *Jacobi Operators and Completely Integrable Nonlinear Lattices*, American Mathematical Society, Providence, RI, 2000.

[38] W. Thirring, *Quantum Mechanics of Atoms and Molecules*, Springer-Verlag, New York, 1981.

[39] S. Verblunsky, *On positive harmonic functions*, Proc. London Math. Soc. **40** (1935), 290–320.

[40] J. Weidmann, *Zur Spektraltheorie von Sturm-Liouville-Operatoren*, Math. Z. **98** (1967), 268–302.

[41] J. Weidmann, *Absolut stetiges Spektrum bei Sturm-Liouville-Operatoren und Dirac-Systemen*, Math. Z. **180** (1982), 423–427.

[42] A. Zlatoš, *The Szegő condition for Coulomb Jacobi matrices*, J. Approx. Theory, to appear.