Annals of Mathematics, **158** (2003), 253–321

Sum rules for Jacobi matrices and their applications to spectral theory

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Abstract

We discuss the proof of and systematic application of Case's sum rules for Jacobi matrices. Of special interest is a linear combination of two of his sum rules which has strictly positive terms. Among our results are a complete classification of the spectral measures of all Jacobi matrices J for which $J - J_0$ is Hilbert-Schmidt, and a proof of Nevai's conjecture that the Szegő condition holds if $J - J_0$ is trace class.

1. Introduction

In this paper, we will look at the spectral theory of Jacobi matrices, that is, infinite tridiagonal matrices,

$$J = \begin{pmatrix} b_1 & a_1 & 0 & 0 & \cdots \\ a_1 & b_2 & a_2 & 0 & \cdots \\ 0 & a_2 & b_3 & a_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{1.1}$$

with $a_j > 0$ and $b_j \in \mathbb{R}$. We suppose that the entries of J are bounded, that is, $\sup_n |a_n| + \sup_n |b_n| < \infty$ so that J defines a bounded self-adjoint operator on $\ell^2(\mathbb{Z}_+) = \ell^2(\{1, 2, \ldots\})$. Let δ_j be the obvious vector in $\ell^2(\mathbb{Z}_+)$, that is, with components δ_{jn} which are 1 if $n = j$ and 0 if $n \neq j$.

The spectral measure we associate to J is the one given by the spectral theorem for the vector δ_1. That is, the measure μ defined by

$$m_\mu(E) \equiv \langle \delta_1, (J - E)^{-1} \delta_1 \rangle = \int \frac{d\mu(x)}{x - E}\,. \tag{1.2}$$

*The first named author was supported in part by NSF grant DMS-9729992. The second named author was supported in part by NSF grant DMS-9707661.

There is a one-to-one correspondence between bounded Jacobi matrices and unit measures whose support is both compact and contains an infinite number of points. As we have described, one goes from J to μ by the spectral theorem. One way to find J, given μ, is via orthogonal polynomials. Applying the Gram-Schmidt process to $\{x^n\}_{n=0}^{\infty}$, one gets orthonormal polynomials $P_n(x) = \kappa_n x^n + \cdots$ with $\kappa_n > 0$ and

$$\int P_n(x) P_m(x)\, d\mu(x) = \delta_{nm}. \tag{1.3}$$

These polynomials obey a three-term recurrence:

$$x P_n(x) = a_{n+1} P_{n+1}(x) + b_{n+1} P_n(x) + a_n P_{n-1}(x), \tag{1.4}$$

where a_n, b_n are the Jacobi matrix coefficients of the Jacobi matrix with spectral measure μ (and $P_{-1} \equiv 0$).

The more usual convention in the orthogonal polynomial literature is to start numbering of $\{a_n\}$ and $\{b_n\}$ with $n = 0$ and then to have (1.4) with (a_n, b_n, a_{n-1}) instead of (a_{n+1}, b_{n+1}, a_n). We made our choice to start numbering of J at $n = 1$ so that we could have z^n for the free Jost function (well known in the physics literature with $z = e^{ik}$) and yet arrange for the Jost function to be regular at $z = 0$. (Case's Jost function in [6, 7] has a pole since where we use u_0 below, he uses u_{-1} because his numbering starts at $n = 0$.) There is, in any event, a notational conundrum which we solved in a way that we hope will not offend too many.

An alternate way of recovering J from μ is the continued fraction expansion for the function $m_\mu(z)$ near infinity,

$$m_\mu(E) = \cfrac{1}{-E + b_1 - \cfrac{a_1^2}{-E + b_2 + \cdots}}. \tag{1.5}$$

Both methods for finding J essentially go back to Stieltjes' monumental paper [57]. Three-term recurrence relations appeared earlier in the work of Chebyshev and Markov but, of course, Stieltjes was the first to consider general measures in this context. While [57] does not have the continued fraction expansion given in (1.5), Stieltjes did discuss (1.5) elsewhere. Wall [62] calls (1.5) a J-fraction and the fractions used in [57], he calls S-fractions. This has been discussed in many places, for example, [24], [56].

That every J corresponds to a spectral measure is known in the orthogonal polynomial literature as Favard's theorem (after Favard [15]). As noted, it is a consequence for bounded J of Hilbert's spectral theorem for bounded operators. This appears already in the Hellinger-Toeplitz encyclopedic article [26]. Even for the general unbounded case, Stone's book [58] noted this consequence before Favard's work.

Given the one-to-one correspondence between μ's and J's, it is natural to ask how properties of one are reflected in the other. One is especially interested in J's "close" to the free matrix, J_0 with $a_n = 1$ and $b_n = 0$, that is,

$$J_0 = \begin{pmatrix} 0 & 1 & 0 & 0 & \dots \\ 1 & 0 & 1 & 0 & \dots \\ 0 & 1 & 0 & 1 & \dots \\ 0 & 0 & 1 & 0 & \dots \end{pmatrix}. \tag{1.6}$$

In the orthogonal polynomial literature, the free Jacobi matrix is taken as $\frac{1}{2}$ of our J_0 since then the associated orthogonal polynomials are precisely Chebyshev polynomials (of the second kind). As a result, the spectral measure of our J_0 is supported by $[-2,2]$ and the natural parametrization is $E = 2\cos\theta$.

Here is one of our main results:

THEOREM 1. *Let J be a Jacobi matrix and μ the corresponding spectral measure. The operator $J - J_0$ is Hilbert-Schmidt, that is,*

$$2\sum_n (a_n - 1)^2 + \sum b_n^2 < \infty \tag{1.7}$$

if and only if μ has the following four properties:

(0) (Blumenthal-Weyl Criterion) *The support of μ is $[-2,2] \cup \{E_j^+\}_{j=1}^{N_+} \cup \{E_j^-\}_{j=1}^{N_-}$ where $N_\pm$ are each zero, finite, or infinite, and $E_1^+ > E_2^+ > \cdots > 2$ and $E_1^- < E_2^- < \cdots < -2$ and if $N_\pm$ is infinite, then $\lim_{j\to\infty} E_j^\pm = \pm 2$.*

(1) (Quasi-Szegő Condition) *Let $\mu_{\mathrm{ac}}(E) = f(E)\,dE$ where μ_{ac} is the Lebesgue absolutely continuous component of μ. Then*

$$\int_{-2}^{2} \log[f(E)]\sqrt{4 - E^2}\,dE > -\infty. \tag{1.8}$$

(2) (Lieb-Thirring Bound)

$$\sum_{j=1}^{N_+} |E_j^+ - 2|^{3/2} + \sum_{j=1}^{N_-} |E_j^- + 2|^{3/2} < \infty. \tag{1.9}$$

(3) (Normalization) $\int d\mu(E) = 1$.

Remarks. 1. Condition (0) is just a quantitative way of writing that the essential spectrum of J is the same as that of J_0, viz. $[-2,2]$, consistent with the compactness of $J - J_0$. This is, of course, Weyl's invariance theorem [63], [45]. Earlier, Blumenthal [5] proved something close to this in spirit for the case of orthogonal polynomials.

2. Equation (1.9) is a Jacobi analog of a celebrated bound of Lieb and Thirring [37], [38] for Schrödinger operators. That it holds if $J - J_0$ is Hilbert-Schmidt has also been recently proven by Hundertmark-Simon [27], although

we do not use the $\frac{3}{2}$-bound of [27] below. We essentially reprove (1.9) if (1.7) holds.

3. We call (1.8) the quasi-Szegő condition to distinguish it from the Szegő condition,

$$\int_{-2}^{2} \log[f(E)](4-E^2)^{-1/2}\, dE > -\infty. \tag{1.10}$$

This is stronger than (1.8) although the difference only matters if f vanishes extremely rapidly at ± 2. For example, like $\exp(-(2-|E|)^{-\alpha})$ with $\frac{1}{2} \leq \alpha < \frac{3}{2}$. Such behavior actually occurs for certain Pollaczek polynomials [8].

4. It will often be useful to have a single sequence $e_1(J), e_2(J), \ldots$ obtained from the numbers $\left|E_j^{\pm} \mp 2\right|$ by reordering so $e_1(J) \geq e_2(J) \geq \cdots \to 0$.

By property (1), for any J with $J - J_0$ Hilbert-Schmidt, the essential support of the a.c. spectrum is $[-2, 2]$. That is, $\mu_{\rm ac}$ gives positive weight to any subset of $[-2, 2]$ with positive measure. This follows from (1.8) because f cannot vanish on any such set. This observation is the Jacobi matrix analogue of recent results which show that (continuous and discrete) Schrödinger operators with potentials $V \in L^p$, $p \leq 2$, or $|V(x)| \lesssim (1 + x^2)^{-\alpha/2}$, $\alpha > 1/2$, have a.c. spectrum. (It is known that the a.c. spectrum can disappear once $p > 2$ or $\alpha \leq 1/2$.) Research in this direction began with Kiselev [29] and culminated in the work of Christ-Kiselev [11], Remling [47], Deift-Killip [13], and Killip [28]. Especially relevant here is the work of Deift-Killip who used sum rules for finite range perturbations to obtain an *a priori* estimate. Our work differs from theirs (and the follow-up papers of Molchanov-Novitskii-Vainberg [40] and Laptev-Naboko-Safronov [36]) in two critical ways: we deal with the half-line sum rules so the eigenvalues are the ones for the problem of interest and we show that the sum rules still hold in the limit. These developments are particularly important for the converse direction (i.e., if μ obeys (0–3) then $J - J_0$ is Hilbert-Schmidt).

In Theorem 1, the only restriction on the singular part of μ on $[-2, 2]$ is in terms of its total mass. Given any singular measure $\mu_{\rm sing}$ supported on $[-2, 2]$ with total mass less than one, there is a Jacobi matrix J obeying (1.7) for which this is the singular part of the spectral measure. In particular, there exist Jacobi matrices J with $J - J_0$ Hilbert-Schmidt for which $[-2, 2]$ simultaneously supports dense point spectrum, dense singular continuous spectrum and absolutely continuous spectrum. Similarly, the only restriction on the norming constants, that is, the values of $\mu(\{E_j^{\pm}\})$, is that their sum must be less than one.

In the related setting of Schrödinger operators on $\mathbb{R}$, Denisov [14] has constructed an L^2 potential which gives rise to embedded singular continuous spectrum. In this vein see also Kiselev [30]. We realized that the key to

Denisov's result was a sum rule, not the particular method he used to construct his potentials. We decided to focus first on the discrete case where one avoids certain technicalities, but are turning to the continuum case.

While (1.8) is the natural condition when $J - J_0$ is Hilbert-Schmidt, we have a one-directional result for the Szegő condition. We prove the following conjecture of Nevai [43]:

THEOREM 2. *If $J - J_0$ is in trace class, that is,*

$$\sum_n |a_n - 1| + \sum_n |b_n| < \infty, \tag{1.11}$$

then the Szegő condition (1.10) *holds.*

Remark. Nevai [42] and Geronimo-Van Assche [22] prove the Szegő condition holds under the slightly stronger hypothesis

$$\sum_n (\log n)\,|a_n - 1| + \sum_n (\log n)\,|b_n| < \infty.$$

We will also prove

THEOREM 3. *If $J - J_0$ is compact and*

(i)

$$\sum_j \left|E_j^+ - 2\right|^{1/2} + \sum_j \left|E_j^- + 2\right|^{1/2} < \infty \tag{1.12}$$

(ii) $\limsup_{N\to\infty} a_1 \dots a_N > 0$

then (1.10) *holds.*

We will prove Theorem 2 from Theorem 3 by using a $\frac{1}{2}$ power Lieb-Thirring inequality, as proven by Hundertmark-Simon [27].

For the special case where μ has no mass outside $[-2, 2]$ (i.e., $N_+ = N_- = 0$), there are over seventy years of results related to Theorem 1 with important contributions by Szegő [59], [60], Shohat [49], Geronomius [23], Krein [33], and Kolmogorov [32]. Their results are summarized by Nevai [43] as:

THEOREM 4 (Previously Known). *Suppose μ is a probability measure supported on $[-2, 2]$. The Szegő condition* (1.10) *holds if and only if*

(i) *$J - J_0$ is Hilbert-Schmidt.*

(ii) *$\sum(a_n - 1)$ and $\sum b_n$ are (conditionally) convergent.*

Of course, the major difference between this result and Theorem 1 is that we can handle bound states (i.e., eigenvalues outside $[-2, 2]$) and the methods of Szegő, Shohat, and Geronimus seem unable to. Indeed, as we will see below, the condition of no eigenvalues is very restrictive. A second issue is that we focus on the previously unstudied (or lightly studied; e.g., it is mentioned in [39]) condition which we have called the quasi-Szegő condition (1.8), which is strictly weaker than the Szegő condition (1.10). Third, related to the first point, we do not have any requirement for conditional convergence of $\sum_{n=1}^{N}(a_n-1)$ or $\sum_{n=1}^{N} b_n$.

The Szegő condition, though, has other uses (see Szegő [60], Akhiezer [2]), so it is a natural object independently of the issue of studying the spectral condition.

We emphasize that the assumption that μ has no pure points outside $[-2,2]$ is extremely strong. Indeed, while the Szegő condition plus this assumption implies (i) and (ii) above, to deduce the Szegő condition requires only a very small part of (ii). We

THEOREM 4′. *If* $\sigma(J)\subset[-2,2]$ *and*

(i) $\limsup_N \sum_{n=1}^{N}\log(a_n) > -\infty$,

then the Szegő condition holds. If $\sigma(J)\subset[-2,2]$ *and either* (i) *or the Szegő condition holds*, *then*

(ii) $\sum_{n=1}^{\infty}(a_n-1)^2+\sum_{n=1}^{\infty} b_n^2<\infty$,

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

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

In particular, *if* $\sigma(J)\subset[-2,2]$, *then* (i) *implies* (ii)–(iv).

In Nevai [41], it is stated and proven (see pg. 124) that $\sum_{n=1}^{\infty}|a_n-1|<\infty$ implies the Szegő condition, but it turns out that his method of proof only requires our condition (i). Nevai informs us that he believes his result was probably known to Geronimus.

The key to our proofs is a family of sum rules stated by Case in [7]. Case was motivated by Flaschka's calculation of the first integrals for the Toda lattice for finite [16] and doubly infinite Jacobi matrices [17]. Case's method of proof is partly patterned after that of Flaschka in [17].

To state these rules, it is natural to change variables from E to z via

$$E = z + \frac{1}{z}\,. \tag{1.13}$$

We choose the solution of (1.13) with $|z|<1$, namely

$$z = \tfrac{1}{2}\Big[E-\sqrt{E^2-4}\,\Big], \tag{1.14}$$

where we take the branch of $\sqrt{}$ with $\sqrt{\mu}>0$ for $\mu>0$. In this way, $E\mapsto z$ is the conformal map of $\{\infty\} \cup \mathbb{C}\backslash[-2,2]$ to $D \equiv \{z \mid |z| < 1\}$, which takes ∞ to 0 and (in the limit) ± 2 to ± 1. The points $E \in [-2,2]$ are mapped to $z = e^{\pm i\theta}$ where $E = 2\cos\theta$.

The conformal map suggests replacing m_μ by

$$M_\mu(z) = -m_\mu\Big(E(z)\Big) = -m_\mu\Big(z + z^{-1}\Big) = \int \frac{z\, d\mu(x)}{1 - xz + z^2}\,. \tag{1.15}$$

We have introduced a minus sign so that $\operatorname{Im} M_\mu(z) > 0$ when $\operatorname{Im} z > 0$. Note that $\operatorname{Im} E > 0 \Rightarrow m_\mu(E) > 0$ but $E \mapsto z$ maps the upper half-plane to the lower half-disk.

If μ obeys the Blumenthal-Weyl criterion, M_μ is meromorphic on D with poles at the points $(\gamma_j^\pm)^{-1}$ where

$$|\gamma_j| > 1 \quad \text{and} \quad E_j^\pm = \gamma_j^\pm + (\gamma_j^\pm)^{-1}. \tag{1.16}$$

As with $E_j^\pm$, we renumber $\gamma_j^\pm$ to a single sequence $|\beta_1| \geq |\beta_2| \geq \cdots \geq 1$.

By general principles, M_μ has boundary values almost everywhere on the circle,

$$M_\mu(e^{i\theta}) = \lim_{r\uparrow 1} M_\mu(re^{i\theta}) \tag{1.17}$$

with $M_\mu(e^{-i\theta}) = \overline{M_\mu(e^{i\theta})}$ and $\operatorname{Im} M_\mu(e^{i\theta}) \geq 0$ for $\theta \in (0,\pi)$.

From the integral representation (1.2),

$$\operatorname{Im} m_\mu(E + i0) = \pi \frac{d\mu_{\rm ac}}{dE} \tag{1.18}$$

so using $dE = -2\sin\theta\, d\theta = -(4 - E^2)^{1/2}\, d\theta$, the quasi-Szegő condition (1.8) becomes

$$4\int_0^\pi \log[\operatorname{Im} M_\mu(e^{i\theta})] \sin^2\theta\, d\theta > -\infty$$

and the Szegő condition (1.10) is

$$\int_0^\pi \log[\operatorname{Im} M_\mu(e^{i\theta})]\, d\theta > -\infty.$$

Moreover, we have by (1.18) that

$$\tfrac{2}{\pi}\int_0^\pi \operatorname{Im}[M_\mu(e^{i\theta})] \sin\theta\, d\theta = \mu_{\rm ac}(-2,2) \leq 1. \tag{1.19}$$

With these notational preliminaries out of the way, we can state Case's sum rules. For future reference, we give them names:

$\underline{C_0}$:

$$\frac{1}{4\pi}\int_{-\pi}^{\pi} \log\left[\frac{\sin\theta}{\operatorname{Im} M(e^{i\theta})}\right] d\theta = \sum_j \log|\beta_j| - \sum_j \log|a_j| \tag{1.20}$$

and for $n = 1, 2, \ldots$,

$\mathbf{C_n}$:

$$-\frac{1}{2\pi}\int_{-\pi}^{\pi}\log\left[\frac{\sin\theta}{\operatorname{Im} M(e^{i\theta})}\right]\cos(n\theta)\,d\theta + \frac{1}{n}\sum_j(\beta_j^n - \beta_j^{-n}) = \frac{2}{n}\operatorname{Tr}\left\{T_n\left(\tfrac{1}{2}J\right) - T_n\left(\tfrac{1}{2}J_0\right)\right\} \tag{1.21}$$

where T_n is the n^{th} Chebyshev polynomial (of the first kind).

We note that Case did not have the compact form of the right side of (1.21), but he used implicitly defined polynomials which he did not recognize as Chebyshev polynomials (though he did give explicit formulae for small n). Moreover, his arguments are formal. In an earlier paper, he indicates that the conditions he needs are

$$|a_n - 1| + |b_n| \leq C(1 + n^2)^{-1} \tag{1.22}$$

but he also claims this implies $N_+ < \infty$, $N_- < \infty$, and, as Chihara [9] noted, this is false. We believe that Case's implicit methods could be made to work if $\sum n[|a_n - 1| + |b_n|] < \infty$ rather than (1.22). In any event, we will provide explicit proofs of the sum rules—indeed, from two points of view.

One of our primary observations is the power of a certain combination of the Case sum rules, $C_0 + \frac{1}{2}C_2$. It says

$\mathbf{P_2}$:

$$\frac{1}{2\pi}\int_{-\pi}^{\pi}\log\left(\frac{\sin\theta}{\operatorname{Im} M(\theta)}\right)\sin^2\theta\,d\theta + \sum_j[F(E_j^+) + F(E_j^-)] = \frac{1}{4}\sum_j b_j^2 + \frac{1}{2}\sum_j G(a_j) \tag{1.23}$$

where $G(a) = a^2 - 1 - \log|a|^2$ and $F(E) = \frac{1}{4}[\beta^2 - \beta^{-2} - \log|\beta|^4]$, with β given by $E = \beta + \beta^{-1}$, $|\beta| > 1$ (cf. (1.16)).

As with the other sum rules, the terms on the left-hand side are purely spectral—they can be easily found from μ; those on the right depend in a simple way on the coefficients of J.

The significance of (1.23) lies in the fact that each of its terms is nonnegative. It is not difficult to see (see the end of §3) that $F(E) \geq 0$ for $E \in \mathbb{R} \setminus [-2, 2]$ and that $G(a) \geq 0$ for $a \in (0, \infty)$. To see that the integral is also nonnegative, we employ Jensen's inequality. Notice that $y \mapsto -\log(y)$ is convex and $\frac{2}{\pi}\int_0^\pi \sin^2\theta\,d\theta = 1$ so

$$
\begin{aligned}
(1.24)\quad \frac{1}{2\pi}\int_{-\pi}^{\pi}\log\left[\frac{\sin(\theta)}{\operatorname{Im}M(e^{i\theta})}\right]\sin^2\theta\,d\theta &= \frac{1}{2}\,\frac{2}{\pi}\int_0^{\pi}-\log\left[\frac{\operatorname{Im}M}{\sin\theta}\right]\sin^2(\theta)\,d\theta \\
&\geq -\frac{1}{2}\log\left[\frac{2}{\pi}\int_0^{\pi}(\operatorname{Im}M)\sin(\theta)\,d\theta\right] \\
&= -\frac{1}{2}\log[\mu_{\mathrm{ac}}(-2,2)]\geq 0
\end{aligned}
$$

by (1.19).

The hard work in this paper will be to extend the sum rule to equalities or inequalities in fairly general settings. Indeed, we will prove the following:

THEOREM 5. *If J is a Jacobi matrix for which the right-hand side of* (1.23) *is finite, then the left-hand side is also finite and* LHS $\leq$ RHS.

THEOREM 6. *If μ is a probability measure that obeys the Blumenthal-Weyl criterion and the left-hand side of* (1.23) *is finite, then the right-hand side of* (1.23) *is also finite and* LHS $\geq$ RHS.

In other words, the P_2 sum rule *always* holds although both sides may be infinite. We will see (Proposition 3.4) that $G(a)$ has a zero only at $a=1$ where $G(a)=2(a-1)^2+O((a-1)^3)$ so the RHS of (1.23) is finite if and only if $\sum b_n^2+\sum(a_n-1)^2<\infty$, that is, J is Hilbert-Schmidt. On the other hand, we will see (see Proposition 3.5) that $F(E_j)=(|E_j|-2)^{3/2}+O((|E_j|-2)^2)$ so the LHS of (1.23) is finite if and only if the quasi-Szegő condition (1.8) and Lieb-Thirring bound (1.9) hold. Thus, Theorems 5 and 6 imply Theorem 1.

The major tool in proving the Case sum rules is a function that arises in essentially four distinct guises:

(1) The perturbation determinant defined as

$$
L(z;J)=\det\Big[(J-z-z^{-1})(J_0-z-z^{-1})^{-1}\Big]. \tag{1.25}
$$

(2) The Jost function, $u_0(z;J)$ defined for suitable z and J. The Jost solution is the unique solution of

$$
a_nu_{n+1}+b_nu_n+a_{n-1}u_{n-1}=(z+z^{-1})u_n \tag{1.26}
$$

$n\geq 1$ with $a_0\equiv 1$ which obeys

$$
\lim_{n\to\infty}z^{-n}u_n=1. \tag{1.27}
$$

The Jost function is $u_0(z;J)=u_0$.

(3) Ratio asymptotics of the orthogonal polynomials P_n,

$$
\lim_{n\to\infty}P_n(z+z^{-1})z^n. \tag{1.28}
$$

(4) The Szegő function, normally only defined when $N_+ = N_- = 0$:

$$D(z) = \exp\biggl(\frac{1}{4\pi}\int \log\Bigl|2\pi\sin(\theta)f(2\cos\theta)\Bigr|\,\frac{e^{i\theta}+z}{e^{i\theta}-z}\,d\theta\biggr) \tag{1.29}$$

where $d\mu = f(E)dE + d\mu_{\rm sing}$.

These functions are not all equal, but they are closely related. $L(z;J)$ is defined for $|z| < 1$ by the trace class theory of determinants [25], [53] so long as $J - J_0$ is trace class. We will see in that case it has a continuation to $\{z \mid |z| \le 1,\, z \neq \pm 1\}$ and, when $J - J_0$ is finite rank, it is a polynomial. The Jost function is related to L by

$$u_0(z;J) = \biggl(\prod_1^\infty a_j\biggr)^{-1} L(z;J). \tag{1.30}$$

Indeed, we will define all u_n by formulae analogous to (1.30) and show that they obey (1.26)/(1.27). The Jost solution is normally constructed using existence theory for the difference equation (1.26). We show directly that the limit in (1.28) is $u_0(J,z)/(1-z^2)$. Finally, the connection of $D(z)$ to $u_0(z)$ is

$$D(z) = (2)^{-1/2}\,(1-z^2)\,u_0(z;J)^{-1}. \tag{1.31}$$

Connected to this formula, we will prove that

$$\Bigl|u_0(e^{i\theta})\Bigr|^2 = \frac{\sin\theta}{\operatorname{Im} M_\mu(\theta)}\,, \tag{1.32}$$

from which (1.31) will follow easily when $J - J_0$ is nice enough. The result for general trace class $J - J_0$ is obviously new since it requires Nevai's conjecture to even define D in that generality. It will require the analytic tools of this paper.

In going from the formal sum rules to our general results like Theorems 4 and 5, we will use three technical tools:

(1) That the map $\mu \mapsto \int_{-\pi}^{\pi} \log(\frac{\sin\theta}{\operatorname{Im} M_\mu})\sin^2\theta\,d\theta$ and the similar map with $\sin^2\theta\,d\theta$ replaced by $d\theta$ is weakly lower semicontinuous. As we will see, these maps are essentially the negatives of entropies and this will be a known upper semicontinuity of an entropy.

(2) Rather than prove the sum rules in one step, we will have a way to prove them one site at a time, which yields inequalities that go in the opposite direction from the semicontinuity in (1).

(3) A detailed analysis of how eigenvalues change as a truncation is removed.

In Section 2, we discuss the construction and properties of the perturbation determinant and the Jost function. In Section 3, we give a proof of the Case sum rules for nice enough $J - J_0$ in the spirit of Flaschka's [16] and Case's [7] papers, and in Section 4, a second proof implementing tool (2) above. Section 5 discusses the Szegő and quasi-Szegő integrals as entropies and the associated semicontinuity, and Section 6 implements tool (3). Theorem 5 is proven in Section 7, and Theorem 6 in Section 8.

Section 9 discusses the C_0 sum rule and proves Nevai's conjecture.

The proof of Nevai's conjecture itself will be quite simple—the C_0 sum rule and semicontinuity of the entropy will provide an inequality that shows the Szegő integral is finite. We will have to work quite a bit harder to show that the sum rule holds in this case, that is, that the inequality we get is actually an equality.

In Section 10, we turn to another aspect that the sum rules expose: the fact that a dearth of bound states forces a.c. spectrum. For Schrödinger operators, there are many V's which lead to $\sigma(-\Delta + V) = [0, \infty)$. This always happens, for example, if $V(x) \geq 0$ and $\lim_{|x|\to\infty} V(x) = 0$. But for discrete Schrödinger operators, that is, Jacobi matrices with $a_n \equiv 1$, this phenomenon is not widespread because $\sigma(J_0)$ has two sides. Making $b_n \geq 0$ to prevent eigenvalues in $(-\infty, -2)$ just forces them in $(2, \infty)$! We will prove two somewhat surprising results (the $e_n(J)$ are defined in Remark 6 after Theorem 1).

THEOREM 7. *If J is a Jacobi matrix with $a_n \equiv 1$ and $\sum_n |e_n(J)|^{1/2} < \infty$, then $\sigma_{\rm ac}(J) = [-2, 2]$.*

THEOREM 8. *Let W be a two-sided Jacobi matrix with $a_n \equiv 1$ and no eigenvalues. Then $b_n = 0$, that is, $W = W_0$, the free Jacobi matrix.*

We emphasize that Theorem 8 does *not* presuppose any reflectionless condition.

Acknowledgments. We thank F. Gesztesy, N. Makarov, P. Nevai, M. B. Ruskai, and V. Totik for useful discussions. R.K. would like to thank T. Tombrello for the hospitality of Caltech where this work was initiated.

2. Perturbation determinants and the Jost function

In this section we introduce the perturbation determinant

$$L(z; J) = \det\Big[\Big(J - E(z)\Big)\Big(J_0 - E(z)\Big)^{-1}\Big]; \qquad E(z) = z + z^{-1}$$

and describe its analytic properties. This leads naturally to a discussion of the Jost function commencing with the introduction of the Jost solution (2.63).

The section ends with some remarks on the asymptotics of orthogonal polynomials. We begin, however, with notation, the basic properties of J_0, and a brief review of determinants for trace class and Hilbert-Schmidt operators. The analysis of L begins in earnest with Theorem 2.5.

Throughout, J represents a matrix of the form (1.1) thought of as an operator on $\ell^2(\mathbb{Z}_+)$. The special case $a_n \equiv 1$, $b_n \equiv 0$ is denoted by J_0 and $\delta J = J - J_0$ constitutes the perturbation. If δJ is finite rank (i.e., for large n, $a_n = 1$ and $b_n = 0$), we say that J is *finite range*.

It is natural to approximate the true perturbation by one of finite rank. We define J_n as the semi-infinite matrix,

$$J_n = \begin{pmatrix} b_1 & a_1 & 0 & & & & \\ a_1 & b_2 & a_2 & & & & \\ & \dots & \dots & \dots & & & \\ & \dots & b_{n-1} & a_{n-1} & & & \\ & & a_{n-1} & b_n & 1 & & \\ & & & 1 & 0 & 1 & \\ & & & & 1 & 0 & \dots \end{pmatrix} \tag{2.1}$$

that is, J_n has $b_m = 0$ for $m > n$ and $a_m = 1$ for $m > n - 1$. Notice that $J_n - J_0$ has rank at most n.

We write the $n \times n$ matrix obtained by taking the first n rows and columns of J (or of J_n) as $J_{n;F}$. The $n \times n$ matrix formed from J_0 will be called $J_{0;n;F}$.

A different class of associated objects will be the semi-infinite matrices $J^{(n)}$ obtained from J by dropping the first n rows and columns of J, that is,

$$J^{(n)} = \begin{pmatrix} b_{n+1} & a_{n+1} & 0 & \dots \\ a_{n+1} & b_{n+2} & a_{n+2} & \dots \\ 0 & a_{n+2} & b_{n+3} & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}. \tag{2.2}$$

As the next preliminary, we need some elementary facts about J_0, the free Jacobi matrix. Fix z with $|z| < 1$. Look for solutions of

$$u_{n+1} + u_{n-1} = (z + z^{-1})u_n, \qquad n \geq 2 \tag{2.3}$$

as sequences without any *a priori* conditions at infinity or $n = 1$. The solutions of (2.3) are linear combinations of the two "obvious" solutions $u^\pm$ given by

$$u_n^\pm(z) = z^{\pm n}. \tag{2.4}$$

Note that u^+ is ℓ^2 at infinity since $|z| < 1$. The linear combination that obeys

$$u_2 = (z + z^{-1})u_1$$

as required by the matrix ending at zero is (unique up to a constant)

$$u_n^{(0)}(z) = z^{-n} - z^n. \tag{2.5}$$

Noting that the Wronskian of $u^{(0)}$ and u^+ is $z^{-1}-z$, we see that $(J_0-E(z))^{-1}$ has the matrix elements $-(z^{-1}-z)^{-1}u^{(0)}_{\min(n,m)}(z)u^+_{\max(n,m)}(z)$ either by a direct calculation or standard Green's function formula. We have thus proven that

$$(J_0 - E(z))^{-1}_{nm} = -(z^{-1}-z)^{-1}[z^{|m-n|} - z^{m+n}] \tag{2.6}$$

$$= -\sum_{j=0}^{\min(m,n)-1} z^{1+|m-n|+2j} \tag{2.7}$$

where the second comes from $(z^{-1}-z)(z^{1-n}+z^{3-n}+\cdots+z^{n-1}) = z^{-n}-z^n$ by telescoping. (2.7) has two implications we will need later:

$$|z| \leq 1 \Rightarrow \left|(J_0 - E(z)^{-1}_{nm}\right| \leq \min(n,m)\,|z|^{1+|m-n|} \tag{2.8}$$

and that while the operator $(J_0-E(z))^{-1}$ becomes singular as $|z|\uparrow 1$, the matrix elements do not; indeed, they are polynomials in z.

We need an additional fact about J_0:

Proposition 2.1. *The characteristic polynomial of $J_{0;n;F}$ is*

$$\det(E(z) - J_{0,n;F}) = \frac{(z^{-n-1} - z^{n+1})}{(z^{-1}-z)} = U_n\Big(\tfrac{1}{2}\,E(z)\Big) \tag{2.9}$$

where $U_n(\cos\theta) = \sin[(n+1)\theta]/\sin(\theta)$ is the Chebyshev polynomial of the second kind. In particular,

$$\lim_{n\to\infty} \frac{\det[E(z) - J_{0;n+j;F}]}{\det[E(z) - J_{0;n;F}]} = z^{-j}. \tag{2.10}$$

Proof. Let

$$g_n(z) = \det(E(z) - J_{0;n;F}). \tag{2.11}$$

By expanding in minors

$$g_{n+2}(z) = (z+z^{-1})g_{n+1}(z) - g_n(z).$$

Given that $g_1 = z+z^{-1}$ and $g_0 = 1$, we obtain the first equality of (2.9) by induction. The second equality and (2.10) then follow easily. □

In Section 4, we will need

Proposition 2.2. *Let T_m be the Chebyshev polynomial (of the first kind):*

$$T_m(\cos\theta) = \cos(m\theta). \tag{2.12}$$

Then

$$\operatorname{Tr}\Big[T_m\Big(\tfrac{1}{2}J_{0,n;F}\Big)\Big] = \begin{cases} n & m = 2\ell(n+1);\ \ell \in \mathbb{Z} \\ -\frac{1}{2} - \frac{1}{2}(-1)^m & \textit{otherwise.} \end{cases} \tag{2.13}$$

In particular, for m fixed, once $n > \frac{1}{2}m - 1$ the trace is independent of n.

Proof. As noted above, the characteristic polynomial of $J_{0,n;F}$ is $U_n(E/2)$. That is, $\det[2\cos(\theta) - J_{0;n;F}] = \sin[(n+1)\theta]/\sin[\theta]$. This implies that the eigenvalues of $J_{0;n;F}$ are given by

$$E_n^{(k)} = 2\cos\left(\frac{k\pi}{n+1}\right) \qquad k = 1, \dots, n. \tag{2.14}$$

So by (2.12), $T_m\Big(\frac{1}{2}E_n^{(k)}\Big) = \cos\Big(\frac{km\pi}{n+1}\Big)$. Thus,

$$\begin{aligned} \operatorname{Tr}\Big[T_m\Big(\tfrac{1}{2}J_{0;n;F}\Big)\Big] &= \sum_{k=1}^{n} \cos\left(\frac{km\pi}{n+1}\right) \\ &= -\tfrac{1}{2} - \tfrac{1}{2}(-1)^m + \tfrac{1}{2}\sum_{k=-n}^{n+1} \exp\left(\frac{ikm\pi}{n+1}\right). \end{aligned}$$

The final sum is $2n+2$ if m is a multiple of $2(n+1)$ and 0 if it is not. □

As a final preliminary, we discuss Hilbert space determinants [25], [52], [53]. Let $\mathcal{I}_p$ denote the Schatten classes of operators with norm $\|A\|_p = \operatorname{Tr}(|A|^p)$ as described for example, in [53]. In particular, $\mathcal{I}_1$ and $\mathcal{I}_2$ are the trace class and Hilbert-Schmidt operators, respectively.

For each $A \in \mathcal{I}_1$, one can define a complex-valued function $\det(1+A)$ (see [25], [53], [52]), so that

$$|\det(1+A)| \le \exp(\|A\|_1) \tag{2.15}$$

and $A \mapsto \det(1+A)$ is continuous; indeed [53, pg. 48],

$$|\det(1+A) - \det(1+B)| \le \|A-B\|_1 \exp(\|A\|_1 + \|B\|_1 + 1). \tag{2.16}$$

We will also use the following properties:

$$A, B \in \mathcal{I}_1 \ \Rightarrow\ \det(1+A)\det(1+B) = \det(1+A+B+AB) \tag{2.17}$$

$$AB, BA \in \mathcal{I}_1 \ \Rightarrow\ \det(1+AB) = \det(1+BA) \tag{2.18}$$

$$(1+A) \text{ is invertible if and only if } \det(1+A) \neq 0 \tag{2.19}$$

$$z \mapsto A(z) \text{ analytic} \Rightarrow \det(1+A(z)) \text{ analytic.} \tag{2.20}$$

If A is finite rank and P is a finite-dimensional self-adjoint projection,

$$PAP = A \quad \Rightarrow \quad \det(1+A) = \det_{P\mathcal{H}}(1_{P\mathcal{H}} + PAP), \tag{2.21}$$

where $\det_{P\mathcal{H}}$ is the standard finite-dimensional determinant.

For $A \in \mathcal{I}_2$, $(1+A)e^{-A} - 1 \in \mathcal{I}_1$, so one defines (see [53, pp. 106–108])

$$\det{}_2(1+A) = \det((1+A)e^{-A}). \tag{2.22}$$

Then

$$|\det{}_2(1+A)| \;\leq\; \exp(\|A\|_2^2) \tag{2.23}$$

$$|\det{}_2(1+A) - \det{}_2(1+B)| \;\leq\; \|A-B\|_2 \exp((\|A\|_2 + \|B\|_2 + 1)^2) \tag{2.24}$$

and, if $A \in \mathcal{I}_1$,

$$\det{}_2(1+A) = \det(1+A)e^{-\operatorname{Tr}(A)} \tag{2.25}$$

or

$$\det(1+A) = \det{}_2(1+A)e^{\operatorname{Tr}(A)}. \tag{2.26}$$

To estimate the $\mathcal{I}_p$ norms of operators we use

LEMMA 2.3. *If A is a matrix and $\|\cdot\|_p$ the Schatten $\mathcal{I}_p$ norm* [53], *then*
(i)

$$\|A\|_2^2 = \sum_{n,m} |a_{nm}|^2\,, \tag{2.27}$$

(ii)

$$\|A\|_1 \leq \sum_{n,m} |a_{nm}|\,, \tag{2.28}$$

(iii) *For any j and p,*

$$\sum_n |a_{n,n+j}|^p \leq \|A\|_p^p. \tag{2.29}$$

Proof. (i) is standard. (ii) follows from the triangle inequality for $\|\cdot\|_1$ and the fact that a matrix which a single nonzero matrix element, α, has trace norm $|\alpha|$. (iii) follows from a result of Simon [53], [51] that

$$\|A\|_p^p = \sup\left\{\sum_n |\langle\varphi_n, A\psi_n\rangle|^p \;\middle|\; \{\varphi_n\}, \{\psi_n\} \text{ orthonormal sets}\right\}. \qquad \square$$

The following factorization will often be useful. Define

$$c_n = \max(|a_{n-1}-1|\,, |b_n|\,, |a_n - 1|)$$

which is the maximum matrix element in the n^{th} row and n^{th} column. Let C be the diagonal matrix with matrix elements c_n. Define U by

$$\delta J = C^{1/2} U C^{1/2}. \tag{2.30}$$

Then U is a tridiagonal matrix with matrix elements bounded by 1 so

$$\|U\| \leq 3. \tag{2.31}$$

One use of (2.30) is the following:

THEOREM 2.4. *Let* $c_n = \max(|a_{n-1} - 1|\,, |b_n|\,, |a_n - 1|)$. *For any* $p \in [1, \infty)$,

$$\tfrac{1}{3}\Big(\sum_n |c_n|^p\Big)^{1/p} \leq \|\delta J\|_p \leq 3\Big(\sum_n |c_n|^p\Big)^{1/p}. \tag{2.32}$$

Proof. The right side is immediate from (2.30) and Hölder's inequality for trace ideals [53]. The leftmost inequality follows from (2.29) and

$$\Big(\sum_n |c_n|^p\Big)^{1/p} \leq \Big(\sum_n |b_n|^p\Big)^{1/p} + 2\Big(\sum_n |a_n - 1|^p\Big)^{1/p}. \qquad \square$$

With these preliminaries out of the way, we can begin discussing the perturbation determinant L. For any J with $\delta J \in \mathcal{I}_1$ (by (2.32) this is equivalent to $\sum |a_n - 1| + \sum |b_n| < \infty$), we define

$$L(z; J) = \det\Big[\Big(J - E(z)\Big)\,\Big(J_0 - E(z)\Big)^{-1}\Big] \tag{2.33}$$

for all $|z| < 1$. Since

$$(J - E)(J_0 - E)^{-1} = 1 + \delta J (J_0 - E)^{-1}, \tag{2.34}$$

the determinant in (2.33) is of the form $1 + A$ with $A \in \mathcal{I}_1$.

THEOREM 2.5. *Suppose* $\delta J \in \mathcal{I}_1$.

(i) *$L(z; J)$ is analytic in $D \equiv \{z \mid |z| < 1\}$.*

(ii) *$L(z; J)$ has a zero in D only at points z_j where $E(z_j)$ is an eigenvalue of J, and it has zeros at all such points. All zeros are simple.*

(iii) *If J is finite range, then $L(z; J)$ is a polynomial and so has an analytic continuation to all of $\mathbb{C}$.*

Proof. (i) follows from (2.20).

(ii) If $E_0 = E(z_0)$ is not an eigenvalue of J, then $E_0 \notin \sigma(J)$ since $E : D \to \mathbb{C}\backslash[-2, 2]$ and $\sigma_{\text{ess}}(J) = [-2, 2]$. Thus, $(J - E_0)/(J_0 - E_0)$ has an inverse (namely, $(J_0 - E_0)/(J - E_0)$), and so by (2.19), $L(z; J) \neq 0$. If E_0 is an eigenvalue, $(J - E_0)/(J_0 - E_0)$ is not invertible, so by (2.19), $L(z_0; J) = 0$. Finally, if $E(z_0)$ is an eigenvalue, eigenvalues of J are simple by a Wronskian argument. That L has a simple zero under these circumstances comes from the following.

If P is the projection onto the eigenvector at $E_0 = E(z_0)$, then $(J-E)^{-1}(1-P)$ has a removable singularity at E_0. Define

$$C(E) = (J-E)^{-1}(1-P) + P \tag{2.35}$$

so

$$(J-E)C(E) = 1 - P + (E_0 - E)P. \tag{2.36}$$

Define

$$\begin{aligned} D(E) &\equiv (J_0 - E)C(E) \\ &= -\delta J C(E) + (J-E)C(E) \\ &= 1 - P + (E_0 - E)P - \delta J C(E) \\ &= 1 + \text{trace class.} \end{aligned} \tag{2.37}$$

Moreover,

$$\begin{aligned} D(E)[(J-E)/(J_0-E)] &= (J_0 - E)[1 - P + (E_0 - E)P](J_0 - E)^{-1} \\ &= 1 + (J_0 - E)[-P + (E_0 - E)P](J_0 - E)^{-1}. \end{aligned}$$

Thus by (2.17) first and then (2.18),

$$\begin{aligned} \det(D(E(z)))L(z;J) &= \det(1 + (J_0 - E)[-P + (E_0 - E)P](J_0 - E)^{-1}) \\ &= \det(1 - P + (E_0 - E)P) \\ &= E_0 - E(z), \end{aligned}$$

where we used (2.21) in the last step. Since $L(z;J)$ has a zero at z_0 and $E_0 - E(z) = (z - z_0)[1 - \frac{1}{zz_0}]$ has a simple zero, $L(z;J)$ has a simple zero.

(iii) Suppose δJ has range N, that is, $N = \max\{n \mid |b_n| + |a_{n-1} - 1| > 0\}$ and let $P^{(N)}$ be the projection onto the span of $\{\delta_j\}_{j=1}^N$. As $P^{(N)}\delta J = \delta J$,

$$\delta J (J_0 - E)^{-1} = P^{(N)} P^{(N)} \delta J (J_0 - E)^{-1}.$$

By (2.18),

$$L(z;J) = \det\Big(1 + P^{(N)}\delta J \Big(J_0 - E(z)\Big)^{-1} P^{(N)}\Big).$$

Thus by (2.7), $L(z;J)$ is a polynomial if δJ is finite range. $\square$

Remarks. 1. By this argument, if δJ has range n, $L(z;J)$ is the determinant of an $n \times n$ matrix whose ij element is a polynomial of degree $i + j + 1$. That implies that we have shown $L(z;J)$ is a polynomial of degree at most

$2n(n+1)/2+n=(n+1)^2$. We will show later it is actually a polynomial of degree at most $2n-1$.

2. The same idea shows that if $\sum_n |(a_n-1)\rho^{2n}|+|b_n\rho^{2n}|<\infty$ for some $\rho>1$, then $C^{1/2}(J_0-z-z^{-1})^{-1}C^{1/2}$ is trace class for $|z|<\rho$, and thus $L(z;J)$ has an analytic continuation to $\{z \mid |z|<\rho\}$.

We are now interested in showing that $L(z;J)$, defined initially only on D, can be continued to ∂D or part of ∂D. Our goal is to show:

(i) If

$$\sum_{n=1}^{\infty} n[|a_n-1|+|b_n|]<\infty, \tag{2.38}$$

then $L(z;J)$ can be continued to all of $\bar{D}$, that is, extends to a function continuous on $\bar{D}$ and analytic in D.

(ii) For the general trace class situation, $L(z;J)$ has a continuation to $\bar{D}\backslash\{-1,1\}$.

(iii) As x real approaches ±1, $|L(x;J)|$ is bounded by $\exp\{o(1)/(1-|x|)\}$.

We could interpolate between (i) and (iii) and obtain more information about cases where (2.38) has n replaced by n^α with $0<\alpha<1$ or even $\log n$ (as is done in [42], [22]), but using the theory of Nevanlinna functions and (iii), we will be able to handle the general trace class case (in Section 9), so we forgo these intermediate results.

Lemma 2.6. *Let C be diagonal positive trace class matrix. For $|z|<1$, define*

$$A(z)=C^{1/2}(J_0-E(z))^{-1}C^{1/2}. \tag{2.39}$$

Then, as a Hilbert-Schmidt operator-valued function, $A(z)$ extends continuously to $\bar{D}\setminus\{-1,1\}$. If

$$\sum_n nc_n<\infty, \tag{2.40}$$

it has a Hilbert-Schmidt continuation to $\bar{D}$.

Proof. Let $A_{nm}(z)$ be the matrix elements of $A(z)$. It follows from $|z|<1$ and (2.6)/(2.8) that

$$|A_{nm}(z)| \leq 2c_n^{1/2}c_m^{1/2}\,|z-1|^{-1}\,|z+1|^{-1} \tag{2.41}$$

$$|A_{nm}(z)| \leq \min(m,n)c_n^{1/2}c_m^{1/2} \tag{2.42}$$

and each $A_{n,m}(z)$ has a continuous extension to $\bar{D}$. It follows from (2.41), the dominated convergence theorem, and

$$\sum_{n,m}(c_n^{1/2}c_m^{1/2})^2 = \Big(\sum_n c_n\Big)^2$$

that so long as z stays away from ± 1, $\{A_{mn}(z)\}_{n,m}$ is continuous in the space $\ell^2((1,\infty)\times(1,\infty))$ so $A(z)$ is Hilbert-Schmidt and continuous on $\bar{D}\backslash\{-1,1\}$. Moreover, (2.42) and

$$\sum_{n,m}\Big[\min(m,n)c_n^{1/2}c_m^{1/2}\Big]^2 \le \sum_{mn} mnc_nc_m = \Big(\sum_n nc_n\Big)^2$$

imply that $A(z)$ is Hilbert-Schmidt on $\bar{D}$ if (2.40) holds. □

Remark. When (2.40) holds—indeed, when

$$\sum n^\alpha c_n < \infty \tag{2.43}$$

for some $\alpha > 0$—we believe that one can show $A(z)$ has trace class boundary values on $\partial D\backslash\{-1,1\}$ but we will not provide all the details since the Hilbert-Schmidt result suffices. To see this trace class result, we note that $\operatorname{Im} A(z) = (A(z) - A^*(z))/2i$ has a rank 1 boundary value as $z \to e^{i\theta}$; explicitly,

$$\operatorname{Im} A(e^{i\theta})_{mn} = -c_n^{1/2}c_m^{1/2}\,\frac{(\sin m\theta)(\sin n\theta)}{(\sin\theta)}\,. \tag{2.44}$$

Thus, $\operatorname{Im} A(e^{i\theta})$ is trace class and is Hölder continuous in the trace norm if (2.43) holds. Now $\operatorname{Re} A(e^{i\theta})$ is the Hilbert transform of a Hölder continuous trace class operator-valued function and so trace class. This is because when a function is Hölder continuous, its Hilbert transform is given by a convergent integral, hence limit of Riemann sums. Because of potential singularities at ± 1, the details will be involved.

Lemma 2.7. *Let δJ be trace class. Then*

$$t(z) = \operatorname{Tr}((\delta J)(J_0 - E(z))^{-1}) \tag{2.45}$$

has a continuation to $\bar{D}\backslash\{-1,1\}$. If (2.38) *holds, $t(z)$ can be continued to $\bar{D}$.*

Remark. We are only claiming $t(z)$ can be continued to ∂D, not that it equals the trace of $(\delta J)(J_0 - E(z))^{-1}$ since $\delta J(J_0 - E(z))^{-1}$ is not even a bounded operator for $z \in \partial D$!

Proof. $t(z) = t_1(z) + t_2(z) + t_3(z)$ where

$$\begin{aligned} t_1(z) &= \sum b_n(J_0 - E(z))^{-1}_{nn} \\ t_2(z) &= \sum (a_n - 1)(J_0 - E(z))^{-1}_{n+1,n} \\ t_3(z) &= \sum (a_n - 1)(J_0 - E(z))^{-1}_{n,n+1}\,. \end{aligned}$$

Since, by (2.6), (2.8),

$$\begin{aligned}\left|(J_0-E(z))^{-1}_{nm}\right| &\leq 2\,|z-1|^{-1}\,|z+1|^{-1}\\ \left|(J_0-E(z))^{-1}_{nm}\right| &\leq \min(n,m),\end{aligned}$$

the result is immediate. □

Theorem 2.8. *If δJ is trace class, $L(z;J)$ can be extended to a continuous function on $\bar{D}\backslash\{-1,1\}$ with*

$$|L(z;J)| \leq \exp\left\{c\Big[\|\delta J\|_1 + \|\delta J\|_1^2\Big]\ |z-1|^{-2}\,|z+1|^{-2}\right\} \tag{2.46}$$

for a universal constant, c. If (2.38) *holds, $L(z;J)$ can be extended to all of $\bar{D}$ with*

$$|L(z;J)| \leq \exp\biggl\{\tilde{c}\Big[1+\sum_{n=1}^{\infty} n\Big[\,|a_n-1|+|b_n|\,\Big]\Big]^2\biggr\} \tag{2.47}$$

for a universal constant, $\tilde{c}$.

Proof. This follows immediately from (2.22), (2.23), (2.25), and the last two lemmas and their proofs. □

While we cannot control $\|C^{1/2}(J_0-E(z))^{-1}C^{1/2}\|_1$ for arbitrary z with $|z|\to 1$, we can at the crucial points ± 1 if we approach along the real axis, because of positivity conditions.

Lemma 2.9. *Let C be a positive diagonal trace class operator. Then*

$$\lim_{\substack{|x|\uparrow 1\\ x\ \text{real}}} (1-|x|)\|C^{1/2}(J_0-E(x))^{-1}C^{1/2}\|_1 = 0. \tag{2.48}$$

Proof. For $x<0$, $E(x)<-2$, and $J_0-E(x)>0$, while for $x>0$, $E(x)>2$, so $J_0-E(x)<0$. It follows that

$$\begin{aligned}\|C^{1/2}(J_0-E(x))^{-1}C^{1/2}\|_1 &= \left|\mathrm{Tr}(C^{1/2}(J_0-E(x))^{-1}C^{1/2})\right|\\ &\leq \sum_n c_n\left|(J_0-E(x))^{-1}_{nn}\right|.\end{aligned} \tag{2.49}$$

By (2.6),

$$(1-|x|)\left|(J_0-E(x))^{-1}_{nn}\right| \leq 1$$

and by (2.7) for each fixed n,

$$\lim_{\substack{|x|\uparrow 1\\ x\ \text{real}}} (1-|x|)\left|(J_0-E(x))^{-1}_{nn}\right| = 0.$$

Thus (2.49) and the dominated convergence theorem proves (2.48). □

THEOREM 2.10.

$$\limsup_{\substack{|x|\uparrow 1\\ x\ \text{real}}} (1-|x|)\log|L(x;J)| \leq 0. \tag{2.50}$$

Proof. Use (2.30) and (2.18) to write

$$L(x;J) = \det(1 + UC^{1/2}(J_0 - E(x))^{-1}C^{1/2})$$

and then (2.15) and (2.31) to obtain

$$\begin{aligned}\log|L(x;J)| &\leq \|UC^{1/2}(J_0-E(x))^{-1}C^{1/2}\|_1\\ &\leq 3\|C^{1/2}(J_0-E(x))^{-1}C^{1/2}\|_1.\end{aligned}$$

The result now follows from the lemma. □

Next, we want to find the Taylor coefficients for $L(z;J)$ at $z=0$, which we will need in the next section.

LEMMA 2.11. *For each fixed $h>0$ and $|z|$ small,*

$$\log\biggl(1-\frac{h}{E(z)}\biggr) = \sum_{n=1}^{\infty} \tfrac{2}{n}\Bigl[T_n(0) - T_n(\tfrac12 h)\Bigr]z^n \tag{2.51}$$

where $T_n(x)$ is the n^{th} Chebyshev polynomial of the first kind: $T_n(\cos\theta) = \cos(n\theta)$. In particular, $T_{2n+1}(0)=0$ and $T_{2n}(0)=(-1)^n$.

Proof. Consider the following generating function:

$$g(x,z) \equiv \sum_{n=1}^{\infty} T_n(x)\frac{z^n}{n} = -\tfrac12\log[1-2xz+z^2]. \tag{2.52}$$

The lemma now follows from

$$\log\left[1-\frac{2x}{z+z^{-1}}\right] = 2[g(0,z)-g(x,z)] = \sum \tfrac{2}{n}\Bigl[T_n(0)-T_n(x)\Bigr]z^n$$

by choosing $x=h/2$. The generation function is well known (Abramowitz and Stegun [1, Formula 22.9.8] or Szegő [60, Equation 4.7.25]) and easily proved: for $\theta\in\mathbb{R}$ and $|z|<1$,

$$\begin{aligned}\frac{\partial g}{\partial z}(\cos\theta,z) &= \frac1z\sum_{n=1}^{\infty}\cos(n\theta)z^n\\ &= \frac{1}{2z}\sum_{n=1}^{\infty}\Bigl[\Bigl(ze^{i\theta}\Bigr)^n + \Bigl(ze^{-i\theta}\Bigr)^n\Bigr]\\ &= \frac{\cos(\theta)+z}{z^2-2z\cos\theta+1}\\ &= -\tfrac12\,\frac{\partial}{\partial z}\,\log[1-2xz+z^2]\end{aligned}$$

at $x = \cos\theta$. Integrating this equation from $z = 0$ proves (2.52) for $x \in [-1, 1]$ and $|z| < 1$. For more general x one need only consider $\theta \in \mathbb{C}$ and require $|z| < \exp\{-|\operatorname{Im}\theta|\}$. □

Lemma 2.12. *Let A and B be two self-adjoint $m \times m$ matrices. Then*

$$\log \det \left[\Big(A - E(z)\Big)\,\Big(B - E(z)\Big)^{-1}\right] = \sum_{n=0}^{\infty} c_n(A, B) z^n \tag{2.53}$$

where

$$c_n(A, B) = -\tfrac{2}{n} \operatorname{Tr}\left[T_n\Big(\tfrac{1}{2}A\Big) - T_n\Big(\tfrac{1}{2}B\Big)\right]. \tag{2.54}$$

Proof. Let $\lambda_1, \dots, \lambda_m$ be the eigenvalues of A and $\mu_1, \dots, \mu_m$ the eigenvalues of B. Then

$$\begin{aligned} \det\left[\frac{A - E(z)}{B - E(z)}\right] &= \prod_{j=1}^{m}\left[\frac{\lambda_j - E(z)}{\mu_j - E(z)}\right] \\ \Rightarrow \quad \log \det\left[\frac{A - E(z)}{B - E(z)}\right] &= \sum_{j=1}^{m} \log[1 - \lambda_j/E(z)] - \log[1 - \mu_j/E(z)] \end{aligned}$$

so (2.53)/(2.54) follow from the preceding lemma. □

Theorem 2.13. *If δJ is trace class, then for each n, $T_n(J/2) - T_n(J_0/2)$ is trace class. Moreover, near $z = 0$,*

$$\log[L(z; J)] = \sum_{n=1}^{\infty} c_n(J) z^n \tag{2.55}$$

where

$$c_n(J) = -\frac{2}{n} \operatorname{Tr}\left[T_n\Big(\tfrac{1}{2}J\Big) - T_n\Big(\tfrac{1}{2}J_0\Big)\right]. \tag{2.56}$$

In particular,

$$c_1(J) = -\operatorname{Tr}(J - J_0) = -\sum_{m=1}^{\infty} b_m \tag{2.57}$$

$$c_2(J) = -\tfrac{1}{2} \operatorname{Tr}(J^2 - J_0^2) = -\tfrac{1}{2}\sum_{m=1}^{\infty} [b_m^2 + 2(a_m^2 - 1)]. \tag{2.58}$$

Proof. To prove $T_n(J/2) - T_n(J_0/2)$ is trace class, we need only show that $J^m - J_0^m = \sum_{j=1}^{m-1} J^j\, \delta J\, J^{m-1-j}$ is trace class, and that's obvious! Let $\widetilde{\delta J}_{n;F}$ be $\delta J_{n;F}$ extended to $\ell^2(\mathbb{Z}_+)$ by setting it equal to the zero matrix on $\ell^2(j \geq n)$. Let $\tilde{J}_{0,n}$ be J_0 with a_{n+1} set equal to zero. Then

$$\widetilde{\delta J}_{n;F}(\tilde{J}_{0,n} - E)^{-1} \to \delta J (J_0 - E)^{-1}$$

in trace norm, which means that

$$\det\left(\frac{J_{n;F} - E(z)}{J_{0,n;F} - E(z)}\right) \to L(z;J). \tag{2.59}$$

This convergence is uniform on a small circle about $z = 0$, so the Taylor series coefficients converge. Thus (2.53)/(2.54) imply (2.55)/(2.56). □

Next, we look at relations of $L(z;J)$ to certain critical functions beginning with the Jost function. As a preliminary, we note (recall $J^{(n)}$ is defined in (2.2)),

Proposition 2.14. *Let δJ be trace class. Then for each $z \in \bar{D}\backslash\{-1,1\}$,*

$$\lim_{n\to\infty} L(z;J^{(n)}) = 1 \tag{2.60}$$

uniformly on compact subsets of $\bar{D}\backslash\{-1,1\}$. If (2.38) *holds*, (2.60) *holds uniformly in z for all z in $\bar{D}$.*

Proof. Use (2.16) and (2.24) with $B = 0$ and the fact that $\|\delta J^{(n)}\|_1 \to 0$ in the estimates above. □

Next, we note what is essentially the expansion of $\det(J - E(z))$ in minors in the first row:

Proposition 2.15. *Let δJ be trace class and $z \in \bar{D}\backslash\{-1,1\}$. Then*

$$L(z;J) = (E(z) - b_1)zL(z;J^{(1)}) - a_1^2 z^2 L(z;J^{(2)}). \tag{2.61}$$

Proof. Denote $(J^{(k)})_{n;F}$ by $J^{(k)}_{n;F}$, that is, the $n \times n$ matrix formed by rows and columns $k+1,\dots,k+n$ of J. Then expanding in minors,

$$\det(E - J_{n;F}) = (E - b_1)\det(E - J^{(1)}_{n-1;F}) - a_1^2 \det(E - J^{(2)}_{n-2;F}). \tag{2.62}$$

Divide by $\det(E - J_{0;n;F})$ and take $n \to \infty$ using (2.59). (2.61) follows if one notes

$$\frac{\det(E - J_{0;n-j;F})}{\det(E - J_{0;n;F})} \to z^j$$

by (2.10). □

We now define for $z \in \bar{D}\backslash\{-1,1\}$ and $n = 1,\dots,\infty$,

$$u_n(z;J) \quad = \quad \left(\prod_{j=n}^{\infty} a_j\right)^{-1} z^n L(z;J^{(n)}) \tag{2.63}$$

$$u_0(z;J) \quad = \quad \left(\prod_{j=1}^{\infty} a_j\right)^{-1} L(z;J). \tag{2.64}$$

u_n is called the Jost solution and u_0 the Jost function. The infinite product of the a's converges to a nonzero value since $a_j > 0$ and $\sum_j |a_j - 1| < \infty$. We have:

THEOREM 2.16. *The Jost solution*, $u_n(z; J)$, *obeys*

$$a_{n-1}u_{n-1} + (b_n - E(z))u_n + a_n u_{n+1} = 0, \quad n = 1, 2, \dots \tag{2.65}$$

where $a_0 \equiv 1$. *Moreover*,

$$\lim_{n\to\infty} z^{-n} u_n(z; J) = 1. \tag{2.66}$$

Proof. (2.61) for J replaced by $J^{(n)}$ reads

$$L(z; J^{(n)}) = (E(z) - b_{n+1})zL(z; J^{(n+1)}) - a_{n+1}^2 z^2 L(z; J^{(n+2)}),$$

from which (2.65) follows by multiplying by $z^n(\prod_{j=n+1}^\infty a_j)^{-1}$. Equation (2.66) is just a rewrite of (2.60) because $\lim_{n\to\infty} \prod_{j=n}^\infty a_j = 1$. $\square$

Remarks. 1. If (2.38) holds, one can define u_n for $z = \pm 1$.

2. By Wronskian methods, (2.65)/(2.66) uniquely determine $u_n(z; J)$.

Theorem 2.16 lets us improve Theorem 2.5(iii) with an explicit estimate on the degree of $L(z; J)$.

THEOREM 2.17. *Let* δJ *have range* n, *that is*, $a_j = 1$ *if* $j \geq n$, $b_j = 0$ *if* $j > n$. *Then* $u_0(z; J)$ *and so* $L(z; J)$ *is a polynomial in* z *of degree at most* $2n-1$. *If* $b_n \neq 0$, *then* $L(z; J)$ *has degree exactly* $2n-1$. *If* $b_n = 0$ *but* $a_{n-1} \neq 1$, *then* $L(z; J)$ *has degree* $2n - 2$.

Proof. The difference equation (2.65) can be rewritten as

$$\begin{aligned} \begin{pmatrix} u_{n-1} \\ u_n \end{pmatrix} &= \begin{pmatrix} (E - b_n)/a_{n-1} & -a_n/a_{n-1} \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_n \\ u_{n+1} \end{pmatrix} \\ &= \frac{1}{za_{n-1}} A_n(z) \begin{pmatrix} u_n \\ u_{n+1} \end{pmatrix}, \end{aligned} \tag{2.67}$$

where

$$A_n(z) = \begin{pmatrix} z^2 + 1 - b_n z & -a_n z \\ a_{n-1}z & 0 \end{pmatrix}. \tag{2.68}$$

If δJ has range n, $J^{(n)} = J_0$ and $a_n = 1$. Thus by (2.63), $u_\ell(z; J) = z^\ell$ if $\ell \geq n$. Therefore by (2.67),

$$\begin{pmatrix} u_0 \\ u_1 \end{pmatrix} = (a_1 \cdots a_{n-1})^{-1} z^{-n} A_1(z) \cdots A_n(z) \begin{pmatrix} z^n \\ z^{n+1} \end{pmatrix} \tag{2.69}$$
$$= (a_1 \cdots a_{n-1})^{-1} A_1(z) \cdots A_n(z) \begin{pmatrix} 1 \\ z \end{pmatrix}$$
$$= (a_1 \cdots a_{n-1})^{-1} A_1(z) \cdots A_{n-1}(z) \begin{pmatrix} 1 - b_n z \\ a_{n-1} z \end{pmatrix}.$$

Since $A_j(z)$ is a quadratic, (2.69) implies u_0 is a polynomial of degree at most $2(n-1)+1 = 2n-1$. The top left component of A_j contains z^2 while everything else is of lower order. Proceeding inductively, the top left component of $A_1(z) \cdots A_{n-1}(z)$ is $z^{2n-2} + O(z^{2n-3})$. Thus if $b_n \neq 0$,

$$u_0 = -(a_1 \ldots a_{n-1})^{-1} b_n z^{2n-1} + O(z^{2n-2}),$$

proving u_0 has degree $2n-1$. If $b_n = 0$, then

$$A_{n-1}(z) \begin{pmatrix} 1 \\ a_{n-1} z \end{pmatrix} = \begin{pmatrix} 1 + (1 - a_{n-1}^2) z^2 - b_{n-1} z \\ a_{n-2} z \end{pmatrix}$$

so inductively, one sees that

$$u_0 = (a_1 \ldots a_{n-1})^{-1} (1 - a_{n-1}^2) z^{2n-2} + O(z^{2n-3})$$

and u_0 has degree $2n-2$. $\square$

Remark. Since the degree of u is the number of its zeros (counting multiplicities), this can be viewed as a discrete analog of the Regge [46]-Zworski [64] resonance counting theorem.

Recall the definitions (1.2) and (1.15) of the m-function which we will denote for now by $M(z; J) = (E(z) - J)^{-1}_{11}$.

THEOREM 2.18. *If $\delta J \in \mathcal{I}_1$ then for $|z| < 1$ with $L(z; J) \neq 0$, we have*

$$M(z; J) = \frac{z L(z; J^{(1)})}{L(z; J)} \tag{2.70}$$
$$= \frac{u_1(z; J)}{u_0(z; J)}. \tag{2.71}$$

Proof. (2.71) follows from (2.70) and (2.63)/(2.64). (2.70) is essentially Cramer's rule. Explicitly,

$$\begin{aligned} M(z; J) &= \lim_{n \to \infty} (E(z) - J_{n;F})^{-1}_{11} \\ &= \lim_{n \to \infty} \frac{\det(E - J^{(1)}_{n-1;F})}{\det(E - J_{n;F})} \\ &= \lim_{n \to \infty} w_n x_m y_n \end{aligned}$$

where (by (2.59) and (2.10))

$$\begin{aligned} w_n &= \frac{\det(E - J^{(1)}_{n-1;F})}{\det(E - J_{0;n-1;F})} \to L(z; J^{(1)}) \\ x_n &= \frac{\det(E - J_{0;n;F})}{\det(E - J_{n;F})} \to L(z; J)^{-1} \\ y_n &= \frac{\det(E - J_{0;n-1;F})}{\det(E - J_{0;n;F})} \to z. \end{aligned}$$

□

Theorem 2.18 allows us to link $|u_0|$ and $|L|$ on $|z| = 1$ to $\mathrm{Im}(M)$ there:

THEOREM 2.19. *Let δJ be trace class. Then for all $\theta \neq 0, \pi$, the boundary value* $\lim_{r\uparrow 1} M(re^{i\theta}; J) \equiv M(e^{i\theta}; J)$ *exists. Moreover,*

$$\left| u_0(e^{i\theta}; J) \right|^2 \operatorname{Im} M(e^{i\theta}; J) = \sin\theta. \tag{2.72}$$

Equivalently,

$$\left| L(e^{i\theta}; J) \right|^2 \operatorname{Im} M(e^{i\theta}; J) = \left(\prod_{j=1}^{\infty} a_j^2 \right) \sin\theta. \tag{2.73}$$

Proof. By (2.64), (2.73) is equivalent to (2.72). If $|z| = 1$, then $E(\bar z) = E(z)$ since $\bar z = z^{-1}$. Thus, $u_n(z; J)$ and $u_n(\bar z; J)$ solve the same difference equation. Since $z^{-n} u_n(z; J) \to 1$ and $a_n \to 1$, we have that

$$a_n[u_n(\bar z; J) u_{n+1}(z; J) - u_n(z; J) u_{n+1}(\bar z; J)] \to z - z^{-1}.$$

Since the Wronskian of two solutions is constant, if $z = e^{i\theta}$,

$$a_n[u_n(e^{-i\theta}; J) u_{n+1}(e^{i\theta}; J) - u_n(e^{i\theta}; J) u_{n+1}(e^{-i\theta}; J)] = 2i \sin\theta.$$

Since $a_0 = 1$ and $u_n(\bar z; J) = \overline{u_n(z; J)}$, we have that

$$\operatorname{Im}[\, \overline{u_0(e^{i\theta}; J)}\, u_1(e^{i\theta}; J)] = \sin\theta. \tag{2.74}$$

(2.74) implies that $u_0(e^{i\theta}; J) \neq 0$ if $\theta \neq 0, \pi$, so by (2.71), $M(z; J)$ extends to $\bar D \backslash \{-1, 1\}$. Since $u_1(e^{i\theta}; J) = u_0(e^{i\theta}; J) M(e^{i\theta}; J)$ (by (2.71)), (2.74) is the same as (2.72). □

If J has no eigenvalues in $\mathbb{R} \backslash [-2, 2]$ and (2.38) holds so $u_0(z; J)$ has a continuation to $\bar D$, then

$$u_0(z; J) = \exp\left(\frac{1}{2\pi} \int_0^{2\pi} \frac{e^{i\theta} + z}{e^{i\theta} - z} \log\left| u_0(e^{i\theta}; J) \right| d\theta \right) \tag{2.75}$$

$$ = \exp\left(-\frac{1}{4\pi} \int_0^{2\pi} \frac{e^{i\theta} + z}{e^{i\theta} - z} \log\left[\frac{\left| \operatorname{Im} M(e^{i\theta}; J) \right|}{|\sin\theta|} \right] d\theta \right) \tag{2.76}$$

$$= \exp\biggl(-\frac{1}{4\pi}\int_0^{2\pi} \frac{e^{i\theta}+z}{e^{i\theta}-z}\,\log\biggl[\frac{\pi f(2\cos\theta)}{|\sin\theta|}\biggr]\,d\theta\biggr) \tag{2.77}$$

$$= (4\pi)^{-1/2}\,(1-z^2)\,D(z)^{-1} \tag{2.78}$$

where D is the Szegő function defined by (1.29) and $f(E) = \frac{d\mu_{\rm ac}}{dE}$. In the above, (2.75) is the Poisson-Jensen formula [48]. It holds because under (2.38), u_0 is bounded on $\bar{D}$ and by (2.74), and the fact that u_1 is bounded, $\log(u_0)$ at worst has a logarithmic singularity at ± 1. (2.76) follows from (2.72) and (2.77) from (1.18). To obtain (2.78) we use

$$\frac{1}{4}\,(1-z^2)^2 = \exp\biggl(\frac{1}{2\pi}\int \frac{e^{i\theta}+z}{e^{i\theta}-z}\,\log[\sin^2\theta]\,d\theta\biggr)$$

which is the Poisson-Jensen formula for $\frac{1}{2}(1-z^2)^2$ if we note that $\Bigl|(1-e^{-2i\theta})^2\Bigr| = 4\sin^2\theta$.

As a final remark on perturbation theory and Jost functions, we note how easy they make Szegő asymptotics for the polynomials:

THEOREM 2.20. *Let J be a Jacobi matrix with δJ trace class. Let $P_n(E)$ be an orthonormal polynomial associated to J. Then for $|z|<1$,*

$$\lim_{n\to\infty} z^n P_n(z+z^{-1}) = \frac{u_0(z;J)}{(1-z^2)} \tag{2.79}$$

with convergence uniform on compact subsets of D.

Remarks. 1. By looking at (2.79) near $z=0$, one gets results on the asymptotics of the leading coefficients of $P_n(E)$, that is, $a_{n,n-j}$ in $P_n(E) = \sum_{k=0}^n a_{n,k}E^k$; see Szegő [60].

2. Alternatively, if Q_n are the monic polynomials,

$$\lim_{n\to\infty} z^n Q_n(z+z^{-1}) = \frac{L(z;J)}{(1-z^2)}. \tag{2.80}$$

Proof. This is essentially (2.59). For let

$$Q_n(E) = \det(E - J_{n;F}). \tag{2.81}$$

Expanding in minors in the last rows shows

$$Q_n(E) = (E-b_n)Q_{n-1}(E) - a_{n-1}^2 Q_{n-2}(E) \tag{2.82}$$

with $Q_0(E)=1$ and $Q_1(E) = E-b_1$. It follows $Q_n(E)$ is the monic orthogonal polynomial of degree n (this is well known; see, e.g. [3]). Multiplying (2.81) by $(a_1,\dots,a_{n-1})^{-1}$, we see that

$$P_n(E) = (a_1\dots a_n)^{-1}Q_n(E) \tag{2.83}$$

obeys (1.4) and so are the orthonormal polynomials. It follows then from (2.59) and (2.9) that

$$L(z;J) = \lim_{n\to\infty} \frac{z^{-1}-z}{z^{-(n+1)}}\, Q_n(z) = \lim_{n\to\infty} (1-z^2)z^n Q_n(z)$$

which implies (2.80) and, given (2.83) and $\lim_{n\to\infty}(a_1\cdots a_n)^{-1}$ exists, also (2.79). □

3. The sum rule: First proof

Following Flaschka [17] and Case [6], [7], the Case sum rules follow from the construction of $L(z;J)$, the expansion (2.55) of $\log[L(z;J)]$ at $z=0$, the formula (2.73) for $\left|L(e^{i\theta};J)\right|$, and the following standard result:

PROPOSITION 3.1. *Let $f(z)$ be analytic in a neighborhood of $\bar D$, let $z_1,\dots,z_m$ be the zeros of f in D and suppose $f(0)\neq 0$. Then*

$$\log|f(0)| = \frac{1}{2\pi}\int_0^{2\pi} \log\left|f(e^{i\theta})\right| d\theta + \sum_{j=1}^m \log|z_j| \tag{3.1}$$

and for $n=1,2,\dots$,

$$\mathrm{Re}(\alpha_n) = \frac{1}{\pi}\int_0^{2\pi} \log\left|f(e^{i\theta})\right| \cos(n\theta)\, d\theta - \mathrm{Re}\left[\sum_{j=1}^m \frac{z_j^{-n}-\bar z_j^{n}}{n}\right] \tag{3.2}$$

where

$$\log\left[\frac{f(z)}{f(0)}\right] = \sum_{n=1}^\infty \alpha_n z^n \tag{3.3}$$

for $|z|$ small.

Remarks. 1. Of course, (3.1) is Jensen's formula. (3.2) can be viewed as a derivative of the Poisson-Jensen formula, but the proof is so easy we give it.

2. In our applications, $\overline{f(z)} = f(\bar z)$ so α_n are real and the zeros are real or come in conjugate pairs. Therefore, Re can be dropped from both sides of (3.2) and the $^-$ dropped from $\bar z_i$.

Proof. Define the Blaschke product,

$$B(z) = \prod_{j=1}^m \frac{|z_j|}{z_j}\,\frac{z_j - z}{1 - z\bar z_j}$$

for which we have

$$
\begin{aligned}
\log[B(z)] &= \sum_{j=1}^{m} \log|z_j| + \log\left[\left(1-\frac{z}{z_j}\right)\right] - \log(1-z\bar{z}_j) \\
&= \sum_{j=1}^{m} \log|z_j| - \sum_{n=1}^{\infty} z^n \sum_{j=1}^{m} \frac{z_j^{-n}-\bar{z}_j^n}{n}\,.
\end{aligned} \tag{3.4}
$$

By a limiting argument, we can suppose f has no zeros on ∂D. Then $f(z)/B(z)$ is nonvanishing in a neighborhood of $\bar{D}$, so $g(z) \equiv \log[f(z)/B(z)]$ is analytic there and by (3.3)/(3.4), its Taylor series

$$
g(z) = \sum_{n=0}^{\infty} c_n z^n
$$

has coefficients

$$
\begin{aligned}
c_0 &= \log[f(0)] - \sum_{j=1}^{m} \log|z_j| \\
c_n &= \alpha_n + \sum_{j=1}^{m} \frac{[z_j^{-n}-\bar{z}_j^n]}{n}\,.
\end{aligned}
$$

Substituting $d\theta = \frac{dz}{iz}$ and $\cos(n\theta) = \frac{1}{2}(z^n + z^{-n})$ in the Cauchy integral formula,

$$
\frac{1}{2\pi i}\int_0^{2\pi} g(z)\,\frac{dz}{z^{n+1}} = \begin{cases} c_n & \text{if } n \ge 0 \\ 0 & \text{if } n \le -1, \end{cases}
$$

we get integral relations whose real part is (3.1) and (3.2). □

While this suffices for the basic sum rule for finite range δJ, which is the starting point of our analysis, we note three extensions:

(1) If $f(z)$ is meromorphic in a neighborhood of $\bar{D}$ with zeros $z_1, \dots, z_m$ and poles $p_1, \dots, p_k$, then (3.1) and (3.2) remain true so long as one makes the changes:

$$
\sum_{j=1}^{m} \log|z_j| \quad \mapsto \quad \sum_{j=1}^{m} \log|z_j| - \sum_{j=1}^{k} \log|p_j| \tag{3.5}
$$

$$
\sum_{j=1}^{m} \frac{z_j^{-n}-\bar{z}_j^n}{n} \quad \mapsto \quad \sum_{j=1}^{m} \frac{z_j^{-n}-\bar{z}_j^n}{n} - \sum_{j=1}^{k} \frac{p_j^{-n}-\bar{p}_j^n}{n} \tag{3.6}
$$

for we write $f(z) = f_1(z)/\prod_{j=1}^{k}(z-p_j)$ and apply Proposition 3.1 to f_1 and to $\prod_{j=1}^{k}(z-p_j)$. We will use this extension in the next section.

(2) If f has continuous boundary values on ∂D, we know its zeros in D obey $\sum_{j=1}^{\infty}(1-|z_j|) < \infty$ (so the Blaschke product converges) and we have some control on $-\log\left|f(re^{i\theta})\right|$ as $r \uparrow 1$, one can prove (3.1)–(3.2) by a limiting

argument. We could use this to extend the proof of Case's inequalities to the situation $\sum n[|a_n - 1| + |b_n|] < \infty$. We first use a Bargmann bound (see [10], [19], [20], [27]) to see there are only finitely many zeros for L and (2.73) to see the only place $\log|L|$ can be singular is at ± 1. The argument in Section 9 that $\sup_r \int [\log_- \left|L(re^{i\theta})\right|]^2 \, d\theta < \infty$ lets us control such potential singularities. Since Section 9 will have a proof in the more general case of trace class δJ, we do not provide the details. But we would like to emphasize that proving the sum rules in generality Case claims in [6], [7] requires overcoming technical issues he never addresses.

(3) The final (one might say ultimate) form of (3.1)/(3.2) applies when f is a Nevanlinna function, that is, f is analytic in D and

$$\sup_{0<r<1} \frac{1}{2\pi} \int_0^{2\pi} \log_+ \left|f(re^{i\theta})\right| \, d\theta < \infty, \tag{3.7}$$

where $\log_+(x) = \max(\log(x), 0)$. If f is Nevanlinna, then ([48, pg. 311]; essentially one uses (3.1) for $f(z/r)$ with $r < 1$),

$$\sum_{j=1}^{\infty} (1 - |z_j|) < \infty \tag{3.8}$$

and ([48, pg. 310]) the Blaschke product converges. Moreover (see [48, pp. 247, 346]), there is a finite real measure $d\mu^{(f)}$ on ∂D so

$$\log \left|f(re^{i\theta})\right| \, d\theta \to d\mu^{(f)}(\theta) \tag{3.9}$$

weakly, and for Lebesgue a.e. θ,

$$\lim_{r \uparrow 1} \log \left|f(re^{i\theta})\right| = \log \left|f(e^{i\theta})\right| \tag{3.10}$$

and

$$d\mu^{(f)}(\theta) = \log \left|f(e^{i\theta})\right| \, d\theta + d\mu_s^{(f)}(\theta) \tag{3.11}$$

where $d\mu_s^{(f)}(\theta)$ is singular with respect to Lebesgue measure $d\theta$ on ∂D. $d\mu_s^{(f)}(\theta)$ is called the singular inner component.

By using (3.1)/(3.2) for $f(z/r)$ with $r \uparrow 1$ and (3.9), we immediately have:

Theorem 3.2. *Let f be a Nevanlinna function on D and let $\{z_j\}_{j=1}^N$ ($N = 1, 2, \ldots,$ or ∞) be its zeros. Suppose $f(0) \neq 0$. Let $\log \left|f(e^{i\theta})\right|$ be the* a.e. *boundary values of f and $d\mu_s^{(f)}(\theta)$ the singular inner component. Then*

$$\log|f(0)| = \frac{1}{2\pi} \int_0^{2\pi} \log \left|f(e^{i\theta})\right| \, d\theta + \frac{1}{2\pi} \int_0^{2\pi} d\mu_s^{(f)}(\theta) + \sum_{j=1}^{N} \log|z_j| \tag{3.12}$$

and for $n = 1, 2, \dots,$

$$\text{(3.13)} \qquad \operatorname{Re}(\alpha_n) = \frac{1}{\pi}\int_0^{2\pi} \log\left|f(e^{i\theta})\right| \cos(n\theta)\,d\theta + \frac{1}{\pi}\int_0^{2\pi} \cos(n\theta)\,d\mu_s^{(f)}(\theta) - \operatorname{Re}\Big[\sum_{j=1}^{N} \frac{z_j^{-n} - \bar{z}_j^{n}}{n}\Big]$$

where α_n *is given by* (3.3).

We will use this form in Section 9.

Now suppose that δJ has finite range, and apply Proposition 3.1 to $L(z;J)$. Its zeros in D are exactly the image under $E \to z$ of the (simple) eigenvalues of J outside $[-2,2]$ (Theorem 2.5(ii)). The expansion of $\log[L(z;J)]$ at $z=0$ is given by Theorem 2.13 and $\log\left|L(e^{i\theta};J)\right|$ is given by (2.73). We have thus proven:

Theorem 3.3 (Case's Sum Rules: Finite Rank Case). *Suppose δJ has finite rank. Then, with $|\beta_1(J)| \geq |\beta_2(J)| \geq \cdots > 1$ defined so that $\beta_j + \beta_j^{-1}$ are the eigenvalues of J outside $[-2,2]$, we have*

$$\text{(3.14)} \quad C_0: \qquad \frac{1}{4\pi}\int_0^{2\pi} \log\Big(\frac{\sin\theta}{\operatorname{Im} M(e^{i\theta})}\Big)\,d\theta = \sum_j \log|\beta_j| - \sum_{n=1}^{\infty} \log(a_n)$$

$$\text{(3.15)} \quad C_n: \qquad -\frac{1}{2\pi}\int_0^{2\pi} \log\Big(\frac{\sin\theta}{\operatorname{Im} M(e^{i\theta})}\Big)\cos(n\theta)\,d\theta = -\frac{1}{n}\sum_j (\beta_j^n - \beta_j^{-n}) + \frac{2}{n}\operatorname{Tr}\Big(T_n\big(\tfrac12 J\big) - T_n\big(\tfrac12 J_0\big)\Big).$$

In particular,

$$\text{(3.16)} \quad P_2: \frac{1}{2\pi}\int_0^{2\pi} \log\Big(\frac{\sin\theta}{\operatorname{Im} M}\Big)\sin^2\theta\,d\theta + \sum_j F(e_j) = \frac14 \sum_n b_n^2 + \frac12 \sum_n G(a_n),$$

where

$$\text{(3.17)} \qquad G(a) = a^2 - 1 - \log(a^2)$$

and

$$\text{(3.18)} \qquad F(e) = \tfrac14(\beta^2 - \beta^{-2} - \log|\beta|^4); \qquad e = \beta + \beta^{-1},\ |\beta| > 1.$$

Remarks. 1. Actually, when δJ is finite rank all eigenvalues must lie outside $[-2,2]$ —it is easily checked that the corresponding difference equation has no (nonzero) square summable solutions. While eigenvalues may occur at -2 or 2 when $\delta J \in \mathcal{I}_1$, there are none in $(-2,2)$. This follows from the fact that $\lim_{r\uparrow 1} M(re^{i\theta}; J)$ exists for $\theta \in (0, \pi)$ (see Theorem 2.19) or alternately from the fact that one can construct two independent solutions $u_n(e^{\pm i\theta}, J)$ whose linear combinations are all non-L^2.

2. In (2.73),

$$\log |L| = \frac{1}{2} \log\left|\frac{\sin\theta}{\operatorname{Im} M}\right| + \sum_{n=1}^{\infty} \log a_n,$$

the $\sum_{n=1}^{\infty} \log a_n$ term is constant and so contributes only to C_0 because $\int_0^{2\pi} \cos(n\theta)\, d\theta = 0$.

3. As noted, P_2 is $C_0 + \frac{1}{2} C_2$.

4. We have looked at the combinations of sum rules that give $\sin^4\theta$ and $\sin^6\theta$ hoping for another miracle like the one below that for $\sin^2\theta$, the function G and F that result are positive. But we have not found anything but a mess of complicated terms that are not in general positive.

P_2 is especially useful because of the properties of G and F:

Proposition 3.4. *The function $G(a) = a^2 - 1 - 2\log(a)$ for $a \in (0, \infty)$ is nonnegative and vanishes only at $a = 1$. For $a - 1$ small,*

$$G(a) = 2(a-1)^2 + O((a-1)^3). \tag{3.19}$$

Proof. By direct calculations, $G(1) = G'(1) = 0$ and

$$G''(a) = \frac{2(1+a^2)}{a^2} \geq 2$$

so $G(a) \geq (a-1)^2$ (since $G(1) = G'(1) = 0$). (3.19) follows from $G''(1) = 4$. $\square$

Proposition 3.5. *The function $F(e)$ given by* (3.18) *is positive throughout its domain, $\{|e| > 2\}$. It is even, increases with increasing $|e|$, and for $|e| - 2$ small,*

$$F(e) = \tfrac{2}{3}(|e| - 2)^{3/2} + O((|e| - 2)^2). \tag{3.20}$$

In addition,

$$F(e) \leq \tfrac{2}{3}(e^2 - 4)^{3/2}. \tag{3.21}$$

Proof. Let $R(\beta) = \frac{1}{4}(\beta^2 - \beta^{-2} - \log|\beta|^4)$ for $\beta \geq 1$ and compute

$$R'(\beta) = \frac{1}{2}\left(\beta + \beta^{-3} - \frac{2}{\beta}\right) = \frac{1}{2}\left(\frac{\beta+1}{\beta}\right)^2 \frac{1}{\beta}\,(\beta-1)^2.$$

This shows that $R(\beta)$ is increasing. It also follows that

$$R'(\beta) = 2(\beta-2)^2 + O((\beta-1)^3)$$

and since $\beta \geq 1$, $(\beta+1)/\beta \leq 2$ and $\beta^{-1} \leq 1$ so

$$R'(\beta) \leq 2(\beta-1)^2.$$

As $R(1) = 0$, we have

$$R(\beta) \leq \tfrac{2}{3}\,(\beta-1)^3 \tag{3.22}$$

and

$$R(\beta) = \tfrac{2}{3}\,(\beta-1)^3 + O((\beta-1)^4). \tag{3.23}$$

Because $F(-e) = F(e)$, which is simple to check, we can suppose $e > 2$ so $\beta > 1$. As $\beta = \frac{1}{2}[e + \sqrt{e^2-4}\,]$ is an increasing function of e, $F(e) = R(\beta)$ is an increasing function of $e > 2$. Moreover, $\beta - 1 = (e-2)^{1/2} + O(e-2)$ and so (3.23) implies (3.20). Lastly,

$$(\beta-1) \leq \beta - \beta^{-1} = \sqrt{e^2-4}\,,$$

so (3.22) implies (3.21). □

4. The sum rule: Second proof

In this section, we will provide a second proof of the sum rules that never mentions a perturbation determinant or a Jost function explicitly. We do this not only because it is nice to have another proof, but because this proof works in a situation where we *a priori* know the m-function is analytic in a neighborhood of $\bar{D}$ and the other proof does not apply. And this is a situation we will meet in proving Theorem 6. On the other hand, while we could prove Theorems 1, 2, 3, 5, 6 without Jost functions, we definitely need them in our proof in Section 9 of the C_0-sum rule for the trace class case.

The second proof of the sum rules is based on the continued fraction expansion of m (1.5). Explicitly, we need,

$$-M(z;J)^{-1} = -(z+z^{-1}) + b_1 + a_1^2 M(z;J^{(1)}) \tag{4.1}$$

which one obtains either from the Weyl solution method of looking at M (see [24], [56]) or by writing M as a limit of ratio of determinants

$$M(z;J) = \lim_{n\to\infty} \frac{\det(E(z) - J^{(1)}_{n-1;F})}{\det(E(z) - J_{n;F})} \tag{4.2}$$

and expanding the denominator in minors in the first row. For any J, (4.1) holds for $z \in D$. Suppose that we know M has a meromorphic continuation to a neighborhood of $\bar{D}$ and consider (4.1) with $z = e^{i\theta}$:

$$-M(e^{i\theta};J)^{-1} = -2\cos\theta + b_1 + a_1^2 M(e^{i\theta};J^{(1)}). \tag{4.3}$$

Taking imaginary parts of both sides,

$$\frac{\operatorname{Im} M(e^{i\theta};J)}{|M(e^{i\theta};J)|^2} = a_1^2 \operatorname{Im} M(e^{i\theta};J^{(1)}) \tag{4.4}$$

or, letting

$$g(z;J) = \frac{M(z;J)}{z}$$

(*Note*: because

$$M(z;J) = (z+z^{-1}-J)_{11}^{-1} = z(1+z^2-zJ)_{11}^{-1} = z + O(z^2) \tag{4.5}$$

near zero, g is analytic in D), we have

$$\frac{1}{2}\left[\log\left(\frac{\operatorname{Im} M(e^{i\theta};J)}{\sin\theta}\right) - \log\left(\frac{\operatorname{Im} M(e^{i\theta};J^{(1)})}{\sin\theta}\right)\right] = \log a_1 + \log\left|g(e^{i\theta};J)\right|. \tag{4.6}$$

To see where this is heading,

Theorem 4.1. *Suppose $M(z;J)$ is meromorphic in a neighborhood of $\bar{D}$. Then J and $J^{(1)}$ have finitely many eigenvalues outside $[-2,2]$ and if*

$$C_0(J) = \frac{1}{4\pi}\int_0^{2\pi} \log\left(\frac{\sin\theta}{\operatorname{Im} M(e^{i\theta};J)}\right) d\theta - \sum_{j=1}^{N} \log|\beta_j(J)| \tag{4.7}$$

(*with β_j as in Theorem* 3.3), *then*

$$C_0(J) = -\log(a_1) + C_0(J^{(1)}). \tag{4.8}$$

In particular, *if δJ is finite rank*, *then the C_0 sum rule holds*:

$$C_0(J) = -\sum_{n=1}^{\infty} \log(a_n). \tag{4.9}$$

Proof. The eigenvalues, E_j, of J outside $[-2,2]$ are precisely the poles of $m(E;J)$ and so the poles of $M(z;J)$ under $E_j = z_j + z_j^{-1}$. By (4.1), the poles of $M(z;J^{(1)})$ are exactly the zeros of $M(z;J)$. Thus $\{\beta_j(J)^{-1}\}$ are the poles of $M(z;J)$ and $\{\beta_j(J^{(1)})^{-1}\}$ are its zeros. Since $g(0;J)=1$ by (4.5), (3.1)/(3.5) becomes

$$\frac{1}{2\pi}\int \log(\left|g(e^{i\theta},J)\right|\, d\theta = -\sum_j \log(|\beta_j(J)|) + \sum_j \log(\left|\beta_j(J^{(1)})\right|).$$

(4.6) and this formula imply (4.8). By (4.3), if $M(z;J)$ is meromorphic in a neighborhood of $\bar{D}$, so is $M(z;J^{(1)})$. So we can iterate (4.8). The free M function is

$$M(z;J_0) = z \tag{4.10}$$

(e.g., by (2.7) with $m = n = 1$), so $C_0(J_0) = 0$ and thus, if δJ is finite rank, the remainder is zero after finitely many steps. $\square$

To get the higher-order sum rules, we need to compute the power series for $\log(g(z; J))$ about $z = 0$. For low-order, we can do this by hand. Indeed, by (4.1) and (4.5) for $J^{(1)}$,

$$\begin{aligned} g(z; J) &= (z[(z + z^{-1}) - b_1 - a_1^2 z + O(z^2)])^{-1} \\ &= (1 - b_1 z - (a_1^2 - 1)z^2 + O(z^3))^{-1} \\ &= 1 + b_1 z + ((a_1^2 - 1) + b_1^2)z^2 + O(z^3) \end{aligned}$$

so since $\log(1 + w) = w - \frac{1}{2}w^2 + O(w^3)$,

$$\log(g(z; J)) = b_1 z + (\tfrac{1}{2}\, b_1^2 + a_1^2 - 1)z^2 + O(z^3). \tag{4.11}$$

Therefore, by mimicking the proof of Theorem 4.1, but using (3.2)/(3.6) in place of (3.1)/(3.5), we have

THEOREM 4.2. *Suppose $M(z; J)$ is meromorphic in a neighborhood of $\bar{D}$. Let*

$$C_n(J) = -\frac{1}{2\pi} \int_0^{2\pi} \log\biggl(\frac{\sin\theta}{\operatorname{Im} M(e^{i\theta})}\biggr) \cos(n\theta) + \frac{1}{n}\biggl[\sum_j \beta_j(J)^n - \beta_j(J)^{-n}\biggr]. \tag{4.12}$$

Then

$$C_1(J) = b_1 + C_1(J^{(1)}) \tag{4.13}$$

$$C_2(J) = [\tfrac{1}{2}\, b_1^2 + (a_1^2 - 1) \ + C_2(J^{(1)})]. \tag{4.14}$$

If

$$P_2(J) = \frac{1}{2\pi} \int_0^{2\pi} \log\biggl(\frac{\sin\theta}{\operatorname{Im} M(e^{i\theta})}\biggr) \sin^2\theta\, d\theta + \sum_j F(e_j(J)) \tag{4.15}$$

with F given by (3.18), *then writing $G(a) = a^2 - 1 - 2\log(a)$ as in* (3.17)

$$P_2(J) = \tfrac{1}{4}\, b_1^2 + \tfrac{1}{2}\, G(a_1) + P_2(J^{(1)}). \tag{4.16}$$

In particular, if δJ is finite rank, we have the sum rules C_1, C_2, P_2 of (3.15)/(3.16).

To go to order larger than two, we expand $\log(g(z; J))$ systematically as follows: We begin by noting that by (4.2) (Cramer's rule),

$$g(z; J) = \lim_{n\to\infty} g_n(z; J) \tag{4.17}$$

where

$$g_n(z; J) = \frac{z^{-1} \det(z + z^{-1} - J^{(1)}_{n-1;F})}{\det(z + z^{-1} - J_{n;F})} \tag{4.18}$$

$$= \frac{1}{1 + z^2}\, \frac{\det(1 - E(z)^{-1} J^{(1)}_{n-1;F})}{\det(1 - E(z)^{-1} J_{n;F})} \tag{4.19}$$

where we used $z(E(z)) = 1+z^2$ and the fact that because the numerator has a matrix of order one less than the denominator, we get an extra factor of $E(z)$. We now use Lemma 2.11, writing $F_j(x)$ for $\frac{2}{j}[T_j(0) - T_j(x/2)]$,

$$\log g_n(z;J) = -\log(1+z^2) + \sum_{j=1}^{\infty} z^j \Big[\operatorname{Tr}\Big(F_j(J^{(1)}_{n-1;F})\Big) - \operatorname{Tr}\Big(F_j(J_{n;F})\Big)\Big] \tag{4.20}$$

$$= -\log(1+z^2) - \sum_{j=1}^{\infty} \frac{z^{2j}}{j}(-1)^j \tag{4.21}$$

$$+ \sum_{j=1}^{\infty} \frac{2z^j}{j}\Big[\operatorname{Tr}\Big(T_j\Big(\tfrac{1}{2}J_{n;F}\Big)\Big) - \operatorname{Tr}\Big(T_j\Big(\tfrac{1}{2}J^{(1)}_{n-1;F}\Big)\Big)\Big]$$

where we picked up the first sum because $J_{n;F}$ has dimension one greater than $J^{(1)}_{n-1;F}$ so the $T_j(0)$ terms in $F_j(J_{n;F})$ and $J^{(1)}_{n-1;F}$ contribute differently. Notice

$$\sum_{j=1}^{\infty} \frac{z^{2j}}{j}(-1)^j = -\log(1+z^2)$$

so the first two terms cancel! Since $g_n(z;J)$ converges to $g(z;J)$ in a neighborhood of $z=0$, its Taylor coefficients converge. Thus

Proposition 4.3. *For each j,*

$$\alpha_j(J,J^{(1)}) = \lim_{n\to\infty}\Big[\operatorname{Tr}\Big(T_j\Big(\tfrac{1}{2}J_{n;F}\Big)\Big) - \operatorname{Tr}\Big(T_j\Big(\tfrac{1}{2}J^{(1)}_{n-1;F}\Big)\Big)\Big] \tag{4.22}$$

exists, and for z small,

$$\log g(z;J) = \sum_{j=1}^{\infty} \frac{2z^j}{j}\,\alpha_j(J,J^{(1)}). \tag{4.23}$$

Remark. Since

$$(J^{(1)\ell})_{mm} = (J^\ell)_{m+1\,m+1}$$

if $m \ge \ell$, the difference of traces on the right side of (4.22) is constant for $n > j$, so one need not take the limit.

Plugging this into the machine that gives Theorem 4.1 and Theorem 4.2, we obtain

Theorem 4.4. *Suppose $M(z;J)$ is meromorphic in a neighborhood of $\bar{D}$. Let $C_n(J)$ be given by* (4.12) *and α by* (4.22). *Then*

$$C_n(J) = \frac{2}{n}\,\alpha_n(J,J^{(1)}) + C_n(J^{(1)}). \tag{4.24}$$

In particular, if δJ is finite rank, we have the sum rule C_n of (3.15).

Proof. The only remaining point is why if δJ is finite rank, we have recovered the same sum rule as in (3.15). Iterating (4.24) when J has rank m gives

$$\begin{aligned} C_n(J) &= \frac{2}{n}\sum_{j=1}^{m} \alpha_n(J^{(j-1)}, J^{(j)}) \\ &= \lim_{\ell\to\infty} \frac{2}{n}\Big[\mathrm{Tr}\Big[T_n\Big(\tfrac{1}{2}J_{\ell;F}\Big) - T_n\Big(\tfrac{1}{2}J_{0,\ell-m;F}\Big)\Big]\Big] \end{aligned} \tag{4.25}$$

while (3.15) reads

$$\begin{aligned} C_n(J) &= \frac{2}{n}\,\mathrm{Tr}\Big[T_n\Big(\tfrac{1}{2}J\Big) - T_n\Big(\tfrac{1}{2}J_0\Big)\Big] \\ &= \lim_{\ell\to\infty} \frac{2}{n}\Big[\mathrm{Tr}\Big[T_n\Big(\tfrac{1}{2}J_{\ell;F}\Big)\Big] - \mathrm{Tr}\Big[T_n\Big(\tfrac{1}{2}J_{0,\ell;F}\Big)\Big]\Big]. \end{aligned} \tag{4.26}$$

That (4.25) and (4.26) are the same is a consequence of Proposition 2.2. □

5. Entropy and lower semicontinuity of the Szegő and quasi-Szegő terms

In the sum rules C_0 and P_2 of most interest to us, there appear two terms involving integrals of logarithms:

$$Z(J) = \frac{1}{4\pi}\int_0^{2\pi} \log\bigg(\frac{\sin\theta}{\mathrm{Im}\, M(e^{i\theta}, J)}\bigg)\, d\theta \tag{5.1}$$

and

$$Q(J) = \frac{1}{2\pi}\int_0^{2\pi} \log\bigg(\frac{\sin\theta}{\mathrm{Im}\, M(e^{i\theta}, J)}\bigg)\sin^2\theta\, d\theta. \tag{5.2}$$

One should think of M as related to the original spectral measure on $\sigma(J) \supset [-2,2]$ as

$$\mathrm{Im}\, M(e^{i\theta}) = \pi\, \frac{d\mu_{\mathrm{ac}}}{dE}\,(2\cos\theta) \tag{5.3}$$

in which case, (5.1), (5.2) can be rewritten

$$Z(J) = \frac{1}{2\pi}\int_{-2}^{2} \log\bigg(\frac{\sqrt{4-E^2}}{2\pi\, d\mu_{\mathrm{ac}}/dE}\bigg)\frac{dE}{\sqrt{4-E^2}} \tag{5.4}$$

and

$$Q(J) = \frac{1}{4\pi}\int_{-2}^{2} \log\bigg(\frac{\sqrt{4-E^2}}{2\pi\, d\mu_{\mathrm{ac}}/dE}\bigg)\sqrt{4-E^2}\, dE. \tag{5.5}$$

Our main result in this section is to view Z and Q as functions of μ and to prove if $\mu_n \to \mu$ weakly, then $Z(\mu_n)$ (resp. $Q(\mu_n)$) obeys

$$Z(\mu) \le \liminf Z(\mu_n); \qquad Q(\mu) \le \liminf Q(\mu_n), \tag{5.6}$$

that is, that Z and Q are weakly lower semicontinuous. This will let us prove sum rule-type inequalities in great generality.

The basic idea of the proof will be to write variational principles for Z and Q as suprema of weakly continuous functions. Indeed, as Totik has pointed out to us, Szegő's theorem (as extended to the general, not only a.c., case [2], [18]) gives what is essentially $Z(J)$ by a variational principle; explicitly,

$$\exp\left\{\frac{1}{2\pi}\int_0^{2\pi}\log\left(\frac{d\mu_{\rm ac}}{d\theta}\right)d\theta\right\} = \inf_P\left[\frac{1}{2\pi}\int_{-\pi}^{\pi}\left|P(e^{i\theta})\right|^2\,d\mu(\theta)\right] \tag{5.7}$$

where P runs through all polynomials with $P(0) = 1$, which can be used to prove the semicontinuity we need for Z. It is an interesting question of what is the relation between (5.7) and the variational principle (5.16) below. It also would be interesting to know if there is an analog of (5.7) to prove semicontinuity of Q.

We will deduce the semicontinuity by providing a variational principle. We originally found the variational principle based on the theory of Legendre transforms, then realized that the result was reminiscent of the inverse Gibbs variation principle for entropy (see [55, pg. 271] for historical remarks; the principle was first written down by Lanford-Robinson [35]) and then realized that the quantities of interest to us aren't merely reminiscent of entropy, they are exactly relative entropies where μ is the second variable rather than the first one that is usually varied. We have located the upper semicontinuity of the relative entropy in the second variable in the literature (see, e.g., [12], [34], [44]), but not in the generality we need it, so especially since the proof is easy, we provide it below. We use the notation

$$\log_\pm(x) = \max(\pm\log(x), 0). \tag{5.8}$$

Definition. Let μ, ν be finite Borel measures on a compact Hausdorff space, X. We define the entropy of μ relative to ν, $S(\mu \mid \nu)$, by

$$S(\mu \mid \nu) = \begin{cases} -\infty & \text{if } \mu \text{ is not } \nu\text{-ac} \\ -\int \log(\frac{d\mu}{d\nu})d\mu & \text{if } \mu \text{ is } \nu\text{-ac.} \end{cases} \tag{5.9}$$

Remarks. 1. Since $\log_-(x) = \log_+(x^{-1}) \le x^{-1}$ and

$$\int\left(\frac{d\mu}{d\nu}\right)^{-1}d\mu = \nu\left(\left\{x \;\Big|\; \frac{d\mu}{d\nu} \neq 0\right\}\right) \le \nu(X) < \infty,$$

the integral in (5.9) can only diverge to $-\infty$, not to $+\infty$.

2. If $d\mu = f\,d\nu$, then

$$S(\mu \mid \nu) = -\int f \log(f)\,d\nu, \tag{5.10}$$

the more usual formula for entropy.

Lemma 5.1. *Let μ be a probability measure. Then*

$$S(\mu \mid \nu) \leq \log \nu(X). \tag{5.11}$$

In particular, if ν is also a probability measure,

$$S(\mu \mid \nu) \leq 0. \tag{5.12}$$

Equality holds in (5.12) *if and only if $\mu = \nu$.*

Proof. If μ is not ν-ac, (5.11)/(5.12) is trivial, so suppose $\mu = f\,d\nu$ and let

$$d\tilde{\nu} = \chi_{\{x \mid f(x) \neq 0\}}\,d\nu \tag{5.13}$$

so $\tilde{\nu}$ and μ are mutually ac. Then,

$$\begin{aligned} S(\mu \mid \nu) &= \int \log\left(\frac{d\tilde{\nu}}{d\mu}\right) d\mu && (5.14)\\ &\leq \log\left(\int \left(\frac{d\tilde{\nu}}{d\mu}\right) d\mu\right) \\ &= \log \tilde{\nu}(X) && (5.15)\\ &\leq \log \nu(X) \end{aligned}$$

where we used Jensen's inequality for the concave function $\log(x)$. For equality to hold in (5.12), we need equality in (5.15) (which says $\nu = \tilde{\nu}$) and in (5.14), which says, since log is strictly convex, that $d\nu/d\mu$ is a constant. When $\nu(X) = \mu(X) = 1$, this says $\nu = \mu$. □

Theorem 5.2. *For all μ, ν,*

$$S(\mu \mid \nu) = \inf\left[\int F(x)\,d\nu - \int (1 + \log F)\,d\mu(x)\right] \tag{5.16}$$

where the inf *is taken over all real-valued continuous functions F with* $\min_{x \in X} F(x) > 0$.

Proof. Let us use the notation

$$\mathcal{G}(F, \mu, \nu) = \int F(x)\,d\nu - \int (1 + \log F)\,d\mu(x)$$

for any nonnegative function F with $F \in L^1(d\nu)$ and $\log F \in L^1(d\mu)$.

Suppose first that μ is ν-ac with $d\mu = f\,d\nu$ and F is positive and continuous. Let $A = \{x \mid f(x) \neq 0\}$ and define $\tilde{\nu}$ by (5.13). As $\log(a)$ is concave, $\log(a) \leq a - 1$ so for $a, b > 0$,

$$ab^{-1} \geq 1 + \log(ab^{-1}) = 1 + \log(a) - \log b. \tag{5.17}$$

Thus for $x \in A$,

$$F(x)f(x)^{-1} \geq 1 + \log F(x) - \log f(x).$$

Integrating with $d\mu$ and using

$$\int F(x)\,d\nu \geq \int F(x)\,d\tilde{\nu} = \int_A F(x)f(x)^{-1}\,d\mu,$$

we have that

$$\int F(x)\,d\nu \geq \int (1 + \log F(x))\,d\mu(x) + S(\mu \mid \nu)$$

or

$$S(\mu \mid \nu) \leq \mathcal{G}(F, \mu, \nu). \tag{5.18}$$

To get equality in (5.16), take $F = f$ so $\int d\mu$ and $\int F\,d\nu$ cancel. Of course, f may not be continuous or strictly positive, so we need an approximation argument. Given N, ε, let

$$f_{N,\varepsilon}(x) = \begin{cases} N & \text{if } f(x) \geq N \\ f(x) & \text{if } \varepsilon \leq f(x) \leq N \\ \varepsilon & \text{if } f(x) \leq \varepsilon. \end{cases}$$

Let $f_{\ell,N,\varepsilon}(x)$ be continuous functions with $\varepsilon \leq f_{\ell,N,\varepsilon} \leq N$ so that as $\ell \to \infty$, $f_{\ell,N,\varepsilon} \to f_{N,\varepsilon}$ in $L^1(X, d\mu + d\nu)$. For $N > 1$, $f f_{N,\varepsilon}^{-1} \leq 1 + f$, so we have

$$\begin{aligned} -\int \log(f_{N,\varepsilon})\,d\mu &= \mu(X) \int \log(f_{N,\varepsilon}^{-1})\,\frac{d\mu}{\mu(X)} \\ &\leq \mu(X) \log\biggl[\int f f_{N,\varepsilon}^{-1}\,\frac{d\nu}{\mu(X)}\biggr] \\ &\leq \mu(X) \log\biggl[1 + \frac{\nu(X)}{\mu(X)}\biggr] < \infty \end{aligned}$$

and thus, since $-\log(f_{N,\varepsilon})$ increases as $\varepsilon \downarrow 0$, $f_{N,\varepsilon=0} \equiv \lim_{\varepsilon\downarrow 0} f_{N,\varepsilon}$ has $\log f_{N,\varepsilon=0} \in L^1(d\mu)$ and the integrals converge. It follows that as $\ell \to \infty$ and then $\varepsilon \downarrow 0$,

$$\mathcal{G}(f_{\ell,N,\varepsilon}, \mu, \nu) \to \mathcal{G}(f_{N,\varepsilon}, \mu, \nu) \to \mathcal{G}(f_{N,\varepsilon=0}, \mu, \nu).$$

We now take $N \to \infty$. By monotonicity, $-\int \log f_{N,\varepsilon=0}\,d\mu$ converges to $-\int \log f\,d\mu$ which may be infinite. In addition, $\int f_{N,\varepsilon=0}\,d\nu - \int d\mu \to 0$ so $\mathcal{G}(f_{N,\varepsilon=0}, \mu, \nu) \to S(\mu \mid \nu)$, and we have proven (5.18).

Next, suppose μ is not ν-ac. Thus, there is a Borel subset $A \subset X$ with $\mu(A) > 0$ and $\nu(A) = 0$. By regularity of measures, we can find $K \subset A$ compact and for any ε, U_ε open so $K \subset A \subset U_\varepsilon$ and

$$\mu(K) > 0 \qquad \nu(U_\varepsilon) < \varepsilon. \tag{5.19}$$

By Urysohn's lemma, find F_ε continuous with

$$1 \leq F_\varepsilon(x) \leq \varepsilon^{-1} \text{ all } x, \qquad F_\varepsilon \equiv \varepsilon^{-1} \text{ on } K,\ F_\varepsilon \equiv 1 \text{ on } X \backslash U_\varepsilon. \tag{5.20}$$

Then

$$\int F_\varepsilon \, d\nu \leq \nu(X \backslash U_\varepsilon) + \varepsilon^{-1}\nu(U_\varepsilon) \leq \nu(X) + 1$$

while

$$\int (1 + \log F_\varepsilon) \, d\mu \geq \log(\varepsilon^{-1})\mu(K)$$

so

$$\mathcal{G}(F_\varepsilon, \mu, \nu) \leq \nu(X) + 1 - \log(\varepsilon^{-1})\mu(K) \to -\infty$$

as $\varepsilon \downarrow 0$, proving the right side of (5.16) is $-\infty$. $\square$

As an infimum of continuous functions is upper semicontinuous, we have

COROLLARY 5.3. *$S(\mu \mid \nu)$ is jointly weakly upper semicontinuous in μ and ν, that is, if $\mu_n \xrightarrow{w} \mu$ and $\nu_n \xrightarrow{w} \nu$, then*

$$S(\mu \mid \nu) \geq \limsup_n S(\mu_n \mid \nu_n).$$

Remarks. 1. In our applications, μ_n will be fixed.

2. This proof can handle functions other than log. If $\int \log((d\nu/d\mu)^{-1}) \, d\mu$ is replaced by $\int G((d\nu/d\mu)) \, d\mu$ where G is an arbitrary increasing concave function with $\lim_{y \downarrow 0} G(y) = \infty$, there is a variational principle where $1 + \log F$ in (5.18) is replaced by $H(F(x))$ with $H(y) = \inf_x (xy - G(x))$.

To apply this to Z and Q, we note

PROPOSITION 5.4.
(a) *Let*

$$d\mu_0(E) = \frac{1}{2\pi} \sqrt{4 - E^2} \, dE. \tag{5.21}$$

Then

$$Q(J) = -\tfrac{1}{2} S(\mu_0 \mid \mu_J). \tag{5.22}$$

(b) *Let*

$$d\mu_1(E) = \frac{1}{\pi} \frac{dE}{\sqrt{4 - E^2}} \,. \tag{5.23}$$

Then

$$Z(J) = -\tfrac{1}{2}\,\log(2) - \tfrac{1}{2}\,S(\mu_1 \mid \mu_J). \tag{5.24}$$

Remarks. 1. Both μ_0 and μ_1 are probability measures, as is easily checked by setting $E = 2\cos\theta$.

2. $d\mu_0$ is the spectral measure for J_0. For $M(z;J_0) = z$ and thus $\operatorname{Im} M(e^{i\theta};J_0) = \sin\theta$ so $m(E;J_0) = \frac{1}{2}\sqrt{4-E^2}$ and $\frac{1}{\pi}\operatorname{Im} m\,dE = d\mu_0$.

3. $d\mu_1$ is the spectral measure for the whole-line free Jacobi matrix and also for the half-line matrix with $b_n = 0$, $a_1 = \sqrt{2}$, $a_2 = a_3 = \cdots = 1$. An easy way to see this is to note that after $E = 2\cos\theta$, $d\mu_1(\theta) = \frac{1}{\pi}\,d\theta$ and so the orthogonal polynomials are precisely the normalized scaled Chebyshev polynomials of the first kind that have the given values of a_j.

Proof. (a) Follows immediately from (5.16) if we note that

$$\frac{d\mu_0}{d\mu} = \frac{d\mu_0}{dE}\bigg/\frac{d\mu_{\rm ac}}{dE} = \frac{\sqrt{4-E^2}}{2\pi\,d\mu_{\rm ac}/dE}\,.$$

(b) As above,

$$\frac{d\mu_1}{d\mu} = 2(4-E^2)^{-1}\,\frac{\sqrt{4-E^2}}{2\pi\,d\mu_{\rm ac}/dE}\,.$$

Thus

$$Z(J) = c - \tfrac{1}{2}\,S(\mu_1 \mid \mu_J),$$

where

$$\begin{aligned} c &= -\frac{1}{2\pi}\int_{-2}^{2} \log\biggl[\frac{2}{4-E^2}\biggr]\sqrt{4-E^2}\,dE \\ &= \frac{1}{4\pi}\int_0^{2\pi} \log[2\sin^2\theta]\,d\theta \\ &= \frac{1}{2}\,\log(2) + \frac{1}{2\pi}\int_0^{2\pi} \log\lvert\sin\theta\rvert\,d\theta \\ &= \frac{1}{2}\,\log(2) + \frac{1}{2\pi}\int_0^{2\pi} \log\biggl\lvert\frac{1-e^{i\theta}}{2}\biggr\rvert\,d\theta \\ &= \frac{1}{2}\,\log(2) + \log\Bigl(\frac{1}{2}\Bigr) = -\frac{1}{2}\,\log(2) \end{aligned}$$

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

Remark. As a check on our arithmetic, consider the Jacobi matrix $\tilde{J}$ with $a_1 = \sqrt{2}$ and all other a's and b's the same as for J_0 so $d\mu_{\tilde{J}}$ is $d\mu_1$. The sum rule, C_0, for this case says that

$$Z(\tilde{J}) = -\log(\sqrt{2}) = -\tfrac{1}{2}\,\log 2$$

since there are no eigenvalues and $a_1 = \sqrt{2}$. But $\mu_1 = \mu_J$, so $S(\mu_1 \mid \mu_J) = 0$. This shows once again that $c = -\frac{1}{2}\log 2$ (actually, it is essentially the calculation we did—done the long way around!).

Given this proposition, Lemma 5.1, and Corollary 5.3, we have

THEOREM 5.5. *For any Jacobi matrix*,

$$Q(J) \geq 0 \tag{5.25}$$

and

$$Z(J) \geq -\tfrac{1}{2}\,\log(2). \tag{5.26}$$

If $\mu_{J_n} \to \mu_J$ weakly, then

$$Z(J) \leq \liminf\, Z(J_n). \tag{5.27}$$

and

$$Q(J) \leq \liminf\, Q(J_n). \tag{5.28}$$

We will call (5.27) and (5.28) lower semicontinuity of Z and Q.

6. Fun and games with eigenvalues

Recall that J_n denotes the Jacobi matrix with truncated perturbation, as given by (2.1). In trying to get sum rules, we will approximate J by J_n and need to estimate eigenvalues of J_n in terms of eigenvalues of J. Throughout this section, X denotes a continuous function on $\mathbb{R}$ with $X(x) = X(-x)$, $X(x) = 0$ if $|x| \leq 2$, and X is monotone increasing in $[2,\infty)$. Our goal is to prove:

THEOREM 6.1. *For any J and all n, we have $N^{\pm}(J_n) \leq N^{\pm}(J) + 1$ and*

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

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

In particular, for any function X of the type described above,

$$\sum_{j=1}^{N^{\pm}(J_n)} X(E_j^{\pm}(J_n)) \leq X(E_1^{\pm}(J)+1) + \sum_{j=1}^{N^{\pm}(J)} X(E_j^{\pm}(J)). \tag{6.1}$$

THEOREM 6.2. *If $J - J_0$ is compact, then*

$$\lim_{n\to\infty} \sum_{j=1}^{N^{\pm}(J_n)} X(E_j^{\pm}(J_n)) = \sum_{j=1}^{N^{\pm}(J)} X(E_j^{\pm}(J)). \tag{6.2}$$

This quantity may be infinite.

Proof of Theorem 6.1. To prove these results, we pass from J to J_n in several intermediate steps.

(1) We pass from J to $J_{n;F}$.

(2) We pass from $J_{n;F}$ to $J_{n;F} \pm d_{n,n} \equiv J^{\pm}_{n;F}$ where $d_{n,n}$ is the matrix with 1 in the n, n place and zero elsewhere.

(3) We take a direct sum of $J^{\pm}_{n;F}$ and $J_0 \pm d_{1,1}$.

(4) We pass from this direct sum to J_n.

Step 1. $J_{n;F}$ is just a restriction of J (to $\ell^2(\{1, \dots, n\})$). The min-max principle [45] implies that under restrictions, the most positive eigenvalues become less positive and the most negative, less negative. It follows that

$$N^{\pm}(J_{n;F}) \leq N^{\pm}(J) \tag{6.3}$$

$$\pm E^{\pm}_j(J_{n;F}) \leq \pm E^{\pm}_j(J). \tag{6.4}$$

Step 2. To study E^+_j, we add $d_{n,n}$, and to study E^-_j, we subtract $d_{n,n}$. The added operator $d_{n,n}$ has two critical properties: It is rank one and its norm is one. From the norm condition, we see

$$\left| E^{\pm}_1(J^{\pm}_{n;F}) - E^{\pm}_1(J_{n;F}) \right| \leq 1 \tag{6.5}$$

so

$$\begin{aligned} E^+_1(J^+_{n;F}) &\leq E^+_1(J_{n;F}) + 1 \\ &\leq E^+_1(J) + 1. \end{aligned} \tag{6.6}$$

(Note (6.5) and (6.6) hold for all indices j, not just $j = 1$, but we only need $j = 1$.) Because $d_{n,n}$ is rank 1, and positive, we have

$$E^+_{m+1}(J_{n;F}) \leq E^+_{m+1}(J^+_{n;F}) \leq E^+_m(J_{n;F})$$

and so, by (6.4),

$$E^+_{m+1}(J^+_{n;F}) \leq E^+_m(J) \tag{6.7}$$

and thus also

$$N^{\pm}(J^{\pm}_{n;F}) \leq N^{\pm}(J) + 1. \tag{6.8}$$

Step 3. Take the direct sum of $J^{\pm}_{n;F}$ and $J_0 \pm d_{11}$. This should be interpreted as a matrix with entries

$$\left[J^{\pm}_{n;F} \oplus (J_0 \pm d_{11}) \right]_{k,\ell} = \begin{cases} (J^{\pm}_{n;F})_{k,\ell} & k, \ell \leq n \\ (J_0 \pm d_{11})_{k-n,\ell-n} & k, \ell > n \\ 0 & \text{otherwise.} \end{cases}$$

Since $J_0 \pm d_{11}$ has no eigenvalues, (6.7) and (6.8) still hold.

Step 4. Go from the direct sum to J_n. In the $+$ case, we add the 2×2 matrix in sites $n, n+1$:

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

and, in the $-$ case,

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

dJ^+ is negative, so it moves eigenvalues down, while dJ^- is positive. Thus

$$E^+_{m+1}(J_n) \le E^+_{m+1}(J^+_{n;F}) \le E^+_m(J)$$

and

$$N^\pm(J_n) \le N^\pm(J^\pm_{n;F}) \le N^\pm(J) + 1. \qquad \square$$

Proof of Theorem 6.2. We have, since $J - J_0$ is compact, that

$$\|J_n - J\| \le \sup_{m \ge n+1} |b_m| + 2 \sup_{m \ge n} |a_m| \to 0.$$

Thus

$$\left| E^\pm_j(J_n) - E^\pm_j(J) \right| \le \|J_n - J\| \to 0. \tag{6.9}$$

If $\sum_{j=1}^{N^\pm(J)} X(E^\pm_j(J)) = \infty$, then, by (6.9), for all fixed m,

$$\begin{aligned} \liminf \sum_{j=1}^{N^\pm(J_n)} X(E^\pm_j(J_n)) \quad &\ge \quad \liminf \sum_{j=1}^{m} X(E^\pm_j(J_n)) \\ &= \quad \sum_{j=1}^{m} X(E^\pm_j(J)) \end{aligned}$$

so taking m to infinity, (6.2) results.

If the sum is finite, (6.9), dominated convergence and (6.1) imply (6.2). $\square$

7. Jacobi data dominate spectral data in P_2

Our goal in this section is to prove Theorem 5. Explicitly, for a Jacobi matrix, J, let

$$D_2(J) = \tfrac{1}{4} \sum_{j=1}^{\infty} b_j^2 + \tfrac{1}{2} \sum_{j=1}^{\infty} G(a_j) \tag{7.1}$$

with $G = a^2 - 1 - 2\log(a)$ as in (3.17). For a probability measure, μ on $\mathbb{R}$, define

$$P_2(\mu) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \log\biggl(\frac{\sin\theta}{\operatorname{Im} M_\mu(e^{i\theta})}\biggr) \sin^2\theta\, d\theta + \sum_j F(E_j) \tag{7.2}$$

where E_j are the mass points of μ outside $[-2,2]$ and F is given by (3.18). Recall that $\operatorname{Im} M_\mu(e^{i\theta}) \equiv \pi\, d\mu_{\rm ac}/dE$ at $E = 2\cos\theta$. We will let μ_J be the measure associated with J by the spectral theorem and J_μ the Jacobi matrix associated to μ.

Then Theorem 5 says

THEOREM 7.1. *If $J - J_0$ is Hilbert-Schmidt so that $D_2(J) < \infty$, then $P_2(\mu_J) < \infty$ and*

$$P_2(\mu_J) \le D_2(J). \tag{7.3}$$

Proof. Let J_n be a truncation of J given by (2.1). Then $D_2(J_n)$ is monotone increasing with limit $D_2(J)$. This is finite because $J - J_0$ is Hilbert-Schmidt. By the definition (5.5),

$$\begin{aligned} P_2(\mu) &= Q(J) + \sum_j F(E_j) \\ &= -\tfrac{1}{2}\, S(\mu_0,\mu) + \sum_j F(E_j) \end{aligned} \tag{7.4}$$

by (5.22). Since $Q \ge 0$ (5.25) and $F > 0$ (Proposition 3.5), (7.4) is a sum of positive terms. Moreover, by Theorem 6.2, $\sum_j F(E_j(J_n)) \to \sum_j F(E_j(J))$ even if the right side is infinite. As $J_n \to J$ in Hilbert-Schmidt sense, $(J_n - E)^{-1}$ converges (in norm) to $(J-E)^{-1}$ for all $E \in \mathbb{C}\setminus\mathbb{R}$. This implies that μ_{J_n} converges weakly to μ and so by (5.28), $Q(J) \le \limsup Q(J_n)$. It follows that

$$\begin{aligned} P_2(J_\mu) &\le \limsup \Bigl[Q(J_n) + \sum F\bigl(E_j(J_n)\bigr)\Bigr] \\ &= \limsup D_2(J_n) \qquad \text{(by Theorem 3.3)} \\ &= D_2(J). \end{aligned}$$

Thus $P_2(\mu_J) < \infty$ and (7.3) holds. $\square$

The result in this section is essentially a quantitative version of the main result in Deift-Killip [13].

8. Spectral data dominate Jacobi data in P_2

Our goal in this section is to prove the following, which is essentially Theorem 6:

THEOREM 8.1. *If μ is a probability measure with $P_2(\mu) < \infty$, then*

$$D_2(J_\mu) \leq P_2(\mu) \tag{8.1}$$

and so J_μ is Hilbert-Schmidt.

The idea of the proof is to start with a case where we have the sum rule and then pass to successively more general cases where we can prove an inequality of the form (8.1). There will be three steps:

(1) Prove the inequality in the case M_μ is meromorphic in a neighborhood of $\bar{D}$.

(2) Prove the inequality in the case $\mu \geq \delta\mu_0$ where δ is a positive real number and μ_0 is the free Jacobi measure (5.18).

(3) Prove the inequality in the case $P_2(\mu) < \infty$.

PROPOSITION 8.2. *Let J be a Jacobi matrix for which M_μ has a meromorphic continuation to a neighborhood of $\bar{D}$. Then*

$$D_2(J) \leq P_2(J). \tag{8.2}$$

Proof. By Theorem 4.2,

$$P_2(J) = \tfrac{1}{4}\, b_1^2 + \tfrac{1}{2}\, G(a_1) + P_2(J^{(1)}).$$

so iterating,

$$\begin{aligned} P_2(J) &= \tfrac{1}{4}\sum_{j=1}^{m} b_j^2 + \tfrac{1}{2}\sum_{j=1}^{m} G(a_j) + P_2(J^{(m)}) \\ &\geq \tfrac{1}{4}\sum_{j=1}^{m} b_j^2 + \tfrac{1}{2}\sum_{j=0}^{m} G(a_j) \end{aligned}$$

since $P_2(J^{(m)}) \geq 0$. Now $G \geq 0$, so we can take $m \to \infty$ and obtain (8.2). □

Remark. If M_μ has a meromorphic continuation into $\{z \mid |z| < \eta\}$ for some $\eta > 1$, then by a theorem of Geronimo [21], $\sum |a_n - 1|\,\rho^n + |b_n|\,\rho^n < \infty$ for all $\rho < \eta$, so the sum rule also follows from the methods of Section 3. We prefer to avoid the use of Geronimo's theorem.

Given any J and associated M-function $M(z; J)$, there is a natural approximating family of M-functions meromorphic in a neighborhood of $\bar{D}$.

LEMMA 8.3. *Let M_μ be the M-function of a probability measure μ obeying the Blumenthal-Weyl condition, and define*

$$M^{(r)}(z) = r^{-1} M_\mu(rz) \tag{8.3}$$

for $0 < r < 1$. Then, there is a set of probability measures $\mu^{(r)}$ so that $M^{(r)} = M_{\mu^{(r)}}$.

Proof. Return to the E variable. Since $M^{(r)}(z)$ is meromorphic in a neighborhood of $\bar{D}$ with $\operatorname{Im} M^{(r)}(z) > 0$ if $\operatorname{Im} z > 0$,

$$m^{(r)}(E) = -M^{(r)}(z(E))$$

(where $z(E) + z(E)^{-1} = E$ with $|z| < 1$) is meromorphic on $\mathbb{C}\backslash[-2,2]$ and Herglotz. It follows that it is the Borel transform of a measure $\mu^{(r)}$ of total weight $\lim_{E\to\infty} -Em^{(r)}(E) = \lim_{z\downarrow 0} z^{-1} M_\mu^{(r)}(z) = 1$. □

Proposition 8.4. *Let μ be a probability measure obeying the Blumenthal-Weyl condition and*

$$\mu \geq \delta\mu_0 \tag{8.4}$$

where μ_0 is the free Jacobi measure (*the measure with $M_{\mu_0}(z) = z$*) *and $\delta > 0$. Then*

$$D_2(J_\mu) \leq P_2(\mu). \tag{8.5}$$

Proof. We claim that

$$\limsup_{r\uparrow 1} \int -\log\left|\operatorname{Im} M_{\mu^{(r)}}(e^{i\theta})\right| \, d\theta \leq \int -\log\left|\operatorname{Im} M_\mu(e^{i\theta})\right| \, d\theta. \tag{8.6}$$

Accepting (8.6) for the moment, let us complete the proof. The eigenvalues of $\mu^{(r)}$ that lie outside $[-2,2]$ correspond to β's of the form

$$\beta_k(J_{\mu^{(r)}}) = \frac{\beta_k(J)}{r}$$

for those k with $|\beta_k(J)| < r$. Thus $\sum F(E_k^\pm(J_{\mu^{(r)}}))$ is monotone increasing to $\sum F(E_k^\pm(J_\mu))$, so (8.6) shows that

$$P_2(\mu) \geq \limsup P_2(\mu^{(r)}). \tag{8.7}$$

Moreover, $M_{\mu^{(r)}}(z) \to M_\mu(z)$ uniformly on compact subsets of D which means that the continued fraction parameters for $m^{(r)}(E)$, which are the Jacobi coefficients, must converge. Thus for any N,

$$\begin{aligned}
\tfrac{1}{4}\sum_{j=1}^{N} b_j^2 + \tfrac{1}{2}\sum_{j=1}^{N-1} G(a_j) &= \lim_{r\uparrow 1} \tfrac{1}{4}\sum_{j=1}^{N}\left(b_j^{(r)}\right)^2 + \tfrac{1}{2}\sum_{j=1}^{N-1} G(a_j^{(r)}) \\
&\leq \liminf D_2(J_{\mu^{(r)}}) \\
&\leq \liminf P_2(\mu^{(r)}) \qquad \text{(by Proposition 8.2)} \\
&\leq P_2(\mu) \qquad \text{(by (8.7))}
\end{aligned}$$

so (8.5) follows by taking $N \to \infty$.

Thus, we need only prove (8.6). Since $M_{\mu^{(r)}}(\theta) = r^{-1}M_\mu(re^{i\theta}) \to M_\mu(e^{i\theta})$ for a.e. θ, Fatou's lemma implies that

$$\liminf_{r\uparrow 1} \int \log_+ \left|\operatorname{Im} M_{\mu^{(r)}}(e^{i\theta})\right| \, d\theta \geq \int \log_+ \left|\operatorname{Im} M_\mu(\theta)\right| \, d\theta. \tag{8.8}$$

On the other hand, (8.4) implies $|\operatorname{Im} M_\mu(z)| \geq \delta\, |\operatorname{Im} z|$, so $\left|\operatorname{Im} M_{\mu^{(r)}}(z)\right| \geq \delta\, |\operatorname{Im} z|$. Thus uniformly in r,

$$\left|\operatorname{Im} M_{\mu^{(r)}}(e^{i\theta})\right| \geq \delta\, |\sin\theta| \, . \tag{8.9}$$

Thus

$$\log_- \left|\operatorname{Im} M_{\mu^{(r)}}(e^{i\theta})\right| \leq -\log\delta - \log|\sin\theta| \, ,$$

so, by the dominated convergence theorem,

$$\lim \int \log_-(\left|\operatorname{Im} M_{\mu^{(r)}}\right|) \, d\theta = \int \log_-(|\operatorname{Im} M_\mu(\theta)|) \, d\theta.$$

This, together with (8.8) and $-\log(x) = -\log_+(x) + \log_-(x)$ implies (8.6). □

Remark. Semicontinuity of the entropy and (8.9) actually imply one has equality for the limit in (8.6) rather than inequality for the lim sup.

Proof of Theorem 8.1. For each $\delta \in (0,1)$, let $\mu_\delta = (1-\delta)\mu + \delta\mu_0$. Since μ_δ obeys (8.4) and the Blumenthal-Weyl criterion,

$$D_2(J_{\mu_\delta}) \leq P_2(\mu_\delta). \tag{8.10}$$

Let $M_\delta \equiv M_{\mu_\delta}$ and note that

$$\operatorname{Im} M_\delta(e^{i\theta}) = (1-\delta)\operatorname{Im} M(e^{i\theta}) + \delta\sin\theta$$

so

$$\log\left|\operatorname{Im} M_\delta(e^{i\theta})\right| = \log(1-\delta) + \log\left|\operatorname{Im} M(e^{i\theta}) + \frac{\delta}{1-\delta}\sin\theta\right|.$$

We see that up to the convergent $\log(1-\delta)$ factor, $\log\left|\operatorname{Im} M_\delta(e^{i\theta})\right|$ is monotone in δ, so by the monotone convergence theorem,

$$P_2(\mu) = \lim_{\delta\downarrow 0} P_2(\mu_\delta) \tag{8.11}$$

(the eigenvalue terms are constant in δ, since the point masses of μ_δ have the same positions as those of μ!).

On the other hand, since $\mu_\delta \to \mu$ weakly, as in the last proof,

$$D_2(J_\mu) \leq \liminf D_2(J_{\mu_\delta}). \tag{8.12}$$

(8.10)–(8.12) imply (8.1). □

9. Consequences of the C_0 sum rule

In this section, we will study the C_0 sum rule and, in particular, we will prove Nevai's conjecture (Theorem 2) and several results showing that control of the eigenvalues can have strong consequences for J and μ_J, specifically Theorems $4'$ and 7. While Nevai's conjecture will be easy, the more complex results will involve some machinery, so we provide this overview:

(1) By employing semicontinuity of the Szegő term, we easily get a C_0-inequality that implies Theorems 2 and 7 and the part of Theorem $4'$ that says $J - J_0$ is Hilbert-Schmidt.

(2) We prove Theorem 4.1 under great generality when there are no eigenvalues and use that to prove a semicontinuity in the other direction, and thereby show that the Szegő condition implies a C_0-equality when there are no eigenvalues, including conditional convergence of $\sum_n (a_n - 1)$.

(3) We use the existence of a C_0-equality to prove a C_1-equality, and thereby conditional convergence of $\sum_n b_n$.

(4) Returning to the trace class case, we prove that the perturbation determinant is a Nevanlinna function with no singular inner part, and thereby prove a sum rule in the Nevai conjecture situation.

THEOREM 9.1 ($\equiv$ Theorem 3). *Let J be a Jacobi matrix with $\sigma_{\text{ess}}(J) \subset [-2, 2]$ and*

$$\sum_k e_k(J)^{1/2} < \infty, \tag{9.1}$$

$$\limsup_{N \to \infty} \sum_{j=1}^{N} \log(a_j) > -\infty. \tag{9.2}$$

Then

(i) $\sigma_{\text{ess}}(J) = [-2, 2]$.

(ii) *The Szegő condition holds*; *that is*,

$$Z(J) < \infty$$

with Z given by (5.1).

(iii) $\sigma_{\text{ac}}(J) = [-2, 2]$; *indeed, the essential support of* σ_{ac} *is* $[-2, 2]$.

Remarks. 1. We emphasize (9.2) says $> -\infty$, not $< \infty$, that is, it is a condition which prevents the a_n's from being too small (on average).

2. We will see below that (9.1) and (9.2) also imply $|a_j - 1| \to 0$ and $|b_j| \to 0$ and that at least inequality holds for the C_0 sum rule:

$$Z(J) \leq \sum_k \log|\beta_k(J)| - \limsup_N \sum_{j=1}^{N} \log(a_j) \tag{9.3}$$

holds.

Proof. Pick $N_1, N_2, \dots$ (tending to ∞) so that

$$\inf_\ell \Big(\sum_{j=1}^{N_\ell} \log(a_j) \Big) > -\infty \tag{9.4}$$

and let J_{N_ℓ} be given by (2.1). By Theorem 3.3,

$$\begin{aligned} Z(J_{N_\ell}) &\leq -\sum_{j=1}^{N_\ell} \log(a_j) + \sum \log(|\beta_k(J_{N_\ell})|) \\ &\leq -\inf_\ell \sum_{j=1}^{N_\ell} \log(a_j) + \sum \log(|\beta_k(J)|) + 2\log(|\beta_1(J)| + 2) \end{aligned} \tag{9.5}$$

where in (9.5) we used Theorem 6.1 and the fact that the $\tilde\beta$ solving $e_1(J)+1 = \tilde\beta + \tilde\beta^{-1}$ (i.e., $1 + \beta_1 + \beta_1^{-1} = \tilde\beta + \tilde\beta^{-1}$) has $\tilde\beta \leq \beta_1(J) + 2$. For later purposes, we note that if $|b_n(J)| + |a_n(J) - 1| \to 0$, Theorem 6.2 implies we can drop the last term in the limit.

Now use (5.27) and (9.5) to see that

$$Z(J) \quad \leq \liminf Z(J_{N_\ell}) < \infty.$$

This proves (ii). But (ii) implies $\frac{d\mu_{\mathrm{ac}}}{dE} > 0$ a.e. on $E \in [-2, 2]$, that is, $[-2, 2]$ is the essential support of μ_{ac}. That proves (iii). (i) is then immediate. ☐

Proof of Theorem 2 (*Nevai's conjecture*). We need only check that $J - J_0$ trace class implies (9.1) and (9.2). The finiteness of (9.1) follows from a bound of Hundertmark-Simon [27],

$$\sum \big[\, |e_k(J)| \; |e_k(J) + 4| \,\big]^{1/2} \leq \sum_n |b_n| + 2\,|a_n - 1|$$

where $e_k(J) = |E^\pm| - 2$ so $|e|\;|e+4| = (E^\pm)^2 - 4$.

Condition (9.2) is immediate for, as is well-known, $a_j > 0$ and $\sum(|a_j| - 1) < \infty$ implies $\prod a_j$ is absolutely convergent, that is, $\sum |\log(a_j)| < \infty$. ☐

COROLLARY 9.2 ($\equiv$ Theorem 7). *A discrete half-line Schrödinger operator (i.e.,* $a_n \equiv 1$*) with* $\sigma_{\rm ess}(J) \subset [-2,2]$ *and* $\sum e_n(J)^{1/2} < \infty$ *has* $\sigma_{\rm ac} = [-2,2]$.

This is, of course, a special case of Theorem 9.1 but a striking one discussed further in Section 10. In particular, if $a_n \equiv 1$ and $b_n = n^{-\alpha} w_n$ where $\alpha < \frac{1}{2}$ and w_n are identically distributed independent random variables with distribution $g(\lambda)\, d\lambda$ with $g \in L^\infty$ and $\operatorname{supp}(g)$ bounded, then it is known that $[-2,2]$ is dense pure point spectrum (see Simon [54]). It follows that J must also have infinitely many eigenvalues outside $[-2,2]$, indeed, enough that $\sum e_n(J)^{1/2} = \infty$.

Next, we deduce some additional aspects of Theorem 4$'$:

COROLLARY 9.3. *If* $\sigma_{\rm ess}(J) \subset [-2,2]$ *and* (9.1), (9.2) *hold, then* $J - J_0 \in \mathcal{I}_2$, *that is*,

$$\sum b_n^2 + \sum (a_n - 1)^2 < \infty. \tag{9.6}$$

Proof. By Theorem 6, (9.6) holds if $\sum_k e_k(J)^{3/2} < \infty$, and $Q(J)$ (given by (5.21)) is finite. By (9.1) and $e_k(J)^{3/2} \le e_1(J) e_k(J)^{1/2}$, we have that $\sum e_k(J)^{3/2} < \infty$. Moreover, $Z(J) < \infty$ (i.e., Theorem 9.1) implies $Q(J) < \infty$. For, in any event, $\int \operatorname{Im} M \, d\theta < \infty$ implies

$$\int_0^{2\pi} \log_-\left(\frac{\sin\theta}{\operatorname{Im} M}\right) \sin^2(\theta)\, d\theta < \infty \quad \text{and} \quad \int_0^{2\pi} \log_-\left(\frac{\sin\theta}{\operatorname{Im} M}\right) d\theta < \infty.$$

Thus

$$\begin{aligned} Z(J) < \infty \quad &\Rightarrow \quad \int_0^{2\pi} \log_+\left(\frac{\sin\theta}{\operatorname{Im} M}\right) d\theta < \infty \\ &\Rightarrow \quad \int_0^{2\pi} \log_+\left(\frac{\sin\theta}{\operatorname{Im} M}\right) \sin^2\theta \, d\theta < \infty \\ &\Rightarrow \quad Q(J) < \infty. \end{aligned}$$

□

What remains to be shown of Theorem 4$'$ is the existence of the conditional sums. We will start with $\sum (a_n - 1)$. Because $\sum (a_n - 1)^2 < \infty$, it is easy to see that $\sum (a_n - 1)$ is conditionally convergent if and only if $\sum \log(a_n)$ is conditionally convergent. By (9.5) and the fact that $J - J_0$ is compact, we have:

PROPOSITION 9.4. *If* (9.2) *holds and* $\sigma(J) \subset [-2,2]$, *that is, no eigenvalues outside* $[-2,2]$, *then*

$$Z(J) \le -\limsup \left[\sum_{j=1}^N \log(a_j) \right]. \tag{9.7}$$

We are heading towards a proof that

$$Z(J) \geq -\liminf\Big[\sum_{j=1}^{N} \log(a_j)\Big] \tag{9.8}$$

from which it follows that the limit exists and equals $Z(J)$.

LEMMA 9.5. *If $\sigma(J) \subset [-2,2]$, then $\log[z^{-1}M(z;J)]$ lies in every $H^p(D)$ space for $p < \infty$. In particular, $z^{-1}M(z;J)$ is a Nevanlinna function with no singular inner part.*

Proof. In $D\backslash(-1,0)$, we can define $\operatorname{Arg} M(z;J) \subset (-\pi,\pi)$ and $\operatorname{Arg} z \subset (-\pi,\pi)$ since $\operatorname{Im} M(z;J)/\operatorname{Im} z > 0$. Thus $g(z;J) = z^{-1}M(z;J)$ in the same region has argument in $(-\pi,\pi)$. But $\operatorname{Arg} g$ is single-valued and continuous across $(-1,0)$ since M has no poles and precisely one zero at $z=0$. Thus $\operatorname{Arg} g \in L^\infty$. It follows by Riesz's theorem on conjugate functions ([48, pg. 351]) that $\log(g) \in H^p(D)$ for any $p < \infty$. Since it lies in H^1, g is Nevanlinna. Since for $p > 1$, any H^p function, F, has boundary values $F(re^{i\theta}) \to F(e^{i\theta})$ in L^p, $\log(g)$ has no singular part in its boundary value. □

PROPOSITION 9.6. *Let $\sigma(J) \subset [-2,2]$. Suppose $Z(J) < \infty$. Let C_0, C_n be given by* (4.10) *and* (4.15) (*where the $\beta(J)$ terms are absent*). *Then the step-by-step sum rules*, (4.8), (4.13), (4.14), (4.24) *hold. In particular*,

$$Z(J) = -\log(a_1) + Z(J^{(1)}) \tag{9.9}$$

$$C_1(J) = b_1 + C_1(J^{(1)}). \tag{9.10}$$

Proof. (4.4) and therefore (4.1) hold. Thus, we only need apply Theorem 3.2 to g, noting that we have just proven that g has no singular inner part. □

THEOREM 9.7. *If J is such that $Z(J) < \infty$ and $\sigma(J) \subset [-2,2]$, then*

(i) $\lim_{N\to\infty} \sum_{j=1}^{N} \log(a_j)$ *exists.*

(ii) *The limit in* (i) *is* $-Z(J)$.

(iii)

$$\lim_{n\to\infty} Z(J^{(n)}) = 0 \qquad (= Z(J_0)) \tag{9.11}$$

Proof. By (9.9),

$$Z(J) + \sum_{j=1}^{n} \log(a_j) = Z(J^{(n)}). \tag{9.12}$$

Since $J - J_0 \in \ell_2$, $\mu_{J^{(n)}} \to \mu_{J_0}$ weakly, and so, by (5.27), $\liminf Z(J^{(n)}) \geq 0$, or by (9.12),

$$\liminf \Big[\sum_{j=1}^{n} \log(a_j) \Big] \geq -Z(J). \tag{9.13}$$

But (9.7) says

$$\limsup \Big[\sum_{j=1}^{n} \log(a_j) \Big] \leq -Z(J).$$

Thus the limit exists and equals $Z(J)$, proving (i) and (ii). Moreover, by (9.12), (i) and (ii) imply (iii). □

If $Z(\,\cdot\,)$ had a positive integrand, (9.11) would immediately imply that $C_1(J^{(n)}) \to 0$ as $n \to \infty$, in which case, iterating (9.10) would imply that $\sum_{j=1}^{n} b_j$ is conditionally convergent. $Z(\,\cdot\,)$ does not have a positive integrand but a theme is that concavity often lets us treat it as if it does. Our goal is to use (9.11) and the related $\lim_{n\to\infty} Q(J^{(n)}) = 0$ (which follows from Theorem 5) to still prove that $C_1(J^{(n)}) \to 0$. We begin with

Lemma 9.8. *Let $d\mu$ be a probability measure and suppose $f_n \geq 0$, $\int f_n \, d\mu \leq 1$, and*

$$\lim_{n\to\infty} \int \log(f_n) \, d\mu = 0. \tag{9.14}$$

Then

$$\int |\log(f_n)| \; d\mu + \int |f_n - 1| \; d\mu \to 0. \tag{9.15}$$

Proof. Let

$$H(y) = -\log(y) - 1 + y. \tag{9.16}$$

Then

(i) $H(y) \geq 0$ for all y.

(ii) $\inf_{|y-1|\geq\varepsilon} H(y) > 0$.

(iii) $H(y) \geq \frac{1}{2} y$ if $y > 8$.

(i) is concavity of $\log(y)$, (ii) is strict concavity, and (iii) holds because $-\log y - 1 + \frac{1}{2} y$ is monotone on $(2, \infty)$ and > 0 at $y = 8$ since $\log(8)$ is slightly more than 2.

Since $\int (f_n - 1) \, d\mu \leq 0$, (9.14) and (i) implies that

$$\int f_n(x) \, d\mu(x) \to 1 \tag{9.17}$$

and

$$\lim_{n\to\infty} \int H(f_n(x))\, d\mu(x) \to 0. \tag{9.18}$$

Since $H \geq 0$, (ii) and the above imply $f_n \to 1$ in measure:

$$\mu(\{x \mid |f_n(x) - 1| > \varepsilon\}) \to 0. \tag{9.19}$$

By (i), (iii) and (9.18),

$$\int_{f_n(x)>8} |f_n(x)|\; d\mu \to 0. \tag{9.20}$$

Now (9.19)/(9.20) imply that

$$\int |f_n(x) - 1|\; d\mu(x) \to 0$$

and this together with (9.18) implies $\int |\log(f_n)|\; d\mu = 0$. □

Proposition 9.9. *Suppose $Z(J) < \infty$ and $\sigma(J) \subset [-2, 2]$. Then*

$$\lim_{n\to\infty} \int_{-\pi}^{\pi} \left| \log\left(\frac{\sin\theta}{\operatorname{Im} M(e^{i\theta}, J^{(n)})} \right) \right| d\theta = 0. \tag{9.21}$$

Proof. By (9.11), the result is true if $|\cdot|$ is dropped. Thus it suffices to show

$$\lim_{n\to\infty} \int_{-\pi}^{\pi} \log_-\left(\frac{\sin\theta}{\operatorname{Im} M(e^{i\theta}, J^{(n)})} \right) d\theta = 0$$

or equivalently,

$$\lim_{n\to\infty} \int_{-\pi}^{\pi} \log_+\left(\frac{\operatorname{Im} M(e^{i\theta}, J^{(n)})}{\sin\theta} \right) d\theta = 0. \tag{9.22}$$

Now, let $d\mu_0(\theta) = \frac{1}{\pi}\sin^2\theta\, d\theta$ and $f_n(\theta) = (\sin\theta)^{-1} \operatorname{Im} M(e^{i\theta}, J^{(n)})$. By (1.19),

$$\int_{-\pi}^{\pi} f_n(\theta)\, d\mu_0(\theta) \leq 1 \tag{9.23}$$

and by Theorem 5 (and Corollary 9.3, which implies $\|J^{(n)} - J_0\|_2^2 \to 0$),

$$\int \log(f_n(\theta))\, d\mu_0(\theta) \to 0$$

so, by Lemma 9.8, we control $|\log|$ and so $\log_+$; that is,

$$\lim_{n\to\infty} \int_{-\pi}^{\pi} \log_+\left(\frac{\operatorname{Im} M(e^{i\theta}, J^{(n)})}{\sin\theta} \right) \sin^2\theta\, d\theta = 0. \tag{9.24}$$

Thus, to prove (9.22), we need only prove

$$\lim_{\varepsilon\downarrow 0} \limsup_{n\to\infty} \int_{\substack{|\theta|<\varepsilon \\ \text{or}\,|\pi-\theta|<\varepsilon}} \log_+\left(\frac{\operatorname{Im} M(e^{i\theta}, J^{(n)})}{\sin\theta} \right) d\theta = 0. \tag{9.25}$$

To do this, use

$$\begin{aligned}\log_+\left(\frac{a}{b}\right) &\leq \log_+(a)+\log_-(b) = 2\log_+(a^{1/2})+\log_-(b)\\ &\leq 2a^{1/2}+\log_-(b)\end{aligned}$$

with $a=\sin\theta \operatorname{Im} M(e^{i\theta},J^{(n)})$ and $b=\sin^2\theta$. The contribution of $\log_-(b)$ in (9.25) is integrable and n-independent, and so goes to zero as $\varepsilon\downarrow 0$. The contribution of the $2a^{1/2}$ term is, by the Schwartz inequality, bounded by

$$(4\varepsilon)^{1/2}\left(4\int_{-\pi}^{\pi} f_n(\theta)\,d\mu_0(\theta)\right)^{1/2}$$

also goes to zero as $\varepsilon\downarrow 0$. Thus (9.25) is proven. □

The following concludes the proofs of Theorems 4 and 4′.

THEOREM 9.10. *If $Z(J)<\infty$ and $\sigma(J)\subset[-2,2]$, then*

$$\lim_{N\to\infty}\sum_{j=1}^{N} b_j \text{ exists and equals } -\frac{1}{2\pi}\int_0^{2\pi}\log\left(\frac{\sin\theta}{\operatorname{Im} M(e^{i\theta})}\right)\cos(\theta)\,d\theta. \tag{9.26}$$

Proof. By Proposition 9.9, $C_1(J^{(n)})\to 0$ and, by (9.10),

$$C_1(J)=\sum_{j=1}^{n} b_j + C_1(J^{(n)}).$$ □

As a final topic in this section, we return to the general trace class case where we want to prove that the C_0 (and other) sum rules hold; that is, we want to improve the inequality (9.5) to an equality. The key will be to show that in this case, the perturbation determinant is a Nevanlinna function with vanishing inner singular part.

PROPOSITION 9.11. *Let $J-J_0$ be trace class. Then, the perturbation determinant $L(z;J)$ is in Nevanlinna class.*

Proof. By (2.19), if J_n is given by (2.1), then

$$L(z;J_n)\to L(z;J) \tag{9.27}$$

uniformly on compact subsets of D. Thus

$$\begin{aligned}\sup_{0<r<1}\int_0^{2\pi}\log_+\left|L(re^{i\theta};J)\right|\frac{d\theta}{2\pi} &\leq \sup_n\sup_{0<r<1}\int_0^{2\pi}\log_+\left|L(re^{i\theta};J_n)\right|\frac{d\theta}{2\pi}\\ &= \sup_n\int_0^{2\pi}\log_+\left|L(e^{i\theta};J_n)\right|\frac{d\theta}{2\pi}\end{aligned} \tag{9.28}$$

where (9.28) follows from the monotonicity of the integral in r (see [48, pg. 336]) and the fact that $L(z; J_n)$ is a polynomial.

In (9.28), write $\log_+ |L| = \log |L| + \log_- |L|$. By Jensen's formula, (3.1), and $L(0; J) = 1$,

$$\int_0^{2\pi} \log \left| L(e^{i\theta}; J_n) \right| \frac{d\theta}{2\pi} = -\sum_{j=1}^{N_n} \log |\beta_j(J_n)|$$

and this is uniformly bounded in n by the $\frac{1}{2}$ Lieb-Thirring inequality of Hundertmark-Simon [27], together with Theorem 6.1. On the other hand, by (2.73),

$$\begin{aligned} (9.29) \qquad 2\log_- \left| L(e^{i\theta}; J_n) \right| &= \log_- \left(\prod_{j=1}^{n-1} a_j^2 \frac{\sin\theta}{\operatorname{Im} M(e^{i\theta}; J_n)} \right) \\ &\leq 2 \sum_{j=1}^{n-1} \log_-(a_j) + 2\log(\sin\theta) + \log_+ \left(\operatorname{Im} M(e^{i\theta}; J_n) \sin\theta \right) \end{aligned}$$

since $\log_- |ab/c| = [\log(a) + \log(b) - \log(c)]_- \leq \log_-(a) + \log_-(b) + \log_+(c)$.

The first term in (9.29) is θ-independent and uniformly bounded in n since $\sum_{j=1}^\infty |a_j - 1| < \infty$. The second term is integrable. For the final term, we note that $\log_+(y) \leq y$ so by (1.19), the integral over θ is uniformly bounded. $\square$

Remark. Our proof that L is Nevanlinna used $\sum_k (e_k(J))^{1/2} < \infty$ as input. If we could find a proof that did not use this *a priori*, we would have, as a consequence, a new proof that $\sum_k e_k(J)^{1/2} < \infty$ since $\sum [1 - \beta_k(J)^{-1}] < \infty$ is a general property of Nevanlinna functions.

Proposition 9.12. *If $\delta J \in \mathcal{I}_1$, the singular inner part of $L(z; J)$, if any, is a positive point mass at $z = 1$ and/or at $z = -1$.*

Proof. By Theorem 2.8, $L(z; J)$ is continuous on $\bar{D} \backslash \{-1, 1\}$ and by (2.73), it is nonvanishing on $\{e^{i\theta} \mid \theta \neq 0, \pi\}$. It follows that on any closed interval, $I \subset (0, \pi) \cup (\pi, 2\pi)$, $\log \left| L(re^{i\theta}, J) \right| d\theta$ converges to an absolutely continuous measure, so the support of the singular inner part is $\{\pm 1\}$.

Returning to (9.29) and using $\log_+(x) = 2\log_+(x^{1/2}) \leq 2x^{1/2}$, we see that $\log_- |L|$ lies in L^2; that is,

$$\sup_n \sup_{0<r<1} \int [\log_- \left| L(re^{i\theta}, J_n) \right|]^2 \frac{d\theta}{2\pi} < \infty$$

and this implies $\log_- \left| L(re^{i\theta}, J) \right|$ has an a.c. measure as its boundary value. Thus ± 1 can only be positive pure points. $\square$

Remark. We will shortly prove L has no singular inner part. However, we can ask a closely related question. If $|\sum \log(a_n)| < \infty$ and $\sum e_k(J)^{1/2} < \infty$ so $Z(J) < \infty$, does the sum rule always hold or is there potentially a positive singular part in some suitable object?

Theorem 2.10 will be the key to proving that $L(x; J)$ has no pure point singular part. The issue is whether the Blaschke product can mask the polar singularity, since, if not, (2.46) says there is no polar singularity in L which combines the singular inner part, outer factor, and Blaschke product. Experts that we have consulted tell us that the idea that Blaschke products cannot mask poles goes back to Littlewood and is known to experts, although our approach in the next lemma seems to be a new and interesting way of discussing this:

Lemma 9.13. *Let $f(z)$ be a Nevanlinna function on D. Then for any $\theta_0 \in \partial D$,*

$$\lim_{r\uparrow 1} [\log(1-r)^{-1}]^{-1} \int_0^r \log \left| f(ye^{i\theta_0}) \right| dy = 2\mu_s(\{\theta_0\}). \tag{9.30}$$

Proof. Let B be a Blaschke product for f. Then ([48, pg. 346]),

$$\log |f(z)| = \log |B(z)| + \int_{-\pi}^{\pi} P(z,\theta)\, d\mu(\theta) \tag{9.31}$$

where P is the Poisson kernel

$$P(re^{i\phi}, \theta) = \frac{(1-r^2)}{(1+r^2-2r\cos(\theta-\varphi))}$$

and $d\mu(\theta)$ is the boundary value of $\log \left| f(re^{i\theta}) \right| d\theta$, that is, outer plus singular inner piece. By an elementary estimate,

$$\sup_{r,\theta,\varphi} (1-r)P(re^{i\theta}, \varphi) < \infty$$

and

$$\lim_{r\uparrow 1} (1-r)P(re^{i\theta}, \varphi) = \begin{cases} 0 & \theta \neq \varphi \\ 2 & \theta = \varphi \end{cases}$$

and thus

$$(1-r)\int_{-\pi}^{\pi} P(re^{i\varphi}, \theta)\, d\mu(\theta) \to 2\mu_s(\{\varphi\}).$$

This means (9.30) is equivalent to

$$\lim_{r\uparrow 1} [\log(1-r)^{-1}]^{-1} \int_0^r \log \left| B(ye^{i\theta_0}) \right| dy = 0 \tag{9.32}$$

for any Blaschke product. Without loss, we can take $\theta_0 = 0$ in (9.32). Now let

$$b_\alpha(z) = \frac{|\alpha|}{\alpha} \frac{\alpha - z}{1 - \bar{\alpha} z}$$

so

$$B(z) = \prod_{z_i} b_{z_i}(z)$$

and note that for $0 < x < 1$ and any $\alpha \in D$,

$$1 > |b_\alpha(x)| \geq \left| b_{|\alpha|}(x) \right|,$$

so

$$0 < -\log|B(x)| \leq \sum_{z_i} -\log\left| b_{|z_i|}(x) \right|. \tag{9.33}$$

Thus, also without loss, we can suppose all the zeros z_i lie on $(0, 1)$.

If $\alpha \in (0, 1)$, a straightforward calculation (or Maple!) shows

$$\int_0^1 -\log|b_\alpha(x)|\, dx = \alpha \log\left(\frac{1}{\alpha}\right) + \frac{1-\alpha^2}{\alpha} \log\left(\frac{1}{1-\alpha}\right). \tag{9.34}$$

We claim that for a universal constant C and $r > \frac{3}{4}$, $\alpha > \frac{1}{2}$,

$$-\int_0^r \log|b_\alpha(x)|\, dx \leq C(1-\alpha)\log(1-r)^{-1}. \tag{9.35}$$

Accepting (9.35) for the moment, by (9.33), we have for $r > \frac{3}{4}$,

$$-\int_0^r \log|B(x)|\, dx \leq \sum_{j=1}^n \eta(\alpha_j) + C\left(\sum_{j=n+1}^\infty (1-\alpha_j)\right)\log(1-r)^{-1}$$

where $\eta(\alpha)$ is the right side of (9.34). Dividing by $\log(1-r)^{-1}$ and using $\eta(\alpha) < \infty$, we see

$$\limsup\left[\frac{1}{\log(1-r)^{-1}}\left\{-\int_0^r \log|B(x)|\, dx\right\}\right] \leq C \sum_{j=n+1}^\infty (1-\alpha_j).$$

Taking $n \to \infty$, we see that the lim sup is 0. Since $-\log|B(x)| > 0$, the limit is 0 as required by (9.32). Thus, the proof is reduced to establishing (9.35).

Note first that if $1 > \alpha > \frac{1}{2}$, $\frac{1}{\alpha}(1+\alpha) < 4$. Moreover, if $g(\alpha) = \alpha\log(\frac{1}{\alpha})$, then $g''(\alpha) = -\frac{1}{\alpha^2} < 0$, so $g(\alpha) \leq (1-\alpha)$. Thus, if $\eta(\alpha)$ is the right side of (9.34) and $\alpha > \frac{1}{2}$, then

$$\eta(\alpha) \leq 1 - \alpha + 4(1-\alpha)\log\left(\frac{1}{1-\alpha}\right). \tag{9.36}$$

Suppose now

$$1 - \alpha \geq (1-r)^2. \tag{9.37}$$

Then

$$-\int_0^r \log|b_\alpha(x)|\,dx \;\leq\; \eta(\alpha) \leq (1-\alpha)\Big[1+4\log\Big(\frac{1}{1-\alpha}\Big)\Big] \;\leq\; (1-\alpha)\Big[1+8\log\Big(\frac{1}{1-r}\Big)\Big] \tag{9.38}$$

by (9.37).

On the other hand, suppose

$$(1-\alpha) \leq (1-r)^2. \tag{9.39}$$

By an elementary estimate (see, e.g., [48, pg. 310]),

$$|1-b_\alpha(x)| \leq \frac{2}{1-x}\,(1-\alpha). \tag{9.40}$$

If (9.39) holds and $x<r$, then, by (9.40),

$$|1-b_\alpha(x)| \leq \frac{2(1-r)^2}{1-x} \leq 2(1-r) < \frac{1}{2} \tag{9.41}$$

since r is supposed larger than $\frac{3}{4}$. If $u \in (\frac{1}{2},1)$, then

$$-\log u = \int_u^1 \frac{dy}{y} \leq 2(1-u)$$

so if (9.41) holds,

$$-\log(b_\alpha(x)) \leq 2(1-b_\alpha(x)) \leq \frac{4(1-\alpha)}{1-x}$$

and so

$$\int_0^r -\log(b_\alpha(x))\,dx \leq 4(1-\alpha)\log(1-r)^{-1}. \tag{9.42}$$

We have thus proven (9.38) if (9.37) holds and (9.42) if (9.39) holds. Together this proves (9.35). ☐

THEOREM 9.14. *Let $J-J_0$ be trace class. Then the Nevanlinna function $L(z;J)$ has a vanishing singular inner component and all the sum rules $C_0, C_1, \dots$ hold with no singular term.*

Proof. By Proposition 9.12, the only possible singular parts are positive points at ± 1. By (9.30) and the estimate (2.50), these point masses are absent. Thus the singular part vanishes and the sum rules hold by Theorem 3.2. ☐

10. Whole-line Schrödinger operators with no bound states

Our goal in this section is to prove Theorem 8 that the only whole-line Schrödinger operator with $\sigma(W) \subset [-2,2]$ is W_0, the free operator. We do this here because it illustrates two themes: that absence of bound states is a strong assertion and that sum rules can be very powerful tools.

Given two sequences of real numbers $\{a_n\}_{n=-\infty}^{\infty}$, $\{b_n\}_{n=-\infty}^{\infty}$ with $a_n > 0$, we will denote by W the operator on $\ell^2(\mathbb{Z})$ defined by

$$(Wu)_n = a_{n-1}u_{n-1} + b_n u_n + a_{n+1}u_{n+1}. \tag{10.1}$$

W_0 is the operator with $a_n \equiv 1$, $b_n \equiv 0$. The result we will prove is:

Theorem 10.1. *Let W be a whole-line operator with $a_n \equiv 1$ and $\sigma(W) \subset [-2,2]$. Then $W = W_0$, that is, $b_n \equiv 0$.*

The proof works if

$$\limsup_{\substack{n\to\infty \\ m\to\infty}} \biggl[\sum_{j=-n}^{m} \log(a_j)\biggr] \geq 0.$$

The strategy of the proof will be to establish analogs of the C_0 and C_2 sum rules. Unlike the half-line case, the integrand inside the Szegő-like integral will be nonnegative. The C_0 sum rule will then imply this integrand is zero and the C_2 sum will therefore yield $\sum_n b_n^2 = 0$. As a preliminary, we note:

Proposition 10.2. *If $a_n \equiv 1$ and $\sigma(W) \subset [-2,2]$, then $\sum_n b_n^2 < \infty$. In particular, $b_n \to 0$ as $|n| \to \infty$.*

Proof. Let J be a Jacobi matrix obtained by restricting to $\{1,2,\dots\}$. By the min-max principle [45], $\sigma(J) \subset [-2,2]$. By Corollary 9.3, $\sum_{n=1}^{\infty} b_n^2 < \infty$. Similarly, by restricting to $\{0,-1,-2,\dots,\}$, we obtain $\sum_{n=-\infty}^{0} b_n^2 < \infty$. □

Let $W^{(n)}$ for $n = 1,2,\dots$ be the operator with

$$\begin{cases} a_j^{(n)} \equiv 1 \\ b_j^{(n)} = b_j & \text{if } |j| \leq n \\ b_j^{(n)} = 0 & \text{if } |j| > n. \end{cases} \tag{10.2}$$

Then, Proposition 10.2 and the proofs of Theorems 6.1 and 6.2 immediately imply:

Theorem 10.3. *If $a_n \equiv 1$ and $\sigma(W) \subset [-2,2]$, then $W^{(n)}$ has at most four eigenvalues in $\mathbb{R}\backslash[-2,2]$ (up to two in each of $(-\infty,-2)$ and $(2,\infty)$) and for $j = 1,\dots,4$,*

$$\Bigl|e_j(W^{(n)})\Bigr| \to 0 \tag{10.3}$$

as $n \to \infty$.

Note. As in the Jacobi case, $e_j(W)$ is a relabeling of $\left|E_j^\pm(W)\right| - 2$ in decreasing order.

To get the sum rules, we need to study whole-line perturbation determinants. We will use the same notation as for the half-line, allowing the context to distinguish the two cases. So, let $\delta W = W - W_0$ be trace class and define

$$L(z;W) = \det((W - E(z)(W_0 - E(z))^{-1}) \tag{10.4}$$
$$= \det(1 + \delta W(W_0 - E(z))^{-1}) \tag{10.5}$$

where as usual, $E(z) = z + z^{-1}$.

The calculation of the perturbation series for L is algebraic and so immediately extends to imply:

Proposition 10.4. *If δW is trace class, for each n, $T_n(W/2)-T_n(W_0/2)$ is trace class. Moreover, for $|z|$ small,*

$$\log[L(z;W)] = \sum_{n=1}^{\infty} c_n(W)z^n \tag{10.6}$$

where $c_n(W)$ is

$$c_n(W) = -\frac{2}{n}\,\mathrm{Tr}\Big(T_n\big(\tfrac{1}{2}W\big) - T_n\big(\tfrac{1}{2}W_0\big)\Big). \tag{10.7}$$

In particular,

$$c_2(W) = -\frac{1}{2}\sum_{m=1}^{\infty} b_m^2 + 2(a_m^2 - 1). \tag{10.8}$$

The free resolvent, $(W_0 - E(z))^{-1}$, has matrix elements that we can compute as we did to get (2.9),

$$(W_0 - E(z))^{-1}_{nm} = -(z^{-1} - z)^{-1} z^{|m-n|}$$

which has poles at $z = \pm 1$. We immediately get

Proposition 10.5. *If δW is finite rank, $L(z;J)$ is a rational function on $\mathbb{C}$ with possible singularities only at $z = \pm 1$.*

Remarks. 1. If δW has $b_0 = 1$, all other elements zero, then

$$L(z;W) = 1 - (z^{-1} - z)^{-1} = \frac{(1 - z - z^2)}{(1 - z^2)}$$

has poles at ± 1, so poles can occur.

2. The rank one operator

$$R(z) = -(z^{-1} - z)^{-1} z^{m+n}$$

is such that if $\delta W = C^{1/2}UC^{1/2}$ with C finite rank, then

$$C^{1/2}[(W_0 - E(z)^{-1} - R(z)]C^{1/2}$$

is entire. Using this, one can see $L(z;J)$ has a pole of order at most 1 when δW is finite rank. We will see this below in another way.

If $z \in \bar{D}\backslash\{-1,1\}$, we can define a Jost solution $u_n^+(z;W)$ so that (2.65) holds for all $n \in \mathbb{Z}$ and

$$\lim_{n\to\infty} z^{-n}u_n^+(z;W) = 1. \tag{10.9}$$

Moreover, if δW has finite rank, u_n^+ is a polynomial in z for each $n \geq 0$. Moreover, for $n < 0$, $z^{-n}u_n^+$ is a polynomial in z by using (2.67).

Similarly, we can construct u_n^- solving (2.65) for all $n \in \mathbb{Z}$ with

$$\lim_{n\to-\infty} z^n u_n^-(z;W) = 1.$$

As above, if δW is finite rank, u_n^- is a polynomial in z if $n \leq 0$ and for $n > 0$, $z^n u_n^-$ is a polynomial.

Proposition 10.6. *Let δW be trace class. Then for $z \in \bar{D}\backslash\{-1,1\}$ and all $n \in \mathbb{Z}$,*

$$\begin{aligned} L(z;W) &= (z^{-1}-z)^{-1}\biggl(\prod_{j=-\infty}^{\infty} a_j\biggr) \\ &\qquad a_n[u_n^+(z;W)u_{n+1}^-(z;W) - u_n^-(z;W)u_{n+1}^+(z;W)]. \end{aligned} \tag{10.10}$$

Proof. Both sides of (10.10) are continuous in W, so we need only prove the result when δW is finite rank. Moreover, by constancy of the Wronskian, the right side of (10.10) is independent of n so we need only prove (10.10) when $|z| < 1$ and n is very negative–so negative it is to the left of the support of δW, that is, choose R so $a_n = 1$, $b_n = 0$ if $n < -R$, and we will prove that (10.10) holds for $n < -R$.

For $n < -R$, z^n and z^{-n} are two solutions of (2.65) so in that region we have

$$u_n^+ = \alpha_\ell z^n + \beta_\ell z^{-n}. \tag{10.11}$$

Taking the Wronskian of u_n^+ given by (10.11) and $u_n^- = z^{-n}$ at some point $n < -R$, we see

$$\text{RHS of (10.10)} = \alpha_\ell\biggl(\prod_{j=-\infty}^{\infty} a_j\biggr). \tag{10.12}$$

Let $W_n, W_{0;n}$ be the Jacobi matrices on $\ell^2(\{n+1, n+2, \dots,\})$ obtained by truncation. On the one hand, as with the proof of (2.74), for $|z| < 1$,

$$L(z;W) = \lim_{n\to-\infty} \det((W_n - E(z))(W_{n;0} - E(z))^{-1}) \tag{10.13}$$

and on the other hand, for $n < -R$, by (2.64),

$$\text{RHS of (10.13)} = \Big(\prod_n a_n\Big) z^{-n} u_n^+(z;W).$$

Thus

$$\begin{aligned} L(z;W) &= \Big(\prod_n a_n\Big) \lim_{n\to-\infty} z^{-n} u_n^+(z;W) \\ &= \Big(\prod_n a_n\Big) \lim_{n\to-\infty} (\alpha_\ell + \beta_\ell z^{-2n}) \\ &= \Big(\prod_n a_n\Big) \alpha_\ell \end{aligned} \tag{10.14}$$

since $|z| < 1$ and $n \to -\infty$. Comparing (10.12) and (10.14) yields (10.10). □

Note. In (10.11), α_ℓ, β_ℓ use "ℓ" for "left" since they are related to scattering from the left.

Corollary 10.7. *If δW is finite rank, then $(1-z^2)L(z;W)$ is a polynomial and, in particular, $L(z;W)$ is a rational function.*

Proof. By (10.10), this is equivalent to $z(u_0^+ u_1^- - u_0^- u_1^+)$ being a polynomial. But u_0^+, zu_1^-, u_0^-, and u_1^+ are all polynomials. □

Let δW be finite rank. Since L is meromorphic in a neighborhood of $\bar{D}$ and analytic in D, Proposition 3.1 immediately implies the following sum rule:

Theorem 10.8. *If δW is finite rank, then*

$$C_0: \quad \frac{1}{2\pi}\int_0^{2\pi} \log\Big|L(e^{i\theta};W)\Big|\, d\theta = \sum_{j=1}^{N(W)} \log|\beta_j(W)| \tag{10.15}$$

$$\begin{aligned} C_n: \quad & \frac{1}{\pi}\int_0^{2\pi} \log\Big|L(e^{i\theta};W)\Big| \cos(n\theta)\, d\theta \\ &= \frac{1}{n}\sum_{j=1}^{N(W)} [\beta_j^n - \beta_j^{-n}] - \frac{2}{n}\operatorname{Tr}\Big(T_n\Big(\tfrac12 W\Big) - T_n\Big(\tfrac12 W_0\Big)\Big) \end{aligned} \tag{10.16}$$

for $n \geq 1$.

The final element of our proof is an inequality for $L(e^{i\theta};W)$ that depends on what a physicist would call conservation of probability.

Proposition 10.9. *Let δW be trace class. Then for all $\theta \neq 0, \pi$,*

$$\Big|L(e^{i\theta};W)\Big| \geq \prod_{j=-\infty}^{\infty} a_j. \tag{10.17}$$

Proof. As above, we can suppose that δW is finite range. Choose R so that all nonzero matrix elements of δW have indices lying within $(-R, R)$. By (10.12), (10.17) is equivalent to

$$|\alpha_\ell| \geq 1 \tag{10.18}$$

where α_ℓ is given by (10.11).

Since $u_n^+(z; W)$ is real for z real, we have

$$u_n^+(\bar{z}; W) = \overline{u_n^+(z; W)}.$$

Thus for $z = e^{i\theta}$, $\theta \neq 0, \pi$, and $n < -R$,

$$\begin{aligned} u_n^+(e^{i\theta}; W) &= \alpha_\ell(e^{i\theta}) e^{in\theta} + \beta_\ell(e^{i\theta}) e^{-in\theta} \\ u_n^+(e^{-i\theta}; W) &= \overline{\alpha_\ell(e^{i\theta})}\, e^{-in\theta} + \overline{\beta_\ell(e^{i\theta})}\, e^{+in\theta}. \end{aligned}$$

Computing the Wronskian of the left-hand sides for $n > R$, where $u_n^+ = z^n$ and then the Wronskian of the right-hand sides for $n < -R$, we find

$$i(\sin\theta) = i(\sin\theta)[|\alpha_\ell|^2 - |\beta_\ell|^2]$$

or, since $\theta \neq 0, \pi$,

$$|\alpha_\ell|^2 = 1 + |\beta_\ell|^2 \tag{10.19}$$

from which (10.18) is obvious. □

Remark. In terms of the transmission and reflection coefficients of scattering theory [61], $\alpha_\ell = 1/t$, $\beta_\ell = r/t$, (10.19) is $|r|^2 + |t|^2 = 1$ and (10.18) is $|t| \leq 1$.

We are now ready for

Proof of Theorem 10.1. Let $W^{(n)}$ be given by (10.2). Then, by (10.3) and C_0 (10.15),

$$\lim_{n\to\infty} \frac{1}{2\pi} \int_0^{2\pi} \log \left| L(e^{i\theta}; W^{(n)}) \right| d\theta = 0. \tag{10.20}$$

Since $a_n \equiv 1$, (10.17) implies $\log \left| L(e^{i\theta}; W^{(n)}) \right| \geq 0$, and so (10.20) implies

$$\lim_{n\to\infty} \frac{1}{2\pi} \int_0^{2\pi} \cos(2\theta) \log \left| L(e^{i\theta}; W^{(n)}) \right| d\theta = 0. \tag{10.21}$$

By (10.8), $a_m \equiv 1$, C_2, and (10.3), we see

$$\lim_{n\to\infty} \sum_{|j|<n} b_j^2 = 0$$

which implies $b \equiv 0$. □

Finally, a remark on why this result holds that could provide a second proof (without sum rules) if one worked out some messy details. Here is a part of the idea:

PROPOSITION 10.10. *Let $\{b_n\}$ be a bounded sequence and W the associated whole-line Schrödinger operator* (*with $a_n \equiv 1$*). *Let*

$$A(\alpha) = \sum b_n e^{-\alpha|n|}. \tag{10.22}$$

If

$$\limsup_{\alpha\downarrow 0}\ A(\alpha) > 0, \tag{10.23}$$

W has spectrum in $(2, \infty)$, and if

$$\liminf_{\alpha\downarrow 0}\ A(\alpha) < 0, \tag{10.24}$$

then W has spectrum in $(-\infty, -2)$.

Proof. Let (10.23) hold and set $\varphi_\alpha(n) = e^{-\alpha|n|/2}$. Then

$$(W_0\varphi_\alpha)(n) = \begin{cases} 2\cosh(\frac{\alpha}{2}) & \text{if } n \neq 0 \\ [2\cosh(\frac{\alpha}{2}) - 2\sinh(\frac{\alpha}{2})]\varphi_\alpha(n) & \text{if } n = 0. \end{cases}$$

It follows that

$$\begin{aligned} (\varphi_\alpha, W\varphi_\alpha)(n) &= 2\cosh\left(\frac{\alpha}{2}\right)\|\varphi_\alpha\|^2 + A(\alpha) - 2\sinh\left(\frac{\alpha}{2}\right) \\ &= 2\|\varphi_\alpha\|^2 + 2\left[\cosh\left(\frac{\alpha}{2}\right) - 1\right]\|\varphi_\alpha\|^2 + A(\alpha) - 2\sinh\left(\frac{\alpha}{2}\right). \end{aligned} \tag{10.25}$$

Now, $\sinh(\alpha/2) \to 0$ as $\alpha \downarrow 0$ and since $\|\varphi_\alpha\|^2 = O(\alpha^{-1})$ and $\cosh(\alpha/2) - 1 = O(\alpha^2)$, $2[\cosh(\alpha/2) - 1]\|\varphi_\alpha\|^2 \to 0$ as $\alpha \downarrow 0$. If there is a sequence with $\lim A(\alpha_n) > 0$, for n large, $(\varphi_{\alpha_n}, (W-2)\varphi_{\alpha_n}) > 0$ which implies there is spectrum in $(2, \infty)$.

If (10.24) holds, use $\varphi_\alpha(n) = (-1)^n e^{-\alpha|n|/2}$ and a similar calculation to deduce $(\varphi_{\alpha_n}, (W+2)\varphi_{\alpha_n}) < 0$. $\square$

This proof is essentially a variant of the weak coupling theory of Simon [50]. Those ideas immediately show that if

$$\sum n\,|b_n| < \infty \tag{10.26}$$

and $\sum b_n = 0$ (so Proposition(10.10) does not apply), then W has eigenvalues in *both* $(2, \infty)$ and $(-\infty, 2)$ unless $b \equiv 0$. This reproves Theorem 10.1 when (10.25) holds by providing explicit eigenvalues outside $[-2, 2]$. It is likely using these ideas as extended in [4], [31], one can provide an alternate proof of Theorem 10.1. In any event, the result is illuminated.

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Added Notes. During the refereeing process, several results were obtained which relate to this paper. In connection with Theorem 10.1, D. Damanik, D. Hundertmark, R. Killip, and B. Simon (to appear) have proved that if the essential spectrum of a whole- or half-line Schrödinger operator is contained in $[-2,2]$, then it is a compact perturbation of the free operator. B. Simon and A. Zlatoš (to appear) have studied when the C_0 sum rule holds, have simplified the proofs of Theorems 7.1 and 9.14, and have extended Theorem $4'$ to the case where one assumes (1.12) rather than that there is no discrete spectrum.

(Received December 13, 2001)