NECESSARY AND SUFFICIENT CONDITIONS IN THE SPECTRAL THEORY OF JACOBI MATRICES AND SCHRÖDINGER OPERATORS

DAVID DAMANIK[1], ROWAN KILLIP[2], AND BARRY SIMON[3]

Abstract. We announce three results in the theory of Jacobi matrices and Schrödinger operators. First, we give necessary and sufficient conditions for a measure to be the spectral measure of a Schrödinger operator $-\frac{d^2}{dx^2}+V(x)$ on $L^2(0,\infty)$ with $V\in L^2(0,\infty)$ and $u(0)=0$ boundary condition. Second, we give necessary and sufficient conditions on the Jacobi parameters for the associated orthogonal polynomials to have Szegő asymptotics. Finally, we provide necessary and sufficient conditions on a measure to be the spectral measure of a Jacobi matrix with exponential decay at a given rate.

1. Introduction

In this note, we want to describe some new results in the spectral and inverse spectral theory of half-line Schrödinger operators and Jacobi matrices. Given $V\in L^1_{\text{loc}}(0,\infty)$ with a mild regularity condition at infinity (ensuring limit-point case there, cf. [21]), one can define a unique selfadjoint operator which is formally

$$H=-\frac{d^2}{dx^2}+V(x) \tag{1.1}$$

with $u(0)=0$ boundary condition (see, e.g., [21]). For any $z\notin\mathbb{R}$, there is a solution $u_+(x;z)$ of $-u''+Vu=zu$ which is L^2 at infinity and unique up to a constant. The Weyl m-function is then defined by

$$m(z)=\frac{u_+'(0;z)}{u_+(0;z)} \tag{1.2}$$

Date: September 5, 2003.

[1] Mathematics 253-37, California Institute of Technology, Pasadena, CA 91125, USA. E-mail: damanik@its.caltech.edu. Supported in part by NSF grant DMS-0227289.

[2] Department of Mathematics, University of California, Los Angeles, Los Angeles, CA 90095. E-mail: killip@math.ucla.edu.

[3] Mathematics 253-37, California Institute of Technology, Pasadena, CA 91125, USA. E-mail: bsimon@caltech.edu. Supported in part by NSF grant DMS-0140592.

It obeys $\operatorname{Im} m(z) > 0$ when $\operatorname{Im} z > 0$, which implies that $\operatorname{Im} m(E + i\varepsilon)$ has a boundary value as $\varepsilon \downarrow 0$ in distributional sense:

$$d\rho(E) = \operatorname*{w-lim}_{\varepsilon \downarrow 0} \frac{1}{\pi} \operatorname{Im} m(E + i\varepsilon)\, dE \tag{1.3}$$

$d\rho$ is called the spectral measure.

In this way, each V gives rise to a spectral measure $d\rho$. In fact, the correspondence is one-to-one: Gel'fand-Levitan [11] (see also Simon [28]) found an inverse procedure to go from $d\rho$ to V.

Similarly, given a Jacobi matrix, $a_n > 0$, $b_n \in \mathbb{R}$:

$$J = \begin{pmatrix} b_1 & a_1 & 0 & 0 & \cdots \\ a_1 & b_2 & a_2 & 0 & \cdots \\ 0 & a_2 & b_3 & a_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{1.4}$$

on $\ell^2(\mathbb{Z}_+)$, we define $d\mu$ to be the measure associated to the vector δ_1 by the spectral theorem. That is,

$$m(z) \equiv \langle \delta_1, (J - z)^{-1} \delta_1 \rangle = \int \frac{d\mu(E)}{E - z} \tag{1.5}$$

In this setting, the inverse procedure dates back to Jacobi, Chebychev, Markov, and Stieltjes. It is easy to describe: By applying Gram-Schmidt to $\{1, E, E^2, \dots\}$ in $L^2(d\mu)$, we obtain the orthonormal polynomials $p_n(E)$. These obey the three-term recursion relation

$$E p_n(E) = a_{n+1} p_{n+1}(E) + b_{n+1} p_n(E) + a_n p_{n-1}(E) \tag{1.6}$$

Alternatively, one can obtain a_n, b_n from a continued fraction expansion of m ([32, 39]).

The main subject of spectral theory is to find relations between general properties of the spectral measures $d\rho$ or $d\mu$ and of the differential/difference equation parameters V and a_n, b_n. Clearly, the gems of the subject are ones that provide necessary and sufficient conditions, that is, a one-to-one correspondence between some explicit family of measures and some explicit set of parameters. In this note, we announce three such results (one involving asymptotics of orthogonal polynomials rather than the measures) whose details will appear elsewhere [20, 4, 5].

In the context of orthogonal polynomials on the unit circle [30], Verblunsky's form [38] of Szegő's theorem [34, 35, 36] is such a one-to-one correspondence between a measure and the recurrence coefficients for its orthogonal polynomials. Baxter's theorem [1, 2] and Ibragimov's theorem [18, 14] can be viewed as other examples.

Our work here is related to and motivated by the more recent result of Killip-Simon [19]:

Theorem 1.1 ([19]). *$J - J_0$ is Hilbert-Schmidt, that is*

$$\sum_{n=1}^{\infty} (a_n - 1)^2 + b_n^2 < \infty \tag{1.7}$$

if and only if the spectral measure $d\mu$ obeys

(i) (Blumenthal-Weyl) $\operatorname{supp}(d\mu) = [-2,2] \cup \{E_j^+\}_{j=1}^{N_+} \cup \{E_j^-\}_{j=1}^{N_-}$ *with* $E_1^+ > E_2^+ > \cdots > 2$ *and* $E_1^- < E_2^- < \cdots < -2$ *with* $\lim_{j\to\infty} E_j^\pm = \pm 2$ *if* $N_\pm = \infty$.

(ii) (Normalization) *μ is a probability measure.*

(iii) (Lieb-Thirring Bound)

$$\sum_{\pm,j} (|E_j^\pm| - 2)^{3/2} < \infty \tag{1.8}$$

(iv) (Quasi-Szegő Condition) *Let $d\mu_{\mathrm{ac}}(E) = f(E)\,dE$. Then*

$$\int_{-2}^{2} \log[f(E)] \sqrt{4 - E^2}\, dE > -\infty \tag{1.9}$$

Our first result is the analog of this theorem for Schrödinger operators. This is discussed in Section 2.

Our second result concerns Szegő asymptotics for orthogonal polynomials. In 1922, Szegő [37] proved that if $d\mu = f(E)\,dE$ where f is supported on $[-2,2]$ and

$$\int \log[f(E)] \frac{dE}{\sqrt{4 - E^2}} > -\infty \tag{1.10}$$

then

$$\lim_{n\to\infty} z^n p_n(z + z^{-1}) \tag{1.11}$$

exists and is nonzero (and finite) for all $z \in \mathbb{D} = \{z \in \mathbb{C} : |z| < 1\}$. There is work by Gončar [15], Nevai [23], and Nikishin [25] that allow point masses outside $[-2,2]$. The following summarizes more recent results on this subject by Peherstorfer-Yuditskii [26], Killip-Simon [19], and Simon-Zlatoš [31]:

Theorem 1.2. *Suppose $d\mu = f(E)\,dE + d\mu_{\mathrm{s}}$ with* $\operatorname{supp}(d\mu_{\mathrm{sc}}) \cup \operatorname{supp}(f) \subset [-2,2]$ *and*

$$\sum_{j,\pm} (|E_j^\pm| - 2)^{1/2} < \infty \tag{1.12}$$

Then the following are equivalent:

(i) $\inf(a_1 \ldots a_n) > 0$

(ii) *All of the following:*

(a)

$$\sum_{n=1}^{\infty} |a_n - 1|^2 + |b_n|^2 < \infty \tag{1.13}$$

(b) $\lim_{n\to\infty} a_n \dots a_1$ *exists and is finite and nonzero.*

(c) $\lim_{n\to\infty} \sum_{j=1}^{n} b_j$ *exists.*

(iii)

$$\int_{-2}^{2} \log[f(E)] \frac{dE}{\sqrt{4-E^2}} > -\infty \tag{1.14}$$

Moreover, if these hold, then the limit (1.11) *exists and is finite for all $z \in \mathbb{D}$ and is nonzero if $z + z^{-1} \notin \{E_j^{\pm}\}$.*

Because (1.12) is required a priori here, this result is not a necessary and sufficient condition with only parameter information on one side and only spectral on the other. In Section 3, we will discuss a necessary and sufficient condition for the asymptotics (1.11) to hold, thereby closing a chapter that began in 1922.

Finally, in Section 4, we discuss necessary and sufficient conditions on the measure for the a's and b's to obey

$$\limsup \left(|a_n - 1| + |b_n|\right)^{1/2n} \leq R^{-1} \tag{1.15}$$

for some $R > 1$. Namely, $d\mu$ must give specified weight to those eigenvalues E_j with $|E_j| < R + R^{-1}$ and the Jost function must admit an analytic continuation to the disk $\{z : |z| < R\}$.

The Jost function is naturally defined in terms of scattering; however, there is a simple procedure for determining it from the measure and vice versa. See (4.2).

Acknowledgment. We would like to thank Roman Romanov for drawing our attention to [9].

2. Schrödinger Operators with L^2 Potential

The proofs of the results in this section will appear in [20]. Given a measure $d\rho$ on $\mathbb{R}$, define $\tilde\sigma$ on $[0,\infty)$ by

$$\int_0^\infty g\big(\sqrt{E}\,\big)\, d\rho(E) = \int_0^\infty g(k)\, d\tilde\sigma(k) \tag{2.1}$$

that is, formally $d\tilde\sigma(k) = \chi_{(0,\infty)}(k^2)\, d\rho(k^2)$. For the Schrödinger operator with $V = 0$,

$$d\rho_0(E) = \pi^{-1}\chi_{[0,\infty)}(E)\sqrt{E}\, dE \tag{2.2}$$

and

$$d\tilde{\sigma}_0(p) = 2\pi^{-1}\chi_{[0,\infty)}(p)p^2\, dp \tag{2.3}$$

Given ρ, define $\tilde{F}$ by

$$\tilde{F}(q) = \pi^{-1/2}\int_{p\geq 1} p^{-1}e^{-(q-p)^2}[d\tilde{\sigma}(p) - d\tilde{\sigma}_0(p)] \tag{2.4}$$

Since $d\rho$ obeys

$$\int \frac{d\rho(E)}{1+E^2} < \infty$$

the integral in (2.4) is convergent.

If $d\rho$ is the spectral measure corresponding to the potential V, $d\rho$ and m are related by a Herglotz representation,

$$m(z) = c + \int \left[\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right] d\rho(\lambda)$$

The constant c is determined by the known asymptotics [13], $m(-k^2) = -k + o(1)$.

Define $M(k)$ by $M(k) = m(k^2)$. Here is our main result on L^2 potentials:

Theorem 2.1. *Let $d\rho$ be the spectral measure associated to a potential, V. Then $V \in L^2([0,\infty))$ if and only if*

(i) (Weyl) $\mathrm{supp}(d\rho) = [0,\infty) \cup \{E_j\}_{j=1}^N$ *with* $E_1 < E_2 < \cdots < 0$ *and* $\lim_j E_j = 0$ *if* $N = \infty$.

(ii) (Local Solubility)

$$\int_0^\infty |\tilde{F}(q)|^2\, dq < \infty \tag{2.5}$$

(iii) (Lieb-Thirring)

$$\sum_j |E_j|^{3/2} < \infty \tag{2.6}$$

(iv) (Quasi-Szegő)

$$\int \log\left[\frac{|M(k)+ik|^2}{4k\,\mathrm{Im}\, M(k)}\right] k^2\, dk < \infty \tag{2.7}$$

Remarks. 1. While there is a parallelism with Theorem 1.1, there are two significant differences. First, the innocuous normalization condition is replaced with (2.5) and, second, (2.7) involves M and not just μ.

2. Equation (2.5) (assuming (2.7) holds) is an expression of the fact that $d\rho$ is the spectral measure of an L^2_{loc} potential essentially because it implies (by [13]) that the A-function of [28] is in L^2_{loc}.

3. That M has a.e. boundary values is standard; compare [8, Ch. 1] or [27, Ch. 17].

4. The integrand in (2.7) is $-\log(1-|R(k)|^2)$ where R is a reflection coefficient. Weak lower semicontinuity of the negative of the entropy used in [19] is replaced by lower semicontinuity of the L^{2n} norm.

5. The key to the proof of Theorem 2.1 is a strong version of the Zaharov-Faddeev [40] sum rules; essentially following [19, 31, 29], we provide a step-by-step sum rule for $V \in L^2_{\text{loc}}$ and take suitable limits. What is interesting is that we use a whole-line, not half-line, sum rule.

We note that prior to our work, $V \in L^2 \Rightarrow$ (2.6) was proved by Gardner et al. in [10]. Bounds of this type are often called Lieb-Thirring inequalities after their work on moments of eigenvalues for $V \in L^p(\mathbb{R}^d)$; see [22]. Deift-Killip, [6], proved that $V \in L^2$ implies $f(E) > 0$ for a.e. $E > 0$. There is related work when $-\frac{d^2}{dx^2} + V \geq 0$ in Sylvester-Winebrenner [33] and Denisov [7].

3. Szegő Asymptotics

The proofs of the results in this section will appear in [4]. For the study of Szegő asymptotics, it is useful to map $\mathbb{D} = \{z : |z| < 1\}$ to $\mathbb{C}\backslash[-2,2]$ by $z \to E = z + z^{-1}$. Our main result on this issue uses the following conditions:

$$\sum_{n=1}^{\infty} |a_n - 1|^2 + |b_n|^2 < \infty \tag{3.1}$$

$$\lim_{N\to\infty} \sum_{n=1}^{N} \log(a_n) \qquad \text{exists (and is finite)} \tag{3.2}$$

$$\lim_{N\to\infty} \sum_{n=1}^{N} b_n \qquad \text{exists (and is finite)} \tag{3.3}$$

Theorem 3.1. *If for some $\varepsilon > 0$, $z^n p_n(z + z^{-1})$ converges uniformly on compact subsets of $\{z : 0 < |z| < \varepsilon\}$ to a non-zero value, then* (3.1)–(3.3) *hold.*

Conversely, if (3.1)–(3.3) *hold, then $z^n p_n(z+z^{-1})$ converges uniformly on compact subsets of $\mathbb{D}$ and has a non-zero limit for those $z \neq 0$ where $z + z^{-1}$ is not an eigenvalue of J.*

Remarks. 1. By Theorem 1.1, (3.1) implies only the quasi-Szegő condition (1.9) whereas all prior discussions of Szegő asymptotics have assumed the stronger Szegő condition (1.14). We have examples in [4] where (3.1)–(3.3) hold and $\sum(|E_n^{\pm}| - 2)^{1/2} = \infty$ which, by [31], implies that (1.14) fails, so we have examples where Szegő asymptotics hold, although the Szegő condition fails.

2. The first step in the proof is to show that for fixed $z \in \mathbb{D}$, Szegő asymptotics hold if and only if there is a solution with Jost asymptotics, that is, for which

$$\lim z^{-n} u_n(z) \tag{3.4}$$

exists and is non-zero.

3. We have two constructions of the Jost solution when (3.1)–(3.3) hold: one using the nonlocal step-by-step sum rule of [29] and the other using perturbation determinants [19]. In either case, one makes a renormalization: In the first approach, one renormalizes Blaschke products and Poisson-Fatou representations, and, in the second case, one uses renormalized determinants for Hilbert-Schmidt operators.

While these are the first results we know for Szegő/Jost asymptotics for Jacobi matrices with only L^2 conditions, Hartman [16] and Hartman-Wintner [17] (see also Eastham [9, Ch. 1]) have found Jost asymptotics for Schrödinger operators with $V \in L^2$ with conditionally convergent integral.

4. Jacobi Parameters With Exponential Decay

The proofs of the results in this section will appear in [5].

If m is given by (1.5), we define $M(z)$ by

$$M(z) = -m(z + z^{-1}) \tag{4.1}$$

Suppose $M(z)$ is the M-function of a Jacobi matrix and that $M(z)$ has an analytic continuation to a neighborhood of $\bar{\mathbb{D}}$ with the only poles in $\bar{\mathbb{D}}$ lying in $\bar{\mathbb{D}} \cap \mathbb{R}$ and all such poles are simple. Then we can define

$$u(z) = \prod_{k=1}^{N} b(z, z_k) \exp\biggl(\int \biggl(\frac{e^{i\theta} + z}{e^{i\theta} - z} \biggr) \log\biggl(\frac{\sin\theta}{\operatorname{Im} M(e^{i\theta})} \biggr) \frac{d\theta}{4\pi} \biggr) \tag{4.2}$$

where $\{z_k\}_{k=1}^{\infty}$ are the poles of M in $\mathbb{D}$. This agrees with the Jost function from scattering theory (see [19]), so we call it by this name.

Given M and the Jost function, u, suppose u is analytic in $\{z : |z| < R\}$ and z_0 is a zero of u (pole of M) with $R^{-1} < |z_0| < 1$. We say M has a canonical weight at z_0 if

$$\lim_{\substack{z \to z_0 \\ z \neq z_0}} (z - z_0) M(z) = (z_0 - z_0^{-1})[u'(z_0) u(z_0^{-1})]^{-1} \tag{4.3}$$

Theorem 4.1. *Let M be the M-function of a Jacobi matrix, J. Then $J - J_0$ is finite rank if and only if*

(i) *M is rational and has only simple poles in $\bar{\mathbb{D}}$ with all such poles in $\mathbb{R}$.*
(ii) *u is a polynomial.*
(iii) *M has canonical weight at each $z \in \mathbb{D}$ which is a pole of M.*

Theorem 4.2. *Let M be the M function of a Jacobi matrix, J. Then the parameters of J obey*

$$(|a_n - 1| + |b_n|) \leq C_\varepsilon (R^{-1} + \varepsilon)^{2n}$$

for some $R > 1$ and all $\varepsilon > 0$ if and only if
(i) *M is meromorphic on $\{z : |z| < R\}$ with only simple poles inside $\bar{\mathbb{D}}$ with all such poles in $\mathbb{R}$.*
(ii) *u is analytic in $\{z : |z| < R\}$.*
(iii) *M has canonical weight at each pole of M, $z_0 \in \mathbb{D}$, with $R^{-1} < |z_0| < 1$.*

Given u and not m, there is a normalization issue, so it is easier to discuss the perturbation determinant [19] which obeys

$$L(z) = \frac{u(z)}{u(0)} = \left(\prod_{n=1}^{\infty} a_n \right) u(z) \tag{4.4}$$

Theorem 4.3. *Let L be a polynomial with $L(0) = 1$. Then L is a perturbation determinant of a Jacobi matrix, J, with $J - J_0$ finite rank if and only if*
(1) *$L(z)$ is real if $z \in \mathbb{R}$.*
(2) *The only zeros of L in $\bar{\mathbb{D}}$ lie on $\bar{\mathbb{D}} \cap \mathbb{R}$ and are simple.*
In that case, there is a unique J with $J - J_0$ finite rank, so L is its perturbation determinant.

Remarks. 1. While there is a unique J with $J - J_0$ finite rank, if L has k zeros in $\mathbb{D}$, there is a k-parameter family of other J's with L as their perturbation determinant (each such J has $|a_n - 1| + |b_n|$ decaying exponentially, but only one has $J - J_0$ finite rank).

2. There is an analog of Theorem 4.3 if L is only analytic in $\{z : |z| < R\}$.

3. The proofs of these results depend on analyzing the map $(u, M) \to (u^{(1)}, M^{(1)})$ where $u^{(1)}, M^{(1)}$ are the Jost function and M-function for $J^{(1)}$, the Jacobi matrix with the top row and leftmost column removed. We control $|||u^{(1)}|||$ in terms of $|||u|||$ where

$$|||u|||^2 = \int |u(R_1 e^{i\theta}) - u(0)|^2 \, \frac{d\theta}{2\pi}$$

with $R_1 < R$, and are thereby able to show $|||u^{(n)}|||$ goes to zero exponentially.

While we are aware of no prior work on the direct subject of this section, we note that Nevai-Totik [24] solved the analogous problem for orthogonal polynomials on the unit circle, that Geronimo [12] has related results for Jacobi matrices (but only under an a priori hypothesis on M), and that there are related results in the Schrödinger operator literature (see, e.g., Chadan-Sabatier [3]).

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