

Spectral Theory via Sum Rules

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Happy Birthday, Barry Simon

ABSTRACT. We survey some results in the spectral theory of certain one-dimensional differential and finite-difference operators: Jacobi matrices, Krein systems, Schrödinger operators and CMV matrices. What ties these results together is the use of sum rules relating the coefficients and the spectral data.

CONTENTS

1. Introduction
 2. Background
 3. Trace Formulae for Jacobi Matrices
 4. Trace Formulae for Other Operators
 5. Point Spectrum
 6. A.C. Spectrum
 7. The Step-by-Step Method
 8. Necessary and Sufficient Conditions
- References

1. Introduction

We survey some results in the spectral theory of certain one-dimensional differential and finite-difference operators. What ties these results together is their use of sum rules relating the coefficients and spectral data. Contemporary mathematicians are perhaps most familiar with these identities in the context of the inverse scattering solution of integrable systems; however, as we will explain, the natural precursor is a formula of Szegő and Verblunsky uncovered in the study of orthogonal polynomials.

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We will describe results for a quartet of operators: Jacobi matrices, Krein systems, Schrödinger operators, and CMV matrices. However, in the interests of brevity and clarity, we limit the discussion of proofs to the case of Jacobi matrices.

2. Background

We start at the very beginning:

THEOREM 2.1. *The sum of the diagonal entries of an $n \times n$ matrix is equal to the sum of its eigenvalues (counting algebraic multiplicity).*

This innocuous sounding result is surprisingly deep; perhaps more importantly, it and its descendants can be surprisingly useful. The key point is the following: in general, one cannot hope to determine the eigenvalues of an operator; however, computing the trace is easy and says something potentially useful about the eigenvalues. A good example of the power of this little fact is shown by the following ingenious application due to Avron, van Mouche, and Simon, [1]:

THEOREM 2.2. *Consider the almost Mathieu operator*

$$[H_\theta u](n) = u(n + 1) + u(n - 1) + \lambda \cos(2\pi n\alpha + \theta)u(n)$$

acting on $\ell^2(\mathbb{Z})$ with $\alpha = p/q$ rational and $\lambda \leq 2$. Then $\sigma_- = \cap_\theta \sigma(H_\theta)$ has Lebesgue measure $4 - 2\lambda$.

Let me outline the proof when q is odd. Due to a remarkable formula of Chambers, [11], it is possible to show that σ_- is the union of q bands; moreover, each band edge corresponds to an eigenfunction of either $H_{\theta=0}$ or $H_{\theta=\pi}$ belonging to a specific symmetry class: periodic/anti-periodic (under translation) and even/odd (under reflection). In this way, one is led to the conclusion that

$$|\sigma_-| = \text{tr}(H_{\theta=\pi}^{p,e}) - \text{tr}(H_{\theta=0}^{a,e}) + \text{tr}(H_{\theta=0}^{a,o}) - \text{tr}(H_{\theta=\pi}^{p,o})$$

where the subscripts indicate the restriction of this operator to the subspace with the corresponding symmetry. This equality comes from regarding the trace as the sum of eigenvalues; the traces are easily evaluated as the sum of diagonal entries, which gives the result. (The result is also true for irrational α ; see [43, 58].)

The proof of Theorem 2.1 is easily found once one pauses to remember the definition of algebraic multiplicity: the number of occurrences on the diagonal in Jordan normal form, or the order of the root in the characteristic polynomial. Of course, one may identify all coefficients of the characteristic polynomial in terms of its roots (the eigenvalues) and in terms of the matrix entries. This leads to

THEOREM 2.3. *For any $n \times n$ matrix, A ,*

$$1 + \sum_{k=1}^n z^k \text{tr}(\wedge^k A) = \det[1 + zA] = 1 + \sum_{k=1}^n z^k \sum_{l_1 > \dots > l_k} \lambda_{l_1} \dots \lambda_{l_k}$$

where $\lambda_1, \dots, \lambda_n$ denote the eigenvalues of A according to algebraic multiplicity.

REMARK. The matrix elements of $\wedge^k A$ —the restriction of $A \otimes \dots \otimes A$ to antisymmetric tensors—are exactly the $k \times k$ minors of A ; thus

$$\text{tr}(\wedge^k A) = \sum_{l_1 > \dots > l_k} A \binom{l_1, \dots, l_k}{l_1, \dots, l_k} = \frac{1}{k!} \sum_{l_1, \dots, l_k} A \binom{l_1, \dots, l_k}{l_1, \dots, l_k}. \tag{1}$$

Our notation for the minors is as follows: the upper list of indices gives the rows used for the minor and the lower, the columns. The second equality comes from summing over permutations of the indices and noting that the (minor) determinant vanishes if two indices coincide.

PROOF. The right-hand equality comes from expanding $\prod(1+z\lambda_i)$. These formulae for the coefficients of a polynomial in terms of its roots are usually attributed to François Viète, a 16th century French lawyer and mathematician.

The determinant is multi-linear in the columns, thus one may expand $\det(1+zA)$ in much the same way as the product in the previous paragraph. A few column operations are all that is required to finish the proof. \square

It is natural to extend this theorem to Banach spaces; it is here that one realizes that things are not so simple after all. An operator on a Banach space E is called nuclear if it can be written as $\sum e_j \langle l_j, \cdot \rangle$ for sequences $e_j \in E$ and $l_j \in E^*$ with $\sum \|e_j\| \|l_j\| < \infty$. The big surprise is that the eigenvalues of nuclear operators are only guaranteed to be absolutely summable if E is isomorphic to a Hilbert space, [44].

In the Hilbert space setting, the space of nuclear operators is better known as trace class, \mathfrak{I}_1 , and the more usual definition is as those compact operators, A , whose singular values are summable. (Recall that the singular values are the eigenvalues of $(A^*A)^{1/2}$.) Here, the sum of the moduli of the eigenvalues is finite; indeed it is bounded by the sum of the singular values. A very general and elegant proof of this fact can be found in [109]; [87] contains three further proofs and historical references.

A second obstruction to the extension of Theorem 2.1 to Banach spaces is more devastating: there is a nuclear operator A on ℓ^1 with $\text{tr}(A) = 1$ and $A^2 = 0$. A textbook presentation of this example can be found in [62, §2.d].

THEOREM 2.4. *Let A be a trace class operator on a Hilbert space. For any orthonormal basis, $\{\phi_j\}$, $\sum \langle \phi_j | A \phi_j \rangle$ is equal to the sum of the eigenvalues repeated according to algebraic multiplicity.*

For a compact operator, the algebraic multiplicity of a non-zero eigenvalue λ can be defined as the rank of $\oint_{\gamma} (z-A)^{-1} dz$ where γ is a small circle around λ excluding the remainder of the spectrum of A . It is not necessary to assign a multiplicity to $\lambda = 0$ as such eigenvalues do not contribute to the sum.

Theorem 2.4 is widely known as Lidskii's theorem, [60]. As pointed out by Pisier, [70], the statement can be found earlier in [40, §4]. Neither paper gives much detail; thorough treatments can be found in several textbooks: [37, 59, 88]. The majority of proofs of this theorem go one step further and treat the determinant:

THEOREM 2.5. *Let A be a trace class operator on a Hilbert space, then*

$$\det(1+zA) := 1 + \sum_{k=1}^{\infty} z^k \text{tr}(\wedge^k A) = \prod (1+z\lambda_i). \quad (2)$$

PROOF. The sum converges to an entire function for any nuclear operator on a Banach space; indeed by applying the Hadamard inequality in (1) one has $\text{tr}(\wedge^k A) = O(C^k k^{-k/2})$. Moreover, by finite-rank approximations, its zeros are $z_l = -\lambda_l^{-1}$ where λ_l are the eigenvalues of A with appropriate multiplicities.

The restriction to Hilbert space has two effects: Firstly, $\sum |z_l|^{-1} < \infty$ and so $\det(1 + zA) = e^{g(z)} \prod (1 + z\lambda_l)$ for some entire function g . Secondly, one can improve the bound on $\text{tr}(\wedge^k A)$ to $O(\epsilon^k/k!)$ for any $\epsilon > 0$. In this way, we obtain $|\det(1 + zA)| \lesssim \exp(\epsilon|z|)$ for every $\epsilon > 0$. With further effort, one can then deduce $\text{Re } g(z) \leq 2\epsilon|z| + C_\epsilon$, which implies that $|g(z)| = o(|z|)$ by the Borel–Carathéodory inequality. Thus g is constant, and taking $z = 0$ shows $g(z) \equiv 0$. \square

The proof outlined above matches the scant details in [40]. It seems to be the simplest approach and was independently discovered by Barry, [87]. Related ideas where used by Carleman, [9], to prove a product representation for the (regularized) determinant of integral operators with Hilbert–Schmidt kernels.

Every entire function has a product representation; the product over the zeros can be made to converge by adding exponential factors. This is a famous idea of Weierstrass. Implementing it in the context of determinants leads to the notion of regularized determinants:

THEOREM 2.6. *Given an integer $p \geq 1$, let $G(x) = \sum_{k=1}^{p-1} x^k/k$ then $\det_p(1 - zA) := \det(1 - zA)e^{\text{tr } G(zA)} = \prod (1 - z\lambda_l)e^{G(z\lambda_l)} = \det[(1 - zA)e^{G(zA)}]$ extends from trace class to a continuous function on \mathfrak{I}_p , the space of operators whose singular values are ℓ^p .*

The notion of regularized determinants entered mathematics incrementally, beginning in the early twentieth century; see [87, §6] for a discussion of the history. One approach to the theory (introduced by Seiler, [86]) is to notice that $(1-x)e^{G(x)}$ can be written as $1 - x^p f(x)$ for some entire function f .

Undoubtedly, the most famous work on infinite determinants is that of Fredholm concerning integral equations, [32]. In addition to constructing the determinant, he obtains a series expansion for the kernel of the inverse operator by analogy with Cramer’s rule. We will use the discrete analogue of these formulae:

THEOREM 2.7. *Suppose $A \in \mathfrak{I}_1$, then $1 + A$ is invertible if and only if*

$$\det(1 + A) = 1 + \sum_{k=1}^{\infty} \sum_{l_1 > \dots > l_k} A^{(l_1, \dots, l_k)}_{(l_1, \dots, l_k)} \tag{3}$$

is non-vanishing. The inverse can then be written as $1 - B$ where

$$B(n, m) = \frac{1}{\det(1 + A)} \sum_{k=0}^{\infty} \sum_{l_1 > \dots > l_k} A^{(n, l_1, \dots, l_k)}_{(m, l_1, \dots, l_k)}. \tag{4}$$

PROOF. The first sentence follows from (1) and Theorem 2.5. Note that $1 + A$ is invertible if and only if -1 is not an eigenvalue of A .

The second statement follows by direct computation. For more detail, see [59, Ch. 24] or [88, Ch. 5]. \square

This theorem can be extended to operators in the higher trace ideals, \mathfrak{I}_p . Specifically, $\det_p(1 + zA)$ can be written as a sum of modified minors: when calculating these determinants as a sum over the symmetric group, one must omit any permutation containing a cycle of length less than p . The modification to (4) is not so simply explained; see [88].

Later, we will use the following consequence of the Fredholm formulae. While I have not seen this precise statement elsewhere, results of this type are well known.

LEMMA 2.8. Let G be a bounded operator with semi-separable kernel, that is,

$$G(n, m) = \begin{cases} f(n)g(m) & : n \geq m, \\ f(m)g(n) & : n \leq m. \end{cases}$$

Suppose K is a finite rank operator with $K(n, m) \neq 0$ only when $m \leq n < N$ for some integer N , then

$$\tilde{f} = [1 + GK]^{-1} f \text{ obeys } \tilde{f}(n) = a^{-1} f(n) \text{ for } n > N$$

where $a = \det(1 + GK)$.

PROOF. We will give the main computation and then justify the steps. Writing A for GK and using the Fredholm formulae from Theorem 2.7, we see that for n sufficiently large,

$$\begin{aligned} \tilde{f}(n) &= f(n) - a^{-1} \sum_{k=0}^{\infty} \sum_{l_1 > \dots > l_k} \sum_m A_{(m, l_1, \dots, l_k)}^{(n, l_1, \dots, l_k)} f(m) \\ &= f(n) - a^{-1} \sum_{k=0}^{\infty} \sum_{m > l_1 > \dots > l_k} A_{(m, l_1, \dots, l_k)}^{(n, l_1, \dots, l_k)} f(m) \\ &= f(n) - a^{-1} \sum_{k=0}^{\infty} \sum_{m > l_1 > \dots > l_k} A_{(m, l_1, \dots, l_k)}^{(m, l_1, \dots, l_k)} f(n) \\ &= f(n)[1 - a^{-1}(a - 1)], \end{aligned}$$

which simplifies to $a^{-1} f(n)$. The second line follows by noting that if $m \leq l_1$ then the top two rows of the minor are linearly dependent; this uses the fact that K is upper triangular and G is semi-separable. For the same reasons, $f(m)A(n, p) = f(n)A(m, p)$ whenever $p \leq \max\{n, m\}$. This justifies the third equality. The last line follows by recognizing the determinant from (3). \square

3. Trace Formulae for Jacobi Matrices

In this section, we will present *a priori* sum rules for Jacobi matrices.

Given two sequences $a_n > 0$ and $b_n \in \mathbb{R}$ indexed over $n = 1, 2, \dots$, the associated Jacobi matrix is the tri-diagonal matrix with these sequences as entries:

$$J = \begin{bmatrix} b_1 & a_1 & & & \\ a_1 & b_2 & a_2 & & \\ & a_2 & b_3 & \ddots & \\ & & & \ddots & \ddots \\ & & & & \ddots & \ddots \end{bmatrix}. \tag{5}$$

This defines a bounded self-adjoint operator if and only if the sequences are bounded. When they are unbounded, the operator may or may not be essentially self-adjoint when defined on finite sequences; see [91] for a discussion of this and its significance for the moment problem.

Given a pair of Jacobi matrices, \tilde{J} and J , that differ at only finitely many entries, we can define the perturbation determinant:

$$a(z) = \det \begin{bmatrix} \tilde{J} - z \\ J - z \end{bmatrix} = \det[1 + G(\tilde{J} - J)] \text{ with } G = G(z) = (J - z)^{-1}, \tag{6}$$

which is an analytic function off $\sigma(J)$ and meromorphic for $z \notin \sigma_{\text{ess}}(J)$. We will derive trace formulae by studying the behaviour of $\log |a(z)|$ at infinity and in a neighbourhood of the spectrum. This is simpler if we assume that J is a bounded operator, which we do henceforth.

The behaviour near infinity is the easiest to describe: for $|z|$ sufficiently large,

$$\begin{aligned} \log[a(z)] &= \log \det \begin{bmatrix} 1-z^{-1}\tilde{J} \\ 1-z^{-1}J \end{bmatrix} = \text{tr}(\log[1-z^{-1}\tilde{J}] - \log[1-z^{-1}J]) \\ &= -\sum_{k=1}^{\infty} \frac{1}{k} z^{-k} \text{tr}(\tilde{J}^k - J^k). \end{aligned} \tag{7}$$

Taking the real part gives the asymptotics of $\log |a(z)|$. Understanding the behaviour of $\log |a(z)|$ near the spectrum is considerably more involved and will require a number of preliminaries.

The vector $e_1 = [1, 0, \dots]^{\dagger}$ is cyclic for J ; we will write $d\mu$ for the corresponding spectral measure. Because of the existence of a cyclic vector, all eigenspaces are one-dimensional and hence all zeros and poles of $a(z)$ are simple. Given a concrete Jacobi matrix, the natural way to determine $d\mu$ is via the m -function:

$$m(z) = \langle e_1 | (J - z)^{-1} e_1 \rangle = \int \frac{d\mu(t)}{t - z}. \tag{8}$$

This requires knowledge of the Green function, which we will now describe. The Green function is constructed from two solutions of the finite difference equation associated to J . Let us define polynomials $p_n(z)$ of degree $n \geq 0$ by the recurrence

$$a_{n+1}p_{n+1}(z) + b_n p_n(z) + a_{n-1}p_{n-1}(z) = z p_n(z) \tag{9}$$

with $p_{-1}(z) \equiv 0$ and $p_0 \equiv 1$. Then $\sum_{n=0}^{\infty} p_n(z)e_{n+1}$ is a formal solution of $Ju = zu$. Moreover, these polynomials form an orthonormal basis for $L^2(d\mu)$ and $p_n(J)e_1 = e_{n+1}$. The second solution is the Weyl solution, which is only defined for $z \notin \sigma(J)$. It is given by

$$\sum_{n=0}^{\infty} \psi_n(z)e_{n+1} = (J - z)^{-1} e_1. \tag{10}$$

In practice, one uses the following equivalent formulation: $\psi_n(z)$ obeys (9) for $n \geq 1$, it is square summable, and $a_1\psi_1 + (b_1 - z)\psi_0 = 1$. It is now easy to check that the Green function is given by

$$G(n+1, n'+1; z) = \langle e_{n+1} | (J - z)^{-1} e_{n'+1} \rangle = p_{\min\{n, n'\}}(z) \psi_{\max\{n, n'\}}(z).$$

The point in introducing all this machinery is the following discrete analogue of a theorem of Jost and Pais, [45]:

THEOREM 3.1. *Suppose \tilde{J} and J are bounded Jacobi matrices differing in only finitely many entries, then for n sufficiently large, the Weyl solutions associated to these Jacobi matrices obey*

$$a(z)\tilde{\psi}_n(z) = \psi_n(z) \prod_{k=1}^{\infty} \frac{\tilde{a}_k}{a_k}. \tag{11}$$

In particular, for a.e. x with respect to $d\mu_{ac}$,

$$\frac{d\tilde{\mu}}{d\mu} = \frac{\text{Im } \tilde{m}(x + i0)}{\text{Im } m(x + i0)} = |a(x + i0)|^{-2} \prod_{k=1}^{\infty} \frac{\tilde{a}_k^2}{a_k^2}. \tag{12}$$

PROOF. Let D be the diagonal matrix with $D_{nn} = \prod_{k=n}^{\infty} \tilde{a}_k/a_k$. By the resolvent identity,

$$D(\tilde{J} - z)^{-1}D^{-1} = (J - z)^{-1} - (J - z)^{-1}[D^{-1}\tilde{J}D - J]D(\tilde{J} - z)^{-1}D^{-1},$$

which implies that the sequence $\xi_n := (D_{nn}/D_{11})\tilde{\psi}_n$ obeys

$$\xi_n = \psi_n - GK\xi_n$$

where G is the Green function for J and K is the matrix $D^{-1}\tilde{J}D - J$, which is lower triangular. As D_{nn} is eventually identically one and

$$\det[1 + GK] = \det[D^{-1}(\tilde{J} - z)D(J - z)^{-1}] = a(z),$$

Lemma 2.8 implies that (11) holds.

To prove (12) we merely combine (11), the fact that

$$\frac{d\mu}{dx} = \lim_{y \downarrow 0} \frac{1}{\pi} \operatorname{Im} m(x + iy) = \lim_{y \downarrow 0} \frac{y}{\pi} \|(J - x - iy)^{-1}e_1\|^2 = \lim_{y \downarrow 0} \frac{y}{\pi} \|\psi_n(x + iy)\|^2$$

Lebesgue almost everywhere, and the corresponding result for \tilde{J} . □

With a little more care, one may use the reasoning above to deduce that $\log |a(z)|$ has a non-tangential limit at $d\mu_{ac}$ -a.e. $x \in \mathbb{R}$. Actually, it is easy to obtain this kind of information about $a(z)$:

LEMMA 3.2. *If $\tilde{J} - J$ has finite rank, then $a(z)$ is a polynomial in z and $m(z)$.*

PROOF. The key observation is that every matrix element of $(J - z)^{-1}(\tilde{J} - J)$ is a polynomial in $m(z)$ and z . This can be justified by noting that

$$\langle e_{n+1} | (J - z)^{-1} e_{m+1} \rangle = \int \frac{p_n(x)p_m(x) d\mu(x)}{x - z}$$

and $x^k(x - z)^{-1} = x^k + zx^{k-1}(x - z)^{-1}$. □

The reader is no doubt familiar with function theory in the unit disk and hence in any simply connected domain. In multiply-connected domains, matters are more complicated, primarily because of the non-existence of Blaschke products. Of course, one may always lift questions to the universal cover and apply results from the disk case, but in general, the covering map can be a horror. We do not wish to get waylaid by these problems and so treat a very simple case.

HYPOTHESIS 3.3. *We assume that J is periodic, that is, the sequences a_n and b_n are periodic.*

Under this hypothesis, $\sigma(J)$ consists of finitely many compact intervals together with finitely many points. (This remains true for finite-rank perturbations.)

Let us write Ω for the complement of $\sigma_{\text{ess}}(J)$ in the Riemann sphere. By applying Joukowski transformations, this region can be transformed to one bounded by finitely many analytic curves; thus we can apply the general results described in [31, 77].

The trace formulae we will derive amount to the relation between $\log |a(z)|$ on $\sigma_{\text{ess}}(J)$ as given in Theorem 3.1 and the asymptotics given in (7). In essence, $\log |a(z)|$ is the Poisson integral of its boundary values; however $a(z)$ may have both

zeros and poles. When Ω is simply connected, the traditional approach has been to remove the problem with Blaschke products. We use Green’s identity:

$$\int_{\Omega} f \Delta g - g \Delta f = \int_{\partial\Omega} f \frac{\partial g}{\partial n} - g \frac{\partial f}{\partial n}. \tag{13}$$

(The Poisson integral representation of harmonic functions follows by choosing g to be the Dirichlet Green function for Ω .)

DEFINITION 3.4. Let $g_0(z)$ denote the (Dirichlet) Green function for Ω with singularity at infinity. That is, g_0 is the unique continuous function on \mathbb{C} that is harmonic on $\mathbb{C} \setminus \sigma_{\text{ess}}(J)$, vanishes on $\sigma_{\text{ess}}(J)$, and has asymptotics

$$g_0(z) = -\frac{1}{2\pi} \log |z| + O(1) \quad \text{as } z \rightarrow \infty.$$

Similarly we introduce functions g_k , $k \geq 1$, that are continuous and harmonic as before, but with asymptotics

$$g_k(z) = -\frac{1}{2\pi} \operatorname{Re} z^k + O(1) \quad \text{as } z \rightarrow \infty.$$

We will also use the analogue of harmonic measure:

$$d\nu_k(x) = -2 \left[\lim_{y \downarrow 0} \frac{\partial}{\partial y} g_k(x + iy) \right] dx,$$

which is supported on $\sigma_{\text{ess}}(J)$.

Note that Green’s identity with $f \equiv 1$ shows that $\int d\nu_k = \delta_{k0}$. These functions are Green functions for infinity in the following sense: if f is smooth and supported in a small neighbourhood of infinity with

$$f(z) \sim \sum_l c_l \operatorname{Re}(z^{-l}) + d_l \operatorname{Im}(z^{-l}), \quad \text{then} \quad \int f \Delta g_k = \begin{cases} kc_k & : k \geq 1, \\ c_0 & : k = 0. \end{cases} \tag{14}$$

THEOREM 3.5. Suppose J is a periodic Jacobi matrix and \tilde{J} is a finite-rank perturbation, then

$$-\sum \log[\tilde{a}_j/a_j] = 2\pi \sum [g_0(\tilde{E}_j) - g_0(E_j)] - \frac{1}{2} \int \log \left[\frac{d\tilde{\mu}}{d\mu} \right] d\nu_0(x), \tag{15}$$

where E_j and \tilde{E}_j enumerate the discrete spectrum of J and \tilde{J} . For $k \geq 1$,

$$-\operatorname{tr}(\tilde{J}^k - J^k) = 2\pi \sum [g_k(\tilde{E}_j) - g_k(E_j)] - \frac{1}{2} \int \log \left[\frac{d\tilde{\mu}}{d\mu} \right] d\nu_k(x). \tag{16}$$

PROOF. The equations follow from Green’s identity, (13), with $f = \log |a(z)|$ and $g = g_k$. As $a(z)$ has simple poles/zeros at the eigenvalues of J and \tilde{J} ,

$$-\Delta f = \sum 2\pi \delta(z - E_j) - \sum 2\pi \delta(z - \tilde{E}_j),$$

while $\int_{\Omega} f \Delta g_k$ can be evaluated with (7) and (14).

We need to show that the integrals over the boundaries can be taken in an almost-everywhere, rather than distributional, sense. Because we have assumed that J is periodic, its m -function is extremely well behaved and so Lemma 3.2 makes this elementary. In more general settings, one needs to use the fact that $m \in H^p(\Omega)$ for any $0 < p < 1$ and hence $a(z) \in H^p(\Omega)$ for p sufficiently small.

From the definition, $a(\bar{z}) = \overline{a(z)}$ and so $f(z) = f(\bar{z})$. This allows us to combine the contributions from upper and lower edges of each slit. The final result follows by re-writing f on the boundary via (12). Note that $\log[\tilde{a}_j/a_j]$ appears with coefficient one in (15) and not at all in (16) because $\int d\nu_k = \delta_{k0}$. \square

These formulae may seem rather far removed from the trace formulae we discussed in Section 2. However, the important property has remained: the left-hand side involves the coefficients of the operator, while the the right, the spectral properties.

The simplest periodic operator has constant coefficients; by scaling and shifting, it suffices to consider $a_k \equiv 1$ and $b_k \equiv 0$. The resulting Jacobi matrix has spectrum $[-2, 2]$, which is purely absolutely continuous,

$$d\mu(x) = \frac{1}{2\pi} \chi_{[-2,2]}(x) \sqrt{4 - x^2} dx.$$

For this choice of J , Theorem 3.5 is due to Case, [10], although he was very much inspired by the trace formulae for Schrödinger operators that we will describe in the next section.

Certain linear combinations of the Case formulae turn out to be more useful for applications; the key ingredient is positivity. The following example synthesizes [47, 54]. Let T_n and U_n denote the usual Chebyshev polynomials:

$$T_n(\cos(\theta)) = \cos(n\theta) \quad \text{and} \quad U_n(\cos(\theta)) = \frac{\sin[(n+1)\theta]}{\sin(\theta)}.$$

Then for each $n \geq 1$,

$$-\frac{n}{\pi} \int_{-2}^2 \log \left[\frac{d\tilde{\mu}}{d\mu} \right] \sqrt{4 - x^2} |U_{n-1}(\frac{x}{2})|^2 dx + \sum G_n(\tilde{E}_j) \tag{17}$$

$$= \text{tr} \left\{ [2T_n(\frac{1}{2}\tilde{J}) - 2T_n(\frac{1}{2}J)]^2 \right\} + 4 \sum_{j=1}^{\infty} F(\tilde{a}_j \cdots \tilde{a}_{j+n-1}) + X_n$$

where $F(x) = x - 1 - \log(x) \geq 0$,

$$G_n(\beta + \beta^{-1}) = \beta^{2n} - \beta^{-2n} - 4n \log |\beta| \quad \text{for } |\beta| > 1, \tag{18}$$

and X_n is a simple function of the first few entries of \tilde{J} . This is most easily deduced by simply repeating the proof of Theorem 3.5 using the harmonic function $g = \frac{1}{2\pi} \text{Re } G_n$ in place of any particular g_k . One further observation is necessary however: $2T_n(\frac{1}{2}J)$ differs from the matrix with ones on the n th sub- and super-diagonals and zeros elsewhere in only a few entries. This implies

$$-8 \text{tr} \left\{ [T_n(\frac{1}{2}\tilde{J}) - T_n(\frac{1}{2}J)] T_n(\frac{1}{2}J) \right\} = X_n - 4 \sum [\tilde{a}_j \cdots \tilde{a}_{j+n-1} - 1],$$

with the proper choice of X_n ; in fact, $X_1 \equiv 0$.

For future reference, let us note that the right-hand side of this equation is finite if and only if $T_n(\frac{1}{2}\tilde{J}) - T_n(\frac{1}{2}J)$ is Hilbert-Schmidt; the sum over $F(\tilde{a}_j \cdots \tilde{a}_{j+n-1})$ is bounded by the sum of the squares of the entries on the n th super-diagonal of this matrix.

The first two terms on the right-hand side of (17) are manifestly positive, as is the sum over the eigenvalues. Strict positivity of the integral is not essential; however, by Lemma 6.2 it is bounded from below. There are several other sum rules for Jacobi matrices that have good positivity properties; see, for example, [47, 53, 81, 100]. A very general (but rather abstract) approach to the positivity problem can be found in [66].

The observation regarding $2T_n(\frac{1}{2}J)$ has an analogue for general periodic Jacobi matrices, which gives rise to similar formulae. Let J be a periodic Jacobi matrix

with period p scaled so that $a_1 a_2 \cdots a_p = 1$ and let Δ denote the corresponding discriminant. For any \tilde{J} differing from J by finite rank,

$$2\pi \sum [g(\tilde{E}_j) - g(E_j)] - \frac{1}{2} \int \log \left[\frac{d\tilde{\mu}}{d\mu} \right] d\nu(x) = \frac{1}{4p} \operatorname{tr} \left\{ [\Delta(\tilde{J}) - \Delta(J)]^2 \right\} + \frac{1}{4p} \sum F(\tilde{a}_j \cdots \tilde{a}_{j+p-1}) + X \tag{19}$$

where $g = \frac{-1}{2\pi p} \operatorname{Re} \left\{ \log \left[\frac{1}{2} \Delta + \frac{1}{2} \sqrt{\Delta^2 - 4} \right] - \frac{1}{4} \Delta \sqrt{\Delta^2 - 4} \right\}$ and $d\nu$ is the probability measure supported on $\sigma_{\text{ess}}(J)$ with density $\frac{d\nu}{dx} = \frac{1}{2\pi p} |\Delta'(x)| \sqrt{4 - \Delta(x)^2}$. These formulae and related results are the topic of forthcoming joint work, [14]. Note also that (17) follows from this formula by considering the case of constant coefficients as a period- n problem.

4. Trace Formulae for Other Operators

As mentioned in the previous section, the derivation of sum rules for Jacobi matrices follows earlier results for Schrödinger operators. The first goal of this section is to describe these results. After that we will briefly discuss certain older results that fit naturally into the same framework. As in the previous section, we will state *a priori* versions of these sum rules; that is, with far stronger hypotheses than turn out to be necessary.

Consider the whole-line Schrödinger operator associated to a smooth compactly supported potential V ,

$$[\tilde{L}u](x) = -u''(x) + V(x)u(x),$$

and write L for the free operator ($V \equiv 0$). In this setting, the perturbation determinant $a(z) = \det[(\tilde{L} - z)/(L - z)]$ happens to be equal to the reciprocal of the transmission coefficient and most references we quote take this point of view. The analogue of Theorem 3.5 is much better known, primarily because of its role in the inverse scattering solution of the KdV equation. As $\sigma(L)$ is not compact, one studies the behaviour of $a(z)$ as z approaches infinity in a particular direction, specifically, along the negative real axis.

THEOREM 4.1. *If V is C^∞ and of compact support, then for $n \geq 0$,*

$$\int_0^\infty \log |a(E + i0)| E^{n-1/2} dE = \frac{(-1)^n \pi}{2^{2n+1}} \int \xi_{2n+1}(x) dx + \frac{(-1)^n 2\pi}{2n+1} \sum E_m^{n+1/2} \tag{20}$$

where $E_m < 0$ enumerate the discrete spectrum and ξ_{2n+1} is defined by the following recurrence: $\xi_0(x) = 0$, $\xi_1(x) = V(x)$ and $\xi_{n+1} + \xi'_n + \sum_{\ell=1}^n \xi_\ell \xi_{n-\ell} = 0$.

The original paper is [110], which builds upon earlier work [7, 34, 35]. The reader may have noticed that Jacobi matrices are parameterized over a half-line, while now we discuss whole-line Schrödinger operators. The trace formulae for half-line Schrödinger operators, [7], contain values of V (and its derivatives) at the origin; this makes them unsuitable for the applications we have in mind.

The formulae for $\int \xi_k dx$ can be simplified by recognizing complete derivatives. We will primarily discuss the $n = 1$ case of (20):

$$\frac{1}{\pi} \int_0^\infty \log |a(E + i0)| E^{1/2} dE + \frac{2}{3} \sum |E_m|^{3/2} = \frac{1}{8} \int |V(x)|^2 dx. \tag{21}$$

If V is supported on the positive half-axis, then we obtain the following analogue of the Jost–Pais theorem: for $k > 0$,

$$|a(k^2 + i0)|^2 = \frac{|m(k^2 + i0) + ik|^2}{4k \operatorname{Im} m(k^2 + i0)} \geq 1 \tag{22}$$

where m denotes the Weyl m -function associated to the half-line Schrödinger operator with potential V and a Dirichlet boundary condition. In Theorem 3.1, we made a direct link to the spectral measure; that is not quite possible here. While $\frac{1}{\pi} \operatorname{Im} m(E + i0)$ is equal to the Radon–Nikodym derivative of the spectral measure, the formula for a involves $\operatorname{Re} m$ and hence the Hilbert transform of the spectral measure.

Jacobi matrices are naturally associated to the theory of orthogonal polynomials for measures supported on the real line. There is an analogous theory of orthogonal polynomials for measures on the unit circle in the complex plane. While this theory is of considerable vintage, the proper analogue of Jacobi matrices was discovered surprisingly recently. We will now describe these operators and describe how the corresponding sum rules relate to certain classical questions.

Given a probability measure $d\mu$ on $S^1 = \{z \in \mathbb{C} : |z| = 1\}$ (with infinite support), we can construct a system of orthonormal polynomials $\phi_k(z)$ by applying the Gram–Schmidt procedure to $1, z, z^2, \dots$. As in the Jacobi case, these polynomials obey a recurrence relation. As it is simpler in this case, we write the relation for the monic orthogonal polynomials:

$$\Phi_{k+1}(z) = z\Phi_k(z) - \bar{\alpha}_k \Phi_k^*(z), \quad \Phi_{k+1}^*(z) = \Phi_k^*(z) - \alpha_k z \Phi_k(z). \tag{23}$$

Here $\alpha_k \in \mathbb{D}$ are the recurrence coefficients, which we call Verblunsky coefficients, and Φ_k^* denotes the reversed polynomial: $\Phi_k^*(z) = z^k \overline{\Phi_k(\bar{z}^{-1})}$.

In general, these polynomials need not form a basis for $L^2(d\mu)$, as can be seen when $d\mu = \frac{1}{2\pi} d\theta$. Instead, we may apply the Gram–Schmidt procedure to $1, z, z^{-1}, z^2, z^{-2}, \dots$; in this way we obtain an orthonormal basis $\chi_k(z)$ for $L^2(d\mu)$, which are related to the orthonormal polynomials by

$$\chi_k(z) = \begin{cases} z^{-k/2} \phi_k^*(z) & : k \text{ even} \\ z^{-(k-1)/2} \phi_k(z) & : k \text{ odd.} \end{cases} \tag{24}$$

Let \mathcal{C} be the matrix representing $f(z) \mapsto zf(z)$ in this basis. The resulting class of matrices are known as CMV matrices and comprise a natural unitary analogue of Jacobi matrices. The name is taken from authors of [8]; however, the original discovery predates this paper as discussed in [95] and [108].

Let us write \mathcal{C}_0 for the CMV matrix associated to $d\mu = \frac{1}{2\pi} d\theta$, which corresponds to $\alpha_k \equiv 0$. The analogue of Theorems 3.1 and 3.5 can be combined into one:

THEOREM 4.2. *Suppose $\mathcal{C} - \mathcal{C}_0$ is of finite rank (that is, $\alpha_k = 0$ for all but finitely many k). Then $d(z) := \det[(1 - z\mathcal{C}^\dagger)/(1 - z\mathcal{C}_0^\dagger)]$ is related to the Szegő function,*

$$D(z) = \exp\left\{ \frac{1}{4\pi} \int \frac{e^{i\theta} + z}{e^{i\theta} - z} \log\left[2\pi \frac{d\mu}{d\theta}\right] d\theta \right\}, \quad \text{by } d(z)D(z) = \prod (1 - |\alpha_k|^2)^{1/2}.$$

Notice that $|D(e^{i\theta})|^2 = 2\pi \frac{d\mu}{d\theta}$.

This result is Theorem 4.2.14 in [94]. By comparing the Taylor coefficients of $d(z)$ and $D(z)$ one easily deduces sum rules resembling (15) and (16).

While the interpretation of $D(z)$ as a perturbation determinant of CMV matrices is very recent, the primary content of this theorem is not. Szegő, [102, 103], proved that when the integral defining D is convergent, $\phi_n^*(z) \rightarrow D(z)^{-1}$ uniformly on compact subsets of \mathbb{D} . By using the recurrence relations for ϕ_n^* , one can deduce the same family of sum rules.

Kreĭn, [52], introduced a continuous analogue of the recurrence (23),

$$\frac{d}{dr}P(r, z) = izP(r, z) - \bar{A}(r)P_*(r, z), \quad \frac{d}{dr}P_*(r, z) = -A(r)P(r, z), \quad (25)$$

where $A(r)$ is a complex function on $[0, \infty)$ and $P_*(0, z) = P(0, z) \equiv 1$. These equations are referred to as the Kreĭn system. Note that $P_*(r, z) = e^{irz}\overline{P(r, \bar{z})}$ and

$$P(r, z) = e^{irz} - \int_0^r \gamma_r(s)e^{i(r-s)z} dz$$

for some integrable function γ_r , which explains the relation of r to the degree of the polynomial. The polynomial analogy is further strengthened by the existence of a measure $d\mu$ on \mathbb{R} so that $\int(1+x^2)^{-1}d\mu(x) < \infty$ and $\int P(r, x)\overline{P(s, x)}d\mu = \delta(r-s)$. While of interest in their own right, results for Kreĭn systems also have consequences for Schrödinger operators; the key observation is that if A is real-valued, then

$$\psi(r; z) = e^{-irz} \frac{P(2r, z) - P_*(2r, \bar{z})}{2iz} \quad \text{solves} \quad -\psi'' + V\psi = z^2\psi$$

where $V(r) = 4A(2r)^2 - 4A'(2r)$.

Kreĭn does not give sum rules *per se*, but under suitable hypotheses, $P_*(r, z) \rightarrow \Pi(z)$ as $r \rightarrow \infty$ where $\Pi(z)$ is the outer function on the upper half-plane that obeys $|\Pi(x+i0)|^{-2} = 2\pi \frac{d\mu}{dx}$. This is essentially equivalent as discussed above. Lastly, the reader should be warned that Kreĭn’s paper contains no proofs; fortunately, details can be found in [84, 105].

5. Point Spectrum

As first noted in [33, p. 115], it follows from (21) that the bound-state energies, E_m , of a whole-line Schrödinger operator with potential $V \in L^2$ obey

$$\frac{2}{3} \sum |E_m|^{3/2} \leq \frac{1}{8} \int |V(x)|^2 dx. \quad (26)$$

This can be justified as follows: Choose $V_n \in C_c^\infty$ converging to V in L^2 . Then $L + V_n$ converges to \tilde{L} in strong resolvent sense, which implies (individual) convergence of the eigenvalues. Applying Fatou’s lemma to the sum over eigenvalues and using the fact that $|a(E+i0)| \geq 1$ for any potential gives (26). The existence of non-trivial reflectionless potentials shows that the constant in this inequality is optimal.

Inequalities of this kind are known as Lieb–Thirring inequalities and hold in considerable generality, including higher dimensions; see [61]. Considerable attention has been paid to the question of the optimal constants. In [57], Laptev and Weidl made a major breakthrough:

THEOREM 5.1. *The negative eigenvalues of $-\Delta + V$ acting in $L^2(\mathbb{R}^d)$ obey*

$$\sum |E_m|^\gamma \leq \frac{\Gamma(\gamma + 1)}{2^d \pi^{d/2} \Gamma(\gamma + \frac{1}{2}d + 1)} \int |V(x)|^{\gamma + \frac{1}{2}d} dx$$

for any $d \geq 1$ and $\gamma \geq \frac{3}{2}$. Moreover, the constant is optimal.

This is proved by extending the inequality (26) to operator-valued potentials (using trace formula methods) and then employing induction in dimension. An alternate proof of the trace formula portion of the argument appears in [5].

It is elementary to apply the reasoning described above to (17); this leads to the following result [47, 54]:

$$[T_n(\frac{1}{2}\tilde{J}) - T_n(\frac{1}{2}J)] \in \mathfrak{I}_2 \quad \Rightarrow \quad \sum [|\tilde{E}_j| - 2]^{3/2} < \infty. \quad (27)$$

(Analogous results can be found in [53, 81].) The particular case $n = 1$, treated in [47], is the natural Jacobi-matrix analogue of (26). For further inequalities of this type, see [41].

For CMV matrices and Kreĭn systems with decaying coefficients, the essential spectrum fills S^1 and \mathbb{R} , respectively. Thus there is no discrete spectrum.

6. A.C. Spectrum

It is well known that a one-dimensional Schrödinger operator with sufficiently rapidly decreasing potential has a.c. spectrum on $[0, \infty)$ —with sufficient decay it will even be purely absolutely continuous. But how quickly is sufficiently quickly?

On the basis of sparse, [50, 68, 72], and random, [18, 19, 51, 89], examples, it was known that there are potentials just outside L^2 which produce no a.c. spectrum whatsoever. Indeed, Simon has shown that this is generic, [90]. Eventually, the weight of this and other evidence led Kiselev, Last, and Simon, [50], to conjecture that L^2 was the correct borderline.

In his thesis, Kiselev made a significant step toward verifying this conjecture. This approach was later refined in [12], while an alternate approach was developed by Remling, [73]. The central conclusion of this work was: If $|V(x)| \lesssim (1+x^2)^{-\epsilon-1/4}$ then for almost every positive energy, all generalized eigenfunctions are bounded. In particular, the essential support of the a.c. spectrum fills $[0, \infty)$. It would be extremely interesting to know whether eigenfunctions are bounded at almost every positive energy when $V \in L^2$; in the regime of infinitesimal coupling, this reduces to Carleson's theorem on a.e. convergence of Fourier integrals. See [104] for more on this perspective.

The spectral question for $V \in L^2$ has been resolved using sum-rule methods, [16]:

THEOREM 6.1. *The absolutely continuous spectrum of a half-line Schrödinger operator with potential $V \in L^2$ is essentially supported by $[0, \infty)$.*

PROOF. Keeping only the imaginary part of m in (22) leads to

$$|a(k^2 + i0)|^2 \geq \frac{[\operatorname{Im} m(k^2 + i0) + k]^2}{4k \operatorname{Im} m(k^2 + i0)} \geq 1$$

Notice that $|a|$ is large wherever $\frac{d\mu}{dx} = \frac{1}{\pi} \operatorname{Im} m$ is small, but by (21), we know that the integral of $\log |a|$ is controlled by the L^2 norm of the potential. The only obstacle is that we only know (21) for compactly supported potentials; this is resolved by choosing a sequence $V_n \rightarrow V$ and applying a simple semi-continuity argument. \square

There are now many results proved by similar means; we will give a brief overview of these and then turn to the Jacobi matrix case, where we offer a more detailed presentation. After that we will describe the analogous results for CMV matrices and Kreĭn systems, which are actually the oldest of all.

Using higher-order sum rules, [65] proves full a.c. spectrum under the hypotheses $V^{(p-1)} \in L^2$ and $V \in L^{p+1}$ for any integer $p \geq 1$. By using the connection to Krein systems, Denisov obtained the same conclusion under the following hypotheses: V is uniformly L^2_{loc} and $V = A'$ with $A \in L^2$, see [20]; or $\limsup V(x) = 0$ and $V' \in L^2$, see [21]. See also [78].

In [46], a modification of the trace formula method was developed that works locally in energy. Specifically, one studies the perturbation determinant in a small region which touches the boundary along an interval, which allows one to consider perturbations of operators with non-zero potentials. In this way, it was shown that the a.c. spectrum of periodic Schrödinger operators is invariant under L^2 perturbation. The Stark operator was also studied; see [69] for further developments in this direction and for references to work on this operator that is not based on sum rules.

Another result from [46] is the following: if $V \in L^3$ and (the distribution) \hat{V} agrees with an L^2 function on an interval $[a^2, b^2]$, then $-\partial_x^2 + V$ has a.c. spectrum throughout the interval $[2a, 2b]$. See also [81], which treats Jacobi matrices. By combining the problems for V and $-V$ as in [83], one can see that the condition $V \in L^3$ can be replaced by $V \in L^4$. This was pointed out to me by O. Safronov.

The most interesting recent development of the trace formula method has been its extension to higher dimensions. For Dirac operators, there are the impressive results of Denisov, [25, 26]. Progress for Schrödinger operators has been slower for two reasons: bound states are especially problematic in the multi-dimensional case and there is no satisfactory WKB theory without smoothness assumptions on the potential. For the state of the art, see [24, 27, 55, 56, 82, 83] and the Denisov–Kiselev contribution to this Festschrift.

We will now present a Jacobi-matrix analogue of Theorem 6.1. The case of discrete Schrödinger operators was discussed in [16]; however, our treatment follows [47] with additional input from [54, 66]. The final result is from [66]. As suggested in the last proof, the main ingredient is a semi-continuity statement:

LEMMA 6.2. *Given probability measures $d\nu$ and $d\sigma$ on \mathbb{R} ,*

$$S(d\nu|d\sigma) := \inf \int e^g d\sigma - \int (g+1) d\nu = \begin{cases} -\int \log[w] d\nu & : d\nu = wd\sigma \\ -\infty & : \text{otherwise} \end{cases}$$

where the infimum is over bounded continuous functions g . As a consequence, if $d\sigma_n$ converges weak-* to $d\sigma$, then $S(d\nu|d\sigma) \geq \limsup S(d\nu|d\sigma_n)$.

PROOF. The case where $d\nu$ is not $d\sigma$ -a.c. is easily dealt with; we suppose $d\nu = wd\sigma$. Let us write $g = c + h$ where $c = \int g d\nu$. By Jensen's inequality,

$$S(d\nu|d\sigma) \leq e^c \int w^{-1} e^h d\nu - c - 1 \leq \exp\{c - \int \log[w] d\nu\} - c - 1.$$

The minimizing value of c is $\int \log[w] d\nu$, which proves $S(d\nu|d\sigma) \leq -\int \log[w] d\nu$.

The fact that this inequality can be saturated follows by choosing g to approximate $\log[w]$, which corresponds to the case of equality in Jensen's inequality. \square

REMARK. By choosing $g \equiv 0$, it follows that $S(d\nu|d\sigma) \leq 0$. Consequently,

$$\int \log \left[\frac{d\tilde{\mu}}{d\mu} \right] d\nu \leq -S(d\nu|d\mu). \quad (28)$$

THEOREM 6.3. *Let J be the Jacobi matrix with $a_k \equiv 1$ and $b_k \equiv 0$. If \tilde{J} is a Jacobi matrix with $[T_n(\frac{1}{2}\tilde{J}) - T_n(\frac{1}{2}J)] \in \mathfrak{I}_2$ for some integer $n \geq 1$, then*

$$\int_{-2}^2 \log \left[\frac{d\tilde{\mu}}{d\mu} \right] \sqrt{4-x^2} |U_{n-1}(\frac{x}{2})|^2 dx < \infty$$

where T_n and U_n represent Chebyshev polynomials as in (17).

PROOF. The result follows by combining (17) and Lemma 6.2 once we know that there are a sequence of operators J_k each differing from J by finite rank such that $J_k \rightarrow \tilde{J}$ strongly (which implies weak-* convergence of the spectral measures) and for which $T_n(\frac{1}{2}J_k) - T_n(\frac{1}{2}J)$ is bounded in Hilbert-Schmidt norm. Such a sequence does exist because $\tilde{a}_n \rightarrow 1$ and $\tilde{b}_n \rightarrow 0$. This can be shown by examining the top three diagonals in $T_n(\frac{1}{2}\tilde{J})$; for details see Lemma 6.6 of [66]. \square

Jacobi matrix results have developed along lines parallel to the Schrödinger case—though the proper analogue of [65] remains particularly stubborn; see [53] for the latest on this problem.

That the a.c. spectrum fills S^1 for CMV matrices with $\alpha_k \in \ell^2$ follows from early work of Szegő, [102, 103]. Indeed much more is true; see Theorem 8.1.

With regard to higher-order sum rules for CMV matrices, see [22, 28, 39, 94, 101].

For Kreĭn systems, we have the following [52]:

THEOREM 6.4. *When $A \in L^2(dr)$, the spectral measure obeys*

$$-\int \log \left[\frac{d\mu}{dx} \right] \frac{dx}{1+x^2} < \infty.$$

In particular, the essential support of the a.c. spectrum is \mathbb{R} .

7. The Step-by-Step Method

As we have seen, the *a priori* sum rules presented in Section 3 are ample for applications in (forward) spectral theory. In the next section, we will be presenting results that incorporate inverse spectral theory and for this purpose, we need to discuss a second kind of *a priori* sum rule. The main idea can be found in [47, §4], but was first emphasized in [100]. The function-theoretic essence of the argument was distilled in [93]. We will present only the simplest case; it is not difficult to extend the results to the generality presented in Section 3.

HYPOTHESIS 7.1. *We assume $d\tilde{\mu}$ is a probability measure with support $[-2, 2] \cup \{\tilde{E}_j\}$ where \tilde{E}_j obeys $\sum[|\tilde{E}_j| - 2]^{3/2} < \infty$ and $\frac{d\tilde{\mu}}{dx} > 0$ almost everywhere in $[-2, 2]$.*

As previously, we write $\tilde{m}(z) = \langle e_1 | (\tilde{J} - z)^{-1} e_1 \rangle = \int \frac{1}{t-z} d\tilde{\mu}(t)$, which is a meromorphic function on Ω , the complement of $[-2, 2]$ in the Riemann sphere. We also enumerate the point spectrum $\{\tilde{E}_j\}$ so that $|\tilde{E}_j|$ is non-increasing.

A single step consists of removing the first row and column from J . We will denote the resulting Jacobi matrix by $\tilde{J}^{(1)}$, its spectral measure by $d\tilde{\mu}^{(1)}$, and m -function, $\tilde{m}^{(1)}(z)$.

LEMMA 7.2. *If $d\tilde{\mu}$ obeys Hypothesis 7.1, then so does $d\tilde{\mu}^{(1)}$.*

PROOF. By the min-max characterization of eigenvalues,

$$|\tilde{E}_j^{(1)}| \leq |\tilde{E}_j|. \tag{29}$$

Indeed, by the theory of rank-one perturbations, the eigenvalues of J and $J^{(1)}$ interlace. By the well-known formulae for inverting block matrices,

$$\tilde{m}(z) = [b_1 - z - a_1^2 \tilde{m}^{(1)}(z)]^{-1}. \tag{30}$$

In particular, taking the imaginary part we find

$$\frac{d\tilde{\mu}^{(1)}}{dx} \div \frac{d\tilde{\mu}}{dx} = \frac{\text{Im } \tilde{m}^{(1)}(x + i0)}{\text{Im } \tilde{m}(x + i0)} = \tilde{a}_1^{-2} |\tilde{m}(x + i0)|^{-2} \tag{31}$$

for a.e. $x \in [-2, 2]$. This completes the proof; Herglotz functions have non-zero boundary values almost everywhere. \square

The step-by-step approach studies $\log |\tilde{m}(z)|$ in very much the same manner as we studied $\log |a(z)|$ in Section 3; its boundary values can be read off (31) while the behaviour at infinity is governed by

LEMMA 7.3. *If $d\tilde{\mu}$ has compact support,*

$$\log[-z\tilde{m}(z)] = \sum_{k=1}^{\infty} -\frac{1}{k} z^{-k} \text{tr}\{\tilde{J}^k - (0 \oplus \tilde{J}^{(1)})^k\} \tag{32}$$

for z sufficiently large. Note, $0 \oplus \tilde{J}^{(1)}$ differs from \tilde{J} by having $a_1 = b_1 = 0$.

PROOF. By writing $m(z) = \text{tr}\{P(\tilde{J} - z)^{-1}\}$ with $P = |e_1\rangle\langle e_1|$ and expanding,

$$\log[-zm(z)] = \sum_{k=1}^{\infty} z^{-k} \sum_{p=1}^k \frac{(-1)^p}{p} \sum_{t_1 + \dots + t_p = k} \text{tr}\{P\tilde{J}^{t_1} P\tilde{J}^{t_2} \dots P\tilde{J}^{t_k}\}$$

where t_1, \dots, t_p are positive integers. Writing out the matrix product, we can regard the trace here as a sum over m -tuples (i_1, \dots, i_m) where $i_s = 1$ whenever s belongs to the set $\{1, 1 + t_1, \dots, 1 + t_1 + \dots + t_{p-1}\}$. Similarly,

$$\text{tr}\{\tilde{J}^k - (0 \oplus \tilde{J}^{(1)})^k\} = - \sum \tilde{J}(j_1, j_2) \tilde{J}(j_2, j_3) \dots \tilde{J}(j_k, j_1)$$

where the sum is taken over k -tuples with $j_s = 1$ for at least one s .

To connect the two, one should perform inclusion/exclusion on the number of times a k -tuple visits the value 1; the role of p is to restrict to k -tuples visiting 1 at least p times. \square

I have not seen (32) in the literature. This is not the simplest proof; however having typed all those indices, I am loath to delete them. A simpler proof was suggested to me by Barry: By (8) and Cramer’s rule, $m(z)$ can be written as a ratio of determinants and thus $\log[-zm(z)]$ can be written as the differences of traces. To make this fully rigorous, one first treats finite Jacobi matrices and then observes that this suffices.

THEOREM 7.4. *Let J denote the Jacobi matrix with $a_j \equiv 1$ and $b_j \equiv 0$. Let us fix $n \geq 1$ and suppose $d\bar{\mu}$ obeys Hypothesis 7.1. Then for each $k \geq 1$,*

$$\begin{aligned}
 & -\frac{n}{\pi} \int_{-2}^2 \log \left[\frac{d\bar{\mu}}{dx} \div \frac{d\bar{\mu}^{(k)}}{dx} \right] \sqrt{4-x^2} |U_{n-1}(\frac{x}{2})|^2 dx + \sum G_n(E_j) - G_n(E_j^{(k)}) \\
 & = \text{tr} \left\{ \left[2T_n(\frac{1}{2}\tilde{J}) - 2T_n(\frac{1}{2}J) \right]^2 - \left[2T_n(\frac{1}{2}\mathbf{0} \oplus \tilde{J}^{(k)}) - 2T_n(\frac{1}{2}\mathbf{0} \oplus J^{(k)}) \right]^2 \right\} \quad (33) \\
 & \quad + 4 \sum_{j=1}^k F(\tilde{a}_j \cdots \tilde{a}_{j+n-1}) + X_n - X_n^{(k)}
 \end{aligned}$$

where $\mathbf{0}$ represents the $k \times k$ zero matrix, $F(x) = x - 1 - \log(x) \geq 0$, G_n is given by (18), and X_n and $X_n^{(k)}$ are simple functions of the first few entries of J and $J^{(k)}$, respectively.

PROOF. It suffices to prove the case $k = 1$ since the general case follows by applying this successively. This case corresponds to Green’s identity with $f(z) = \log |m(z)|$ and $g(z) = G_n(z)$. Note that $m(z)$ has a pole at every eigenvalue of J and a zero at those of $J^{(1)}$. Also, $0 \leq G(x) \lesssim [|x| - 2]^{3/2}$ for $x \in \mathbb{R}$ and so by Lemma 7.2, the sum over each set of eigenvalues is absolutely convergent. \square

Because of the interlacing property of the discrete spectrum and the monotonicity of G_n , it is not necessary to assume that $d\bar{\mu}$ has the Lieb–Thirring property.

8. Necessary and Sufficient Conditions

In this section, our presentation will most closely resemble the historical development; though as previously, we will restrict detailed discussions to the Jacobi case. The primary topic is the optimal versions of the sum rules we have described—the versions with no hypotheses; the left-hand side equals the right, be they finite or infinite.

The first sum rule to reach this stage of development is that of Verblunsky [107]:

THEOREM 8.1. *The coefficients of a CMV matrix, α_k , and its spectral measure, $d\mu$, always obey*

$$\prod_{k=0}^{\infty} (1 - |\alpha_k|^2) = \exp \left\{ \int \log \left[2\pi \frac{d\mu}{d\theta} \right] \frac{d\theta}{2\pi} \right\}.$$

In particular, the right-hand side is finite if and only if $\alpha_k \in \ell^2$.

This result admits several ‘higher order’ analogues where $\frac{d\theta}{2\pi}$ is replaced by $|P(\theta)|^2 \frac{d\theta}{2\pi}$ with P a trigonometric polynomial; see [100] and [94, §2.8].

Theorem 8.1 is often referred to as Szegő’s theorem in deference to [102, 103]; see [94] for a thorough historical discussion. There is a related sum rule which goes under the name ‘strong Szegő theorem’. The definitive version of this is due to Golinskii and Ibragimov, [38, 42]:

THEOREM 8.2. *If $d\mu = \frac{1}{2\pi} e^{h(\theta)} d\theta$, then*

$$\prod_{k=0}^{\infty} (1 - |\alpha_k|^2)^{-k-1} = \exp \left\{ \sum_{n=1}^{\infty} n |\hat{h}(n)|^2 \right\}$$

and the left-hand side is infinite if $d\mu$ cannot be written in this form.

There are two more results of similar nature, although neither has a corresponding trace formula. The first is due to Baxter, [4]:

THEOREM 8.3. $\alpha_k \in \ell^1$ if and only if $d\mu = \frac{1}{2\pi} e^{h(\theta)} d\theta$ with $\hat{h} \in \ell^1$.

This can be interpreted as a statement about the Wiener algebra. As discussed by Baxter, the result extends to other algebras; see also [94].

The second result is from [67]:

THEOREM 8.4. $\limsup |\alpha_k|^{1/k} \leq R^{-1} < 1$ if and only if $d\mu = |f(e^{i\theta})|^{-2} d\theta$ with $f(z)$ an analytic function on $|z| < R$.

This result has recently been the subject of much study, including several extensions in the circle case, [2, 3, 17, 96], and also to Jacobi matrices, [15, 97]. See also the review article [98].

In the remainder of this section, we will discuss analogues of Theorem 8.1 for Jacobi matrices and Schrödinger operators; I am not aware of a corresponding result for Kreĭn systems. It would be interesting to find analogues of Theorems 8.2 and 8.3. As far as I know, the only work on this question is [79, 80], which treats Jacobi matrices. Note that as the rate of decay improves, the analysis becomes more tractable; for instance, the classical theorems of forward and inverse scattering (as used to solve KdV and the Toda lattice), [63, 106], have weighted L^1 hypotheses.

The following result is from [66]; it extends earlier results from [47] and [54]. We give a slightly different proof.

THEOREM 8.5. Fix $n \geq 1$ and write J for the Jacobi matrix with $a_j \equiv 1$ and $b_j \equiv 0$. Then $T_n(\frac{1}{2}\tilde{J}) - T_n(\frac{1}{2}J)$ is Hilbert–Schmidt if and only if the spectral measure $d\tilde{\mu}$ obeys

- (i) (Blumenthal–Weyl) $\text{supp}(d\tilde{\mu})$ is compact and $\text{ess-supp}(d\tilde{\mu}) = [-2, 2]$.
- (ii) (Normalization) $d\tilde{\mu}$ is a probability measure.
- (iii) (Lieb–Thirring Bound)

$$\sum (|\tilde{E}_j| - 2)^{3/2} < \infty \tag{34}$$

- (iv) (Quasi-Szegő Condition) Let $d\tilde{\mu}_{ac}(E) = w(E) dE$. Then

$$\int_{-2}^2 \log[w(E)] |U_{n-1}(\frac{1}{2}E)|^2 \sqrt{4 - E^2} dE > -\infty. \tag{35}$$

REMARK. When n is small, the Hilbert–Schmidt condition can be reduced to simple explicit hypotheses on the coefficients by brute force; the general case was treated in [66] by using the recurrence relation for Chebyshev polynomials. The reformed condition is

$$\begin{aligned} (u_j + u_{j+1} + \dots + u_{j+n-1}) &\in \ell^2, \quad u_j \in \ell^4, \\ (\tilde{b}_j + \tilde{b}_{j+1} + \dots + \tilde{b}_{j+n-1}) &\in \ell^2, \quad \text{and } \tilde{b}_j \in \ell^4, \end{aligned}$$

where $u_j = \tilde{a}_j^2 - 1$.

PROOF. The forward implication follows from Weyl’s theorem (on relatively compact perturbations), (27), and Theorem 6.3.

For the other direction, we use Theorem 7.4. The first observation is that LHS(33) is bounded from above as $k \rightarrow \infty$; naively, it may happen that

$$\frac{n}{\pi} \int_{-2}^2 \log \left[\frac{d\tilde{\mu}^{(k)}}{d\mu} \right] \sqrt{4 - x^2} |U_{n-1}(\frac{x}{2})|^2 dx \rightarrow -\infty$$

but by (28), this sequence cannot diverge to $+\infty$. Therefore, RHS(33) must also be bounded above as $k \rightarrow \infty$.

As $d\tilde{\mu}$ has compact support, the coefficients of \tilde{J} are uniformly bounded. The sequence \tilde{a}_j is bounded from below, for if it were not, trace-class perturbation theory would imply that $d\mu$ is purely singular, [30, 99]. In this way, the bound on RHS(33) translates into

$$\limsup_{k \rightarrow \infty} \sum_{j=1}^k \left\langle e_j \left| [T_n(\frac{1}{2}\tilde{J}) - T_n(\frac{1}{2}J)]^2 e_j \right\rangle < \infty,$$

□

which completes the proof.

An analogous result for perturbations of periodic operators can be found in [14].

The proof of Theorem 8.5 given above avoids a very interesting idea that was employed in [54, 66], namely Denisov’s extension of Rakhmanov’s theorem, [23]:

THEOREM 8.6. *Let J be a bounded Jacobi matrix, and $d\mu$ its spectral measure. If $\sigma_{\text{ess}}(J) = [-2, 2]$ and $\frac{d\mu}{dx} > 0$ a.e. there, then $a_n \rightarrow 1$ and $b_n \rightarrow 0$.*

The original theorem of Rakhmanov, [64, 71], says the following: if the spectral measure of a CMV matrix obeys $\frac{d\mu}{d\theta} > 0$ a.e. on the unit circle, then $\alpha_k \rightarrow 0$.

To obtain the Schrödinger analogue of Theorem 8.5, one must confront two new difficulties.

First, every probability measure is the spectral measure for some Jacobi matrix, but not every positive measure on \mathbb{R} is the spectral measure of a Schrödinger operator. Necessary and sufficient conditions are known, [63]; they involve the large-energy asymptotics of the spectral measure. In addition, for technical reasons, one would like a statement that guarantees the existence of an L^2_{loc} potential.

The second problem is the occurrence of the real part of m in the natural trace formula. By analogy with Theorem 8.5, one would like to have a condition on the logarithmic integrability of the Radon–Nikodym derivative of the spectral measure.

The theorem below is from [48]. But first, a few remarks about how these difficulties are overcome.

Let $d\rho$ denote the spectral measure for a half-line Schrödinger operator (or a candidate for this role) and let $d\rho_0$ denote the measure for the free ($V \equiv 0$) case. We define a signed measure $d\nu$ on $(1, \infty)$ by

$$\frac{2}{\pi} \int f(k^2)k d\nu(k) = \int f(E)[d\rho(E) - d\rho_0(E)], \quad \forall f \in C_c^\infty((1, \infty)). \quad (36)$$

Notice that $d\nu$ is parameterized by momentum, k , rather than energy, E . Using Barry’s A -function approach to the inverse problem, [36, 76, 92], it is possible to show that if $\sum [|\nu(n, n+1)|]^2$ is finite, then $d\rho$ is the spectral measure of a potential $V \in L^2_{\text{loc}}$. Using trace-formula methods, it is possible to show that this sum is finite for any $V \in L^2$.

Following the work of Burkholder, Gundy, and Silverstein, [6], it is understood that L^p bounds on the maximal function are equivalent to such bounds on the conjugate function. This is progress in our setting because it removes the spectre of cancellation. It also unifies the way one measures the size of the singular and absolutely continuous parts of $d\rho$. The specific hypothesis below makes use of a

short-range modification of the usual Hardy–Littlewood maximal function:

$$(M_s\nu)(x) = \sup_{0 < L \leq 1} \frac{|\nu|([x-L, x+L])}{2L}.$$

THEOREM 8.7. *A positive measure $d\rho$ on \mathbb{R} is the spectral measure associated to a (Dirichlet) half-line Schrödinger operator with potential $V \in L^2(\mathbb{R}^+)$ if and only if*

- (i) (Weyl) $\text{supp}(d\rho)$ is bounded from below and $\text{ess-supp}(d\rho) = [0, \infty)$.
- (ii) (Normalization)

$$\int \log \left[1 + \left(\frac{M_s\nu(k)}{k} \right)^2 \right] k^2 dk < \infty \quad (37)$$

- (iii) (Lieb–Thirring)

$$\sum_j |E_j|^{3/2} < \infty \quad (38)$$

- (iv) (Quasi-Szegő)

$$\int_0^\infty \log \left[\frac{1}{4} \frac{d\rho}{d\rho_0} + \frac{1}{2} + \frac{1}{4} \frac{d\rho_0}{d\rho} \right] \sqrt{E} dE < \infty \quad (39)$$

One consequence of this theorem is that L^2 perturbations can give rise to more or less arbitrary embedded singular spectrum. A related result was proved in [29]; indeed, this paper was a major stimulus for [47, 48]. Other results on the nature of embedded singular spectrum (not using trace formula methods) can be found in [13, 49, 74, 75] and the Denisov–Kiselev contribution to this Festschrift.

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