SPECTRAL ANALYSIS OF RANK ONE PERTURBATIONS AND APPLICATIONS

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Abstract. A review of the general theory of self-adjoint operators of the form $A + \alpha B$ where B is rank one is presented. Applications include proofs of localization for Schrödinger operators, results on inverse spectral theory, and examples of operators with singular continuous spectrum.

Lecture given at the Vancouver Summer School in Mathematical Physics, August 10–14, 1993. This material is based upon work supported by the U.S. National Science Foundation under Grant No. DMS-9101715. The Government has certain rights in this material.

Typeset by $\mathcal{A}\mathcal{M}\mathcal{S}$-TEX

CHAPTER I

INTRODUCTION, BOREL TRANSFORMS, THE KREIN SPECTRAL SHIFT, AND ALL THAT

I.0 Introduction

Our goal here is to review the spectral theory (with applications) of rank one perturbations of positive self-adjoint operators on a separable complex Hilbert space, $\mathcal{H}$:

$$A_\alpha = A + \alpha B \qquad B = (\varphi, \cdot)\varphi. \tag{I.1}$$

The cynic might feel that I have finally sunk to my proper level. I started with quantum field theory, analysis in infinitely many variables. That was too hard so I switched to the N-body Schrödinger equation; but that was too hard so I switched to one-body, then one-dimensional, then discrete one-dimensional. Finally to rank one perturbations—maybe something so easy that I can say something useful! Alas, we'll see even this is hard and exceedingly rich.

I should warn you that (I.1) is somewhat more general than you might think. First, I'll bet you thought that φ was a unit vector. It need not be. Big deal, you think—normalize φ and renormalize α. But φ need not be a normalizable vector. We'll consider B's which are rank one but only form bounded perturbations of A. In one fell swoop, we've absorbed the theory of variation of boundary conditions for Sturm-Liouville problems on a half-line!

Moreover, as I'll discuss in §I.5, α may be infinite.

In some ways, my recent relationship with rank one perturbations reminds me of my relationship with trace ideals fifteen years ago. Then it turned out three distinct problems: Yukawa field theories, scattering theory, and semi-classical bounds on the number of bound states led me to similar mathematics, viz estimates on the trace ideal properties of certain pseudo-differential operators.

This past year, three distinct research projects:

(1) my work, in part with del Rio, Jitomirskaya, and Makarov, on singular spectrum;
(2) my trying to understand the work of Aizenman and Molchanov;
(3) my work with Gesztesy on trace formulas

all led to rank one perturbations and enriched my own knowledge of the subject. (1)–(3) are the themes of Chapters II–IV of these notes.

In this chapter I'll discuss the general theory in a new systematic way; many of the ideas were developed in discussions with Fritz Gesztesy, to whom I am grateful.

A key role will be played by

$$F_\alpha(z) = (\varphi, (A_\alpha - z)^{-1}\varphi). \tag{I.2}$$

In terms of a suitable spectral measure $d\mu_\alpha$:

$$F_\alpha(z) = \int \frac{d\mu_\alpha(\lambda)}{\lambda - z} \tag{I.3}$$

so we'll begin with an exhaustive study of the Borel transform of a measure and its relation to the measure in §I.1. That section and §I.2 are the technical core behind most of what follows.

I.1 Borel Transforms of Measures

Throughout, we let $d\mu$ be a (positive) measure on $[a, \infty)$ for some $a > -\infty$ with

$$\int \frac{d\mu(\lambda)}{|\lambda| + 1} < \infty. \tag{I.4}$$

REMARKS. 1. We'll suppose that $\mathrm{supp}(\mu)$ is bounded from below and the operator A in (I.1) is positive. Much of our theory works without those restrictions but the details are a little simpler with them and they hold in the applications I want to make, so I've made them.

2. For some results when one only knows that $\int \frac{d\mu(\lambda)}{1+\lambda^2} < \infty$, see Aronszajn-Donoghue [4].

When I.4 holds, we can define for $z \in \mathbb{C}\backslash(-\infty, a)$:

$$F(z) = \int \frac{d\mu(\lambda)}{\lambda - z} \tag{I.5}$$

the *Borel transform* of μ (also called the Stieltjes transform or the Borel-Stieltjes transform). The key issues concern boundary values of F as $z = x + i\epsilon \downarrow x \in \mathrm{supp}(d\mu)$. We begin with the simple stuff away from $\mathrm{supp}(d\mu)$.

THEOREM I.1. (i) *F is an anlytic function on $\mathbb{C}\backslash(a, \infty)$.*
(ii) *F is positive on $(-\infty, a)$ and* $\mathrm{Im}\ F > 0$ *if* $\mathrm{Im}\ z > 0$.
(iii) $\lim_{\gamma\to\infty} F(-\gamma) = 0$.
(iv) $\lim_{\gamma\to\infty} F(-\gamma)(\gamma) = \int d\mu(\lambda)$ *where $\int d\mu = \infty$ is allowed. Similarly,*

$$\lim_{\gamma\to\infty} F'(-\gamma)(\gamma)^2 = \int d\mu(\lambda).$$

(v) $\lim_{\gamma\to\infty} F'(-\gamma)/F^2(-\gamma) = (\int d\mu(\lambda))^{-1}$ *where $\int d\mu = \infty$ is allowed with $\infty^{-1} = 0$.*

PROOF. (i) and (ii) are elementary. (iii) uses:

$$\text{Im } F(x+i\beta) = \int \frac{\beta}{(x-y)^2+\beta^2}\, d\mu(y). \tag{I.6}$$

(iii) and (iv) follow from the monotone convergence theorem. Actually, by a slightly more involved argument if $|z| \to \infty$ with $|\arg(-z)| < \epsilon$ with $\epsilon > 0$ and small, it is not hard to see that $(-z)F(z) \to \int d\mu$.

If $\int d\mu < \infty$, a similar use of the monotone convergence theorem shows that

$$\gamma^2 F'(-\gamma) = \gamma^2 \int \frac{d\mu(\lambda)}{(\lambda+\gamma)^2} \longrightarrow \int d\mu(\lambda)$$

and (iv) follows. If $\int d\mu = \infty$, we use the fact that $|1/[zF(z)]| \to 0$ as $|z| \to \infty$ with Re $z < 0$. Thus, writing

$$\left(\frac{1}{F}\right)'(z) = (2\pi i)^{-1} \int\limits_{|w-z|=|z|/2} (w-z)^{-2} \frac{1}{F(w)}\, dw$$

we see that $(\frac{1}{F})' \to 0$ but $(\frac{1}{F})' = -\frac{F'}{F^2}$ implying (v). $\square$

Next we talk about boundary values of F. The function

$$G(x) = \int \frac{d\mu(y)}{(x-y)^2}$$

which is defined for $x \in (-\infty, \infty)$ and takes values in $(0, \infty]$ (note ∞ is allowed), will play an important role.

THEOREM I.2. (i) $G(x) < \infty$ *implies that*

$$\int \frac{d\mu(y)}{|x-y|} < \infty. \tag{I.7}$$

(ii) [12,27] $\{x \mid G(x) = \infty\}$ *is a dense* G_δ *in* $\operatorname{supp}(d\mu)$.

(iii) *If* (1.7) *holds, and, in particular if* $G(x) < \infty$, *then* $\lim_{\epsilon \downarrow 0} F(x+i\epsilon)$ *exists and is real.*

(iv) $\lim_{\epsilon \downarrow 0} \epsilon^{-1} \text{Im } F(x+i\epsilon) \to G(x)$.

(v) *If* $G(x) < \infty$, *then* $\lim_{\epsilon \downarrow 0} (i\epsilon)^{-1}[F(x+i\epsilon) - F(x+i0)] = G(x)$.

REMARK. A G_δ is a countable intersection of open sets.

PROOF. (i) is immediate if one notes that

$$\frac{1}{|x-y|} \le \frac{1}{|x-y|^2} + \frac{|x|+2}{|y|+1}$$

since

$$|y| + 1 \le |x| + |x-y| + 1 \le (|x-y|)(|x|+2)$$

if $|x-y| \geq 1$.

(ii) By the lemma below, if $\mu([0,1]) \geq 1$, there is an $x_0 \in [0,1]$ with $\int \frac{d\mu(y)}{|x_0-y|} = \infty$. So, by scaling, if $\mu([a,b]) > 0$, there is an $x_0 \in [a,b]$ with $\int \frac{d\mu(y)}{|x_0-y|} = \infty$. It follows that if $a_0 \in \operatorname{supp}(d\mu)$, then there exists $a_n \to a_0$ with $\int \frac{d\mu(y)}{|a_n-y|} = \infty$. So, by (i), $\{x \mid G(x) = \infty\}$ is dense in $\operatorname{supp}(d\mu)$. It is a G_δ because if we define $G_n(x) = \int (|x-y|^2 + n^{-1})^{-1}\, d\mu(y)$, then G_n is continuous and

$$\{x \mid G(x) = \infty\} = \bigcap_m \bigcup_n \{x \mid G_n(x) > m\}.$$

(iii) By (I.6), for any δ

$$\operatorname{Im} F(x+i\beta) \leq \beta \int_{|x-y|>\delta} |x-y|^{-2}\, d\mu(y) + \int_{|x-y|\leq\delta} |x-y|^{-1}\, d\mu(y)$$

so

$$\varlimsup_{\beta\downarrow 0} \operatorname{Im} F(x+i\beta) \leq \varlimsup_{\delta\downarrow 0} \int_{|x-y|\leq\delta} |x-y|^{-1}\, d\mu(y) = 0$$

if (I.7) holds. (I.7) also implies

$$\lim_{\beta\downarrow 0} \operatorname{Re} F(x+i\beta) = \int (y-x)^{-1}\, d\mu(y)$$

by the dominated convergence theorem.

(iv) follows from (I.6) and the monotone convergence theorem.

(v) If $G(x) < \infty$, then, by the proof of (iii)

$$F(x+i0) = \int \frac{d\mu(y)}{y-x}$$

so

$$(i\epsilon)^{-1}[F(x+i\epsilon) - F(x-i0)] = \int \frac{d\mu(y)}{(y-x)(y-x-i\epsilon)} \to G(x)$$

by the dominated convergence theorem if $G(x) < \infty$. $\square$

Lemma 1.3. *Let $\mu([0,1]) \geq 1$. Then, there exists $x_0 \in [0,1]$ with $\int \frac{d\mu(y)}{|x_0-y|} = \infty$.*

Proof. Define I_n inductively as follows. Let I_1 be one of $[0,\frac{1}{2}], [\frac{1}{2},1]$ with $\mu(I_1) \geq \frac{1}{2}$. Now subdivide I_1 in half and choose I_2 to be one of those halves with $\mu(I_2) \geq \frac{1}{4}$. By induction

$$I_1 \supset I_2 \supset \cdots \quad \text{all closed;} \quad \mu(I_n) \geq 2^{-n}; \quad |I_n| = 2^{-n}.$$

By compactness, $\cap I_n = \{x_0\}$ for some x_0. Obviously

$$\int_{I_n} |x-x_0|^{-1}\, d\mu(x) \geq (2^{-n})^{-1} 2^{-n} = 1.$$

But if $\int |x-x_0|^{-1}\, d\mu(x) < \infty$, $\int_{I_n} |x-x_0|^{-1}\, d\mu(x) \downarrow 0$ by monotone convergence, so we must have $\int |x-x_0|^{-1}\, d\mu(x) = \infty$. $\square$

THEOREM I.4. *$\lim_{\beta\downarrow 0} F(x+i\beta)$ exists and is finite for a.e. x.*

PROOF. This is a standard harmonic analysis result on non-tangential boundary values of analytic maps, see [31], so we'll only sketch the details. Let $g(z) = \frac{z-i}{z+i}$, the fractional linear map of the upper half plane to the unit disc. Thus $\tilde{F} = g \circ F \circ g^{-1}$ is a map of the unit disc to itself. Such maps have boundary values by a standard maximal function argument, see Katznelson [31]. By the same argument as in the next theorem, $\{\theta \mid \lim_{r\uparrow 1} \tilde{F}(re^{i\theta}) = -1\}$ has measure zero, so $\lim_{\beta\downarrow 0} F(x+i\beta) = \infty$ on a set of measure 0 and so F is finite a.e. $\square$

THEOREM I.5. *Let F_1, F_2 be the Borel transforms of two (positive) measures (one may be zero) and fix $\alpha \in \mathbb{C}$. Then*

$$|\{x \mid F_1(x+i0) - F_2(x+i0) = \alpha\}| > 0$$

only if $\alpha = 0$ and $F_1 = F_2$.

PROOF. Let g be defined as in the proof of Theorem I.4 and let

$$h = e^{iF_1 \circ g^{-1}} - (e^{iF_2 \circ g^{-1}})e^{i\alpha}.$$

h is a bounded analytic function on the disc and the theorem asserts that under $h \not\equiv 0$, $\{\theta \mid \lim_{r\uparrow 1} h(re^{i\theta}) = 0\}$ has Lebesgue measure zero. This is a standard theorem; see Katznelson [31]. $\square$

Let $d\mu_{\text{ac}}, d\mu_{\text{sc}}, d\mu_{\text{pp}}$ be the absolutely continuous, singular continuous and pure point parts of a measure $d\mu$. Let $d\mu_{\text{sing}} = d\mu_{\text{sc}} + d\mu_{\text{pp}}$.

The main theorem on Borel transforms is

THEOREM I.6. *Let $F(z)$ be the Borel transform of a measure $d\mu$ obeying* (I.4). *Then*

(i) *$\pi^{-1}\,\text{Im}\; F(E+i\epsilon)dE \to d\mu$ weakly in the sense that*

$$\int \pi^{-1} f(E)\,\text{Im}\; F(E+i\epsilon)\,dE \longrightarrow \int f(E)\,d\mu(E) \tag{I.8}$$

for all continuous functions, f, of compact support.

(ii) *μ_{sing} is supported on $\{E \mid \lim_{\epsilon\downarrow 0} \text{Im}\; F(E+i0) = \infty\}$.*

(iii) *$\mu(\{E_0\}) = \lim_{\epsilon\downarrow 0} \epsilon\; \text{Im}\; F(E_0+i\epsilon)$. Moreover, for any $E_0 \in \mathbb{R}$:*

$$\lim_{\epsilon\downarrow 0} \epsilon\; \text{Re}\; F(E_0+i0) = 0.$$

(iv) *$d\mu_{\text{ac}}(E) = \pi^{-1}\,\text{Im}\; F(E+i0)\,dE$.*

PROOF. (i) It is a well-known calculation that for f, continuous of compact support:

$$\lim_{\epsilon\downarrow 0} \frac{1}{\pi} \int f(E') \frac{\epsilon}{(E-E')^2+\epsilon^2}\,dE' \to f(E).$$

This and the dominated convergence theorem easily imply the result.

(ii) We will prove the weaker fact that μ_{sing} is supported on $\{E \mid \overline{\lim}\ \text{Im}\ F(E + i2^{-n}) = \infty\}$. The stronger fact (theorem of de Vallée Poussin) can be found in Saks ([40]), but for most applications, this weaker fact suffices. Since the stronger result is true and more elegant, we'll use it. For the theorem of Aronszajn on mutual singularity (Theorem II.2(iv)), one does need the stronger fact.

We will prove that for any a

$$\big\{E \mid \sup_n \text{Im}\ F(E + i2^{-n}) \leq a\big\} = A_a$$

has μ_{sing}-measure 0 from which the result follows. Notice that

$$\begin{aligned}\text{Im}\ F(x + i\epsilon) &= \int \frac{\epsilon}{(x-y)^2 + \epsilon^2}\, d\mu(y) \\ &\geq \frac{1}{2\epsilon} \int\limits_{|x-y| \leq \epsilon} d\mu(y).\end{aligned}$$

So for fixed $x \in A_a$

$$\sup_n 2^n \mu\left([x - 2^{-n}, x + 2^{-n}]\right) \leq 2a$$

and so, since any $2^n \leq \epsilon^{-1} \leq 2^{n+1}$ for some n

$$\sup_n \epsilon^{-1} \mu\left([x - \epsilon, x + \epsilon]\right) \leq 4a$$

and thus looking at the two subintervals:

$$\sup_{x \in [\alpha,\beta]} |\beta - \alpha|^{-1} \mu([\alpha, \beta]) \leq 8a.$$

By regularity of measures, for any ϵ, we can find a closed set C and open O with $C \subset O$, so $\mu_{\text{sing}}(\mathbb{R} \backslash C) \leq \epsilon$ and $|O| \leq \epsilon$. We write $O = \bigcup\limits_{n=1}^{\infty} (\alpha_n, \beta_n)$ as a disjoint union of intervals (union of connected components). Then

$$\begin{aligned}\mu_{\text{sing}}(C \cap A_a) &\leq \mu_{\text{sing}}\Bigg(\bigcup_{\{n \mid (\alpha_n, \beta_n) \cap A_a \neq \emptyset\}} (\alpha_n, \beta_n)\Bigg) \\ &\leq \sum_{\{n \mid (\alpha_n, \beta_n) \cap A_a \neq \emptyset\}} \mu(\alpha_n, \beta_n) \\ &\leq 8a \sum_n |\beta_n - \alpha_n| = 8a|O| \leq 8a\epsilon\end{aligned}$$

so

$$\mu_{\text{sing}}(A_a) \leq \mu_{\text{sing}}(C \cap A_a) + \mu_{\text{sing}}(\mathbb{R} \backslash C) \leq \epsilon + 8a\epsilon.$$

Since ϵ is arbitrary, $\mu_{\text{sing}}(A_a) = 0$ as was to be proven.

(iii) The first part is a trivial consequence of the monotone convergence theorem, if we note that $\frac{\epsilon^2}{x^2+\epsilon^2}$ converges monotonically to 0 (resp. 1) if $x \neq 0$, (resp. $x = 0$). For the second:

$$\epsilon \int\limits_{|x-y|\geq 1} \frac{|x-y|}{|x-y|^2+\epsilon^2}\, d\mu(y) \leq \epsilon \int\limits_{|x-y|\geq 1} \frac{1}{|x-y|}\, d\mu(y) \longrightarrow 0$$

while

$$\lim_{\epsilon\downarrow 0} \int\limits_{|x-y|<1} \frac{\epsilon|x-y|}{(x-y)^2+\epsilon^2}\, d\mu(y) = 0$$

by the dominated convergence theorem since $\alpha\beta/(\alpha^2+\beta^2) \leq \frac{1}{2}$.

(iv) Write $d\mu_{\mathrm{ac}}(E) = h(E)\, dE$ and let $F_{\mathrm{ac}}(z)$ be the Borel transform of $d\mu_{\mathrm{ac}}$. By the Lebesgue theorem on the derivatives of the integral (that says if $h \in L^1$, for a.e. x, $h(x) = \lim\limits_{a\to 0}(2a)^{-1} \int\limits_{x-a}^{x+a} h(y)\, dy$; see Katznelson [31]), one sees that $\frac{1}{\pi}$ Im $F_{\mathrm{ac}}(E+i0) = h(E)$ for a.e. E. By Fatou's lemma, for $f \geq 0$ and continuous:

$$\begin{aligned}\pi^{-1} \int [\mathrm{Im}\ F(E+i0)] f(E)\, dE &\leq \underline{\lim}\, \pi^{-1} \int \mathrm{Im}\ F(E+i\epsilon) f(E)\, dE \\ &= \int f(E)\, d\mu(E).\end{aligned}$$

Thus $\pi^{-1}\mathrm{Im}\ F(E+i0)\, dE \leq d\mu$ and so for a.e. E:

$$\frac{1}{\pi}\ \mathrm{Im}\ F(E+i0) \leq h(E) = \frac{1}{\pi}\ \mathrm{Im}\ F_{\mathrm{ac}}(E+i0) \leq \frac{1}{\pi}\ \mathrm{Im}\ F(E+i0)$$

since $d\mu \geq d\mu_{\mathrm{ac}}$ implies Im $F \geq$ Im F_{ac}. Thus

$$h(E) = \frac{1}{\pi}\ \mathrm{Im}\ F(E+i0)$$

as was to be proven. $\square$

I.2 Rank One Perturbations: The Set-Up and Basic Formulas

Let $A \geq 0$ be a possibly unbounded self-adjoint operator on a Hilbert space $\mathcal{H}$. One defines the scale of spaces $\mathcal{H}_s(A)$ associated to A as follows. For $s \geq 0$, $\mathcal{H}_s(A)$ is $D(A^{s/2})$ with the norm

$$\|\varphi\|_s = \|(A+1)^{s/2}\varphi\| \tag{I.9}$$

in which $\mathcal{H}_s$ is easily seen to be complete. For $s < 0$, take $\mathcal{H}$ with the norm given by (I.9) and complete it. In a natural way, $\mathcal{H}_s$ and $\mathcal{H}_{-s}$ are duals in such a way that $\varphi \in \mathcal{H}$ is associated to the functional on $\mathcal{H}_s$ given by $\ell_\varphi(\eta) = (\varphi, \eta)$, so $|\ell_\varphi(\eta)| \leq \|\varphi\|_{-s}\|\eta\|_s$ and $\mathcal{H}_s \subset \mathcal{H}_t$ if $s > t$.

$(A+1)^{-t/2}$ is an isometry from $\mathcal{H}_s$ to $\mathcal{H}_{s+t}$ so for $s > 0$, if Δ is a bounded subset of $\mathbb{R}$, $E_\Delta(A)$, the spectral projection of A, maps $\mathcal{H}_{-s}$ to $\mathcal{H}_s$ since $(A+1)^{+s/2}E_0(A)(A+1)^{s/2}$ is bounded. In particular, we can define a spectral measure $d\mu_A^\varphi$ for any $\varphi \in \mathcal{H}_{-s}(A)$ by

$$\mu_A^\varphi(\Delta) = (\varphi, E_\Delta(A)\varphi).$$

It is easy to see that

$$\int \frac{d\mu_A^\varphi(x)}{(|x|+1)^s} < \infty \tag{I.10}$$

and, in particular, the spectral measures of $\varphi \in \mathcal{H}_{-1}(A)$ have Borel transforms.

Now let $\varphi \in \mathcal{H}_{-1}(A)$ and let b be the quadratic form on $\mathcal{H}_{+1}(A)$ given by

$$b_\varphi(\eta, \eta') = \overline{\ell_\varphi(\eta)}\,\ell_\varphi(\eta').$$

b_φ is positive but if $\varphi \notin \mathcal{H}$, it is neither closed nor closable.

See [30,38] for discussion of forms and their perturbation theory.

PROPOSITION I.7. *For any φ, b_φ is a form bounded perturbation of A with relative bound zero.*

PROOF. Given ϵ, find $\varphi_\epsilon \in \mathcal{H}_{-1}(A)$ so $\|\varphi_\epsilon\|_{-1}^2 \leq \frac{1}{2}\epsilon$ and $\psi_\epsilon \equiv \varphi - \varphi_\epsilon \in \mathcal{H}$. Then

$$\begin{aligned} b_\varphi &= b_{\varphi_\epsilon + \psi_\epsilon} \leq b_{\varphi_\epsilon + \psi_\epsilon} + b_{\varphi_\epsilon - \psi_\epsilon} \\ &= 2b_{\varphi_\epsilon} + 2b_{\psi_\epsilon}. \end{aligned}$$

So, for any $\eta \in \mathcal{H}_{+1}(A)$

$$\begin{aligned} b_\varphi(\eta, \eta) &\leq 2\|\varphi_\epsilon\|_{-1}^2\|\eta\|_{+1}^2 + 2\|\psi_\epsilon\|^2\|\eta\|^2 \\ &\leq \epsilon(\eta, A\eta) + (2\|\psi_\epsilon\|^2 + \epsilon)\|\eta\|^2 \end{aligned}$$

as was to be proven. $\square$

The perturbation theory of forms [30,38] thus implies that for any $\alpha \in \mathbb{R}$, $A + \alpha b$ is the quadratic form of a self- adjoint operator A_α with $\mathcal{H}_s(A_\alpha) = \mathcal{H}_s(A)$ if $|s| \leq 1$. We will write

$$A_\alpha = A + \alpha B = A + \alpha(\varphi, \cdot)\varphi \tag{I.11}$$

although there is no operator B or vector φ in the usual sense if $\varphi \notin \mathcal{H}$. We will occasionally write $\|\varphi\|^2$ which may be infinite if $\varphi \notin \mathcal{H}$.

Since $\mathcal{H}_{-1}(A_\alpha) = \mathcal{H}_{-1}(A)$ and so $(A_\alpha - z)^{-1}\varphi \in \mathcal{H}_{+1}(A_\alpha) = \mathcal{H}_{+1}(A) \subset \mathcal{H}$. The strong resolvent formula holds, viz

$$(A_\alpha - z)^{-1} - (A - z)^{-1} = -\alpha((A_\alpha - \bar{z})^{-1}\varphi, \cdot)(A - z)^{-1}\varphi. \tag{I.12}$$

Don't blink now because in just about one page we're going to present four of the five critical formulas in the subject (the fifth is (I.17) below).

Define

$$F_\alpha(z) = (\varphi, (A_\alpha - z)^{-1}\varphi) \equiv \int \frac{d\mu_\alpha(x)}{x - z}$$

where $d\mu_\alpha \equiv d\mu^\varphi_{A_\alpha}$ is the spectral measure for φ which has a Borel transform by (I.10) and $\mathcal{H}_{-1}(A_\alpha) = \mathcal{H}_{-1}(A)$. We define $F(z) \equiv F_{\alpha=0}(z)$.

Taking matrix elements of (I.12) with φ on both sides, we get $F_\alpha(z) - F(z) = -\alpha F_\alpha(z)$
$F(z)$, or solving for F_α, we get the Aronszajn-Krein formula:

$$F_\alpha(z) = \frac{F(z)}{1 + \alpha F(z)}, \tag{I.13}$$

the first critical formula. Applying (I.12) to φ and using (I.13) to see that $1 - \alpha F_\alpha = [1 + \alpha F(z)]^{-1}$, we get the second key formula:

$$(A_\alpha - z)^{-1}\varphi = (1 + \alpha F(z))^{-1}(A - z)^{-1}\varphi. \tag{I.14}$$

Plugging this into (I.12) we get the third key formula:

$$(A_\alpha - z)^{-1} = (A - z)^{-1} - \frac{\alpha}{1 + \alpha F(z)}((A - \bar{z})^{-1}\varphi, \cdot)(A - z)^{-1}\varphi. \tag{I.15}$$

Notice that I.14 says for η, z fixed, $(\eta, (A_\alpha - z)^{-1}\varphi) = a/(\alpha + b)$, the key to the Aizenman-Molchanov theory.

For the final formula, (I.12) says that $(A_\alpha - z)^{-1} - (A - z)^{-1}$ is rank one, so trace class, and by (I.15) we have

$$\operatorname{Tr}\left[(A - z)^{-1} - (A_\alpha - z)^{-1}\right] = \frac{\alpha}{1 + \alpha F(z)}(\varphi, (A - z)^{-2}\varphi).$$

Notice that $(\varphi, (A - z)^{-2}\varphi) = \frac{d}{dz}F(z)$. Thus, we have what I'll call the trace formula, the key to our discussion of the Krein spectral shift in §I.4 below:

$$\operatorname{Tr}\left[(A - z)^{-1} - (A_\alpha - z)^{-1}\right] = \frac{d}{dz}\ln(1 + \alpha F(z)) \tag{I.16}$$

where we take the branch of the log which is positive for z real and very negative (recall by Theorem I.1 (iii), that even for $\alpha < 0$, $1 + \alpha F(z) > 0$ for z real and very negative).

I.3 The Integral Formula

The critical last formula of the general theory is

THEOREM I.8.
$$\int_{-\infty}^{\infty} [d\mu_\alpha(E)]\, d\alpha = dE \tag{I.17}$$
in the sense that if f is in $L^1(\mathbb{R}, dE)$, then $f \in L^1(\mathbb{R}, d\mu_\alpha)$ for a.e. α, $\int f(E)\, d\mu_\alpha(E)$ $\in L^1(\mathbb{R}, d\alpha)$ and
$$\int \left(\int f(E)\, d\mu_\alpha(E) \right) d\alpha = \int f(E)\, dE. \tag{I.18}$$

PROOF. By an elementary argument, it suffices to prove this result for $f_z(E) = (E - z)^{-1} - (E + i)^{-1}$ for any $z \in \mathbb{C}\backslash\mathbb{R}$ (use analyticity in z and then Stone-Weierstrass approximation). By closing the contour in the upper half plane

$$\begin{aligned} \int_{-\infty}^{\infty} f_z(E)\, dE &= 0 \qquad \text{if } \operatorname{Im} z < 0 \\ &= 2\pi i \qquad \text{if } \operatorname{Im} z > 0. \end{aligned}$$

On the other hand, by (I.13)

$$\begin{aligned} \int f_z(E)\, d\mu_\alpha(E) = F_\alpha(z) - F_\alpha(-i) &= \frac{1}{\alpha + F(z)^{-1}} - \frac{1}{\alpha + F(-i)^{-1}} \\ &\equiv h_z(\alpha). \end{aligned}$$

Now, if $\pm\operatorname{Im} z > 0$, then $\pm\operatorname{Im} F(z) > 0$ so $\pm\operatorname{Im} F(z)^{-1} < 0$. Thus, $h_z(\alpha)$ has either two poles in the lower half plane if $\operatorname{Im} z < 0$ or one in each half plane if $\operatorname{Im} z > 0$. The same contour integral as for E (but now for α!) implies that

$$\begin{aligned} \int_{-\infty}^{\infty} d\alpha\, h_z(\alpha) &= 0 \qquad \text{if } \operatorname{Im} z < 0 \\ &\equiv 2\pi i \qquad \text{if } \operatorname{Im} z > 0 \end{aligned}$$

so I.18 is proven for $f_z(E)$. $\square$

The above implies a regularity result for the density of states in n-dimensional Jacobi matrices (see Theorem I.19 below) due to Wegner [49]. Wegner proved his result by tracking eigenvalues in finite-dimensional approximations, but his underlying result is similar to (I.17) so this is sometimes called a Wegner estimate. The Russian literature, however, has similar results much earlier in the case of boundary condition dependence; see Javrjan [28].

I.4 The Krein Spectral Shift

In this section, we make a presentation of the Krein spectral shift [33] due to Gesztesy and me. By the general theory of Borel transforms, $F(z)$ has a boundary value $F(\lambda + i0)$ for a.e. λ in $\mathbb{R}$. Moreover, by Theorem I.5, if α is fixed, $F(\lambda + i0) \neq -\alpha^{-1}$ for a.e. α. Thus we can define $\text{Arg}(1 + \alpha F(\lambda + i0))$ for a.e. λ. Since $\text{Im } F(\lambda + i0) \geq 0$, if $\alpha > 0$ (resp. $\alpha < 0$), this arg lies in $[0, \pi]$ (resp. $[-\pi, 0]$). If $1 + \alpha F(\lambda + i0) \in (-\infty, 0)$ that sets the argument to $(\text{sgn } \alpha)\pi$.

Definition. The Krein spectral shift, $\xi_\alpha(\lambda)$, is defined by

$$\xi_\alpha(\lambda) = \frac{1}{\pi} \text{ Arg}(1 + \alpha F(\lambda + i0)).$$

Definition. $i(\alpha) \equiv \min(\inf \ \text{spec}(A), \inf \ \text{spec}(A_\alpha))$.

Theorem I.9. (i) $0 \leq \pm\xi_\alpha(\lambda) \leq 1$ *if* $\pm\alpha > 0$; $\xi_\alpha(\lambda) = 0$ *if* $\lambda < i(\alpha)$.
(ii)

$$\text{Tr}((A - z)^{-1} - (A_\alpha - z)^{-1}) = \int (\lambda - z)^{-2} \xi_\alpha(\lambda) \, d\lambda \tag{I.19}$$

if $z \in \mathbb{C} \backslash [i(\alpha), \infty)$.
(iii) *If* $\|\varphi\| < \infty$, *then* $\xi_\alpha \in L^1$ *and*

$$\int \xi_\alpha(\lambda) \, d\lambda = \alpha \|\varphi\|^2. \tag{I.20}$$

Proof. (i) The first part follows from the discussion above. If $\alpha > 0$, $i(\alpha) = \inf \ \text{spec}(A)$ and $F(\lambda + i0) > 0$ for $\lambda < i(\alpha)$ so $\xi_\alpha(\lambda) = 0$. If $\alpha < 0$, $i(\alpha)$ is either $\inf \ \text{spec}(A)$ or the unique $\lambda < i(\alpha)$ with $1 + \alpha F(\lambda) = 0$. Either way, since $F(\lambda)$ is monotone increasing on $(-\infty, i(0))$, below $i(\alpha)$, we have that $1 + \alpha F(\lambda) > 0$.

(ii) Let $H_\alpha(z) = \ln(1 + \alpha F(z))$ on $(-\infty, i(\alpha))$ analytically continued to $\mathbb{C} \backslash [i(\alpha), \infty)$.Consider a contour, C, which goes from $i(\alpha)$ just above the real axis to R, then directly up to $R + iR$, then on a circle of radius $R\sqrt{2}$ to $R - iR$, then up to just above the real axis, then along the bottom of the real axis to $i(\alpha)$. Consider for $z_0 \in (-\infty, i(\alpha))$:

$$\frac{1}{2\pi i} \oint_C \frac{H_\alpha(z)}{(z - z_0)^2} \, dz \equiv I_\alpha(z_0).$$

By Cauchy's formula, once $R\sqrt{2} > |z_0|$, the integral is just dH_α/dz, which is the left side of (I.19) by (I.16).

Since $|\text{Im } H_\alpha| \leq \pi$, and the real parts of the contour from R to $R + iR$ and from R to $R - iR$ cancel, and since $F(z) \to 0$ as $z \to \infty$ with $|\text{Arg } z| > \frac{\pi}{2}$, the infinite part of the contour contributes 0 as $R \to \infty$. Since $|\text{Im } H_\alpha| \leq \pi$, dominated convergence lets us take the contour to the real axis and get $\text{Im } \ln(1 + \alpha F(z)) = \text{Arg}(1 + \alpha F(z))$. Thus, we get the right side of (I.19).

(iii) By Theorem I.1(iii) and (iv) and the fact that $\int d\mu_0(z) = \|\varphi\|^2$, we see that

$$\lim_{\gamma\to\infty} \gamma^2 \frac{d}{dz} H_\alpha(-\gamma) = \alpha\|\varphi\|^2$$

so, by (ii)

$$\lim_{\gamma\to\infty} \int \frac{\gamma^2}{(x+\gamma)^2} \xi_\alpha(x)\, dx = \alpha\|\varphi\|^2.$$

By monotone convergence we obtain (I.20). $\square$

The next result extends (I.19) to more general functions than $f(x) = (x-z)^{-1}$. The formula we want is:

$$\operatorname{Tr}(f(A) - f(A_\alpha)) = -\int f'(x)\xi_\alpha(x)\, dx. \tag{I.21}$$

Formally this holds for any reasonable f since it holds for $f(x) = (x-z)^{-1}$ and those f's are "dense" in reasonable f. One issue is that we don't even know that $f(A) - f(A_\alpha)$ is trace class! Our hypotheses on f aren't optimal but include the critical example $f(x) = e^{-sx}$ (cutoff near $-\infty$).

THEOREM I.10. *Let f be a C^2 on $\mathbb{R}$ with $(1+|x|)^2 f^{(j)} \in L^2(0,\infty)$ for $j = 1,2$. Then for any α, $f(A) - f(A_\alpha)$ is trace class and* (I.21) *holds.*

PROOF. We only sketch the details supposing w.l.o.g. that $\alpha > 0$ and $A \geq 1$ (otherwise, reverse the roles and/or add a constant to A). And we write $B \equiv A_\alpha$ for notational simplicity.

1. $B^{-1} - A^{-1}$ is rank 1 and so trace class. It follows that $B^{-2}e^{isB} - A^{-2}e^{isA}$ is trace class with trace norm bounded by $c(1+|s|)$ since

$$\begin{aligned} B^{-2}e^{isB} - A^{-2}e^{isA} &= B^{-1}e^{isB}(B^{-1} - A^{-1}) \\ &\quad - i\int_0^s e^{iuB}(B^{-1} - A^{-1})e^{i(s-u)A} + (B^{-1} - A^{-1})e^{isA}A^{-1}. \end{aligned}$$

2. Let $\hat{f}$ be the Fourier transform of f. Under the hypotheses

$$\int (1+|k|)\left[\left|\frac{d\hat{f}}{dk}\right| + \left|\frac{d^2\hat{f}}{dk^2}\right|\right] dk < \infty \tag{I.22}$$

and that implies that we can integrate by parts twice to find that

$$f(B) - f(A) = -(2\pi)^{-1/2}\int \left[\frac{d^2\hat{f}}{dk^2}(k)\right][B^{-2}e^{ikB} - A^{-2}e^{ikA}]\, dk.$$

It follows by step 1 that $f(B) - f(A)$ is trace class.

3. From (I.19) one deduces (I.21) for $f(x) = x^{-2}e^{ixs}$ by writing

$$f(x) = \lim_{n\to\infty}[x^{-2}(1 - ixs/n)^{-n}]$$

for one can use analyticity to get (I.21) for $f(x) = (x - z)^{-n}$ and then for this special f.

4. (I.21) for general f follows from the formula in step 2 and the equality proven in step 3. □

REMARK. This does not capture all f for which (I.21) holds. For example, $f(x) = (x+1)^{-\beta}$ with $0 < \beta < 1$ does not obey the hypotheses, but using

$$(A+1)^{-\beta} = \frac{\sin \pi\beta}{\pi} \int_0^\infty (A+1+x)^{-1}|x|^{-\beta}\, dx$$

and $\|(A+x)^{-1} - (A_\alpha + x)^{-1}\|_1 \leq C(|x|+1)^{-2}$ for x large, one can prove (I.21) for such f.

PROPOSITION I.11. *Suppose that* (a,b) *is an interval disjoint from* $\operatorname{spec}(A) \cup \operatorname{spec}(A_\alpha)$. *Then*

(i) $\xi_\alpha(x)$ *is constant on* (a,b).
(ii) *Its value is either* 0 *or* 1.
(iii) $P_{(-\infty,a)}(A_\alpha) - P_{(-\infty,a)}(A)$ *is trace class and its trace is the common value of* $\xi_\alpha(x)$ *in* (a,b).

PROOF. (i) Let $f \in C_0^\infty(a,b)$. Then, $f(A) = f(A_\alpha) = 0$ so $\int f'(x)\xi_\alpha(x)\, dx = 0$ by Theorem I.10. Thus the distributional derivative $d\xi_\alpha/dx = 0$ on (a,b) so ξ_α is constant there.

(iii) Let f be a function in $C^\infty(\mathbb{R})$ which is 1 on $(i(\alpha), a)$, 0 on $[b,\infty)$. Then $f(A) = P_{(-\infty,a)}(A)$, $f(A_\alpha) = P_{(-\infty,a)}(A_\alpha)$, and $-\int f'(x)\xi_\alpha(x) = -\int_a^b f'(x)\xi_\alpha(x) = -\xi_\alpha(x_0)$
$\int_a^b f'(x)\, dx = \xi_\alpha(x_0)$, the common value of $\xi_\alpha(x)$ in (a,b).

(ii) It is a general fact about the trace of a difference of projections that is trace class, that it is an integer [16,5]. Since $0 \leq \xi_\alpha(x) \leq 1$, it must be 0 or 1. [There is a simple argument: Since $(a,b) \cap \operatorname{spec}(A) = \emptyset$, $F(x+i0)$ is real and continuous on (a,b). If $F(x_0 + i0) = -\alpha^{-1}$ anywhere on (a,b), then $F_\alpha(z) = F(z)/[1+\alpha F(z)]$ has a pole at x_0 and so x_0 is an eigenvalue of A_α. Since $(a,b) \cap \operatorname{spec}(A_\alpha) = \emptyset$, this cannot happen; that is, $1 + \alpha F(x+i0)$ has no zeros and so its argument is constant at either 0 or 1.] □

REMARK. Because of (iii), $\xi_\alpha(x)$ is called a spectral shift.

There is an interesting extension of Theorem I.8, an abstraction of a result of Javrjan [28]:

THEOREM I.12. *Let* $\beta < \gamma$. *Then*

$$\int_\beta^\gamma (d\mu_\alpha(E))\, d\alpha = (\xi_\gamma(E) - \xi_\beta(E))\, dE. \tag{I.23}$$

REMARK. If $c \neq 0$, $\lim_{\alpha\to\infty} \operatorname{Arg}(1+\alpha c)-\operatorname{Arg}(1-\alpha c) = \pi$ so $\lim_{\alpha\to\infty} [\xi_\alpha(E)-\xi_{-\alpha}(E)] = 1$ and (I.23) implies (I.17).

PROOF. By (I.13), if Im $z \neq 0$:

$$\begin{aligned}
\int_\beta^\gamma \left[\int \frac{d\mu_\alpha(E)}{(E-z)^2}\right] d\alpha &= \int_\beta^\gamma \frac{d}{dz}\left[\frac{F(z)}{1+\alpha F(z)}\right] d\alpha \\
&= \frac{d}{dz}\int_\beta^\gamma \frac{F(z)}{1+\alpha F(z)}\, d\alpha \\
&= \frac{d}{dz}\left[\ln(1+\gamma F(z)) - \ln(1+\beta F(z))\right] \\
&= \int \frac{\xi_\gamma(E)-\xi_\beta(E)}{(E-z)^2}\, dE
\end{aligned}$$

proving (I.23) smeared with $(E-z)^2$. Such functions have linear combinations which are dense in a big enough space to imply (I.23) as an equality of measures. $\square$

Since $d\mu_\alpha$ obeys $\int d\mu_\alpha(\lambda)(|\lambda|+1)^{-1} < \infty$, with bounds uniform in α on compacts, this result implies a similar estimate for ξ_α. Here's another proof:

THEOREM I.13. (i) *If $\alpha < \infty$, then*

$$\int |\xi_\alpha(E)|(1+|E|)^{-1}\, dE < \infty \tag{I.24}$$

and

$$\int \xi_\alpha(E)(E-z)^{-1}\, dE = \ln(1+\alpha F(z)). \tag{I.25}$$

(ii) $\int |\xi_\alpha(E)|\, dE \equiv \infty$ *if and only if* $\varphi \notin \mathcal{H}$.

PROOF. (i) Integrating

$$\frac{d}{dz}\ln(1+\alpha F(z)) = \int \xi_\alpha(y)(y-z)^{-2}\, dy.$$

¿From $-w$ to $-x$ for $x < w$ real, we get

$$\ln(1+\alpha F(-x)) - \ln(1+\alpha F(-w)) = \int \xi_\alpha(y)\frac{1}{y+x}\left(\frac{w-x}{y+w}\right) dy.$$

As $w \to \infty$, $F(-w) \to 0$ so $\ln(1+\alpha F(-w)) \to 0$ while $\frac{w-x}{y+w} = (1+\frac{y+x}{w-x})^{-1}$ is monotone increasing in w so (I.24) is proven and (1.25) is proven for $z = -x$, x real. By analytic continuation, it holds for all $z \in \mathbb{C}\backslash[i(\alpha),\infty)$.

(ii) By (I.25) and the monotone convergence theorem

$$\begin{aligned}
\int |\xi_\alpha(E)|\, dE &= (\operatorname{sgn}\alpha)\lim_{x\to\infty}\int \frac{x}{E+x}\left[\xi_\alpha(E)\right] dE \\
&= \operatorname{sgn}\alpha \lim_{x\to\infty} x\ln(1+\alpha F(-x)) \\
&= |\alpha|\|\varphi\|^2
\end{aligned}$$

by Theorem I.1(iv). $\square$

REMARK. It is not hard to show that $\int x^n |\xi_\alpha(x)|\, dx < \infty$ if and only if $\varphi \in \mathcal{H}_{n/2}(A)$ and in that case

$$\int x^n \xi_\alpha(x)\, dx = \mathrm{Tr}(A_\alpha^{n+1} - A^{n+1})/(n+1).$$

Appendix to I.4
The Krein Spectral Shift for Trace Class Perturbations

Let $C - A = (\varphi, \cdot)\varphi$ be rank one with $\|\varphi\| < \infty$ and $C \geq A$. Then for nice f, we have

$$\mathrm{Tr}(f(C) - f(A)) = \int f'(x)\xi_{C,A}(x)\, dx \tag{I.26a}$$

where

$$\int \xi_{C,A}(x)\, dx = \mathrm{Tr}(C - A) \tag{1.26b}$$

and

$$\int |\xi_{C,A}(x)|\, dx = \mathrm{Tr}(|C - A|). \tag{I.26c}$$

If $C - A$ is finite rank, we can diagonalize it and get it as a sum of rank one perturbations and (I.26a–c) continue to hold. By (1.26c), ξ has a limit in L^1 norm as $C - A$ approaches a general trace class of operator. This proves

THEOREM I.14 (KREIN'S SPECTRAL SHIFT FORMULA). *If A is self-adjoint and bounded below, B is trace class, and $C = A + B$, then there exists an L^1 function, $\xi_{C,A}(x)$, on $\mathbb{R}$ vanishing for x near $-\infty$ so that* (I.26a–c) *hold.*

REMARK. ξ is no longer given as $\mathrm{Arg}(1 + \alpha F(z))$ with $F(z)$ as simple as in the rank one case. However, in the rank one case

$$\begin{aligned} \mathrm{Tr}(1 + \alpha F(z)) &= (1 + \mathrm{Tr}((C - A)(A - z)^{-1}) \\ &= \det(1 + (C - A)(A - z)^{-1}) \\ &= \det((C - z)(A - z)^{-1}) \end{aligned}$$

and the argument of this has the correct additive properties. The result is [33]

$$\xi_{C,A}(\lambda) = \lim_{\epsilon \downarrow 0} \arg[\det(1 + (C - A)(A - \lambda - i\epsilon)^{-1})]$$

where det is a Fredholm determinant (see [42]).

I.5 Infinite Coupling

In the rank one setting we have been describing, let P be the projection onto the space spanned by φ if $\|\varphi\| < \infty$ and $P = 0$ if $\|\varphi\| = \infty$.

Look at the formula (I.15) for $(A_\alpha - z)^{-1}$. It clearly shows the first part of

THEOREM I.15. (i) *As* $\alpha \to \pm\infty$, $(A_\alpha - z)^{-1}$ *converges in norm to a limit we call* $(A_\infty - z)^{-1}$ *given by*

$$(A_\infty - z)^{-1} = (A - z)^{-1} - F(z)^{-1}((A - \bar{z})^{-1}\varphi, \cdot)(A - z)^{-1}\varphi. \tag{I.27}$$

(ii) *If* $\|\varphi\| = \infty$, *then there is a self-adjoint operator* A_∞ *on* $\mathcal{H}$ *whose resolvent is* $(A_\infty - z)^{-1}$. *If* $\|\varphi\| < \infty$, *then there is a self-adjoint operator,* $\tilde{A}_\infty$, *on* $(1-P)\mathcal{H}$ *so that* $(A_\infty - z)^{-1}\eta = (\tilde{A}_\infty - z)^{-1}(1 - P)\eta$. *(We'll call* $\tilde{A}_\infty$ *as just* A_∞ *with the understanding that* $(A_\infty - z)^{-1} = 0$ *on* $P\mathcal{H}$ *and we'll write* $\mathcal{H}(A_\infty) = (1 - P)\mathcal{H}$.*)*

(iii) $\mathcal{H}_{+1}(A_\infty) = \{\psi \in \mathcal{H}_{+1}(A) \mid (\varphi, \psi) = 0\}$ *and*

$$(\psi, A_\infty\psi) = (\psi, A\psi)$$

for $\psi \in \mathcal{H}_{+1}(A_\infty)$.

PROOF. We have proven (i). To prove (ii), (iii), one uses the following monotone convergence theorem for forms ([30,41]):

Let C_n be a family of non-negative self-adjoint operators with $\mathcal{H}_{+1}(C_{n+1}) \subseteq \mathcal{H}_{+1}(C_n)$ and $(\psi, C_{n+1}\psi) \geq (\psi, C_n\psi)$ if $\psi \in \mathcal{H}_{+1}(C_{n+1})$. Let

$$\mathcal{H}_{+1}(C_\infty) = \Big\{\psi \in \bigcap_n \mathcal{H}_{+1}(C_n) \mid \sup_n (\psi, C_n\psi) < \infty\Big\}.$$

Let c_∞ be the quadratic form on $\mathcal{H}_{+1}(C_\infty)$ given by $c_\infty(\psi, \psi) = \sup\limits_n (\psi, c_n\psi)$. Then, there is a self-adjoint operator C_∞ on $\overline{\mathcal{H}_{+1}(C_\infty)}$ so that if $(C_\infty - z)^{-1}$ is extended to $\mathcal{H}_{+1}(C_\infty)^\perp$ by setting it equal to zero there, then $(C_n - z)^{-1}$ converges strongly to $(C_\infty - z)^{-1}$.

This yields (ii), (iii) if one notes that

$$\sup_\alpha (\psi, A_\alpha\psi) < \infty \Longleftrightarrow (\psi, \varphi) = 0. \quad \square$$

Since $\xi_\alpha(x)$ is monotone in α, and bounded by 1, it has a limit $\xi_\alpha(x)$. In fact

$$\xi_\infty(x) = \operatorname{Arg}(F(x + i0)), \qquad 0 \leq \xi_\infty(x) \leq 1 \tag{I.28}$$

since

$$\xi_\alpha(x) = \operatorname{Arg}(\alpha^{-1} + F(x + i0)).$$

By a limiting argument, $\xi_\infty(x)\,dx = \int\limits_0^\infty (d\mu_\alpha(x))\,d\alpha$.

In addition,

$$\operatorname{Tr}((A-z)^{-1}-(A_\infty-z)^{-1}) = \lim_{\alpha\to\infty} \frac{\alpha F'(z)}{1+\alpha F(z)} = \frac{F'(z)}{F(z)} \tag{I.29a}$$

$$= \frac{d}{dz}\ln F(z) \tag{I.29b}$$

so by mimicking the arguments in the $\alpha<\infty$ case,

$$\operatorname{Tr}(f(A)-f(A_\infty)) = -\int f'(x)\xi_\infty(x)\,dx$$

for the f's in Theorem I.10. One place that ξ_α and ξ_∞ differ though is (compare with (I.24))

PROPOSITION I.16 ([25]).

$$\int (1+|x|)^{-1}\xi_\infty(x)\,dx = \infty$$

PROOF. By monotone convergence,

$$\begin{aligned}\int (1+x)^{-1}\xi_\infty(x)\,dx &= \lim_{\alpha\to\infty}\int (1+x)^{-1}\xi_\alpha(x)\,dx \\ &= \lim_{\alpha\to\infty}\ln(1+\alpha F(-1)) = \infty. \quad \square\end{aligned}$$

If A is bounded, it is easy to see why the integral diverges; $\xi_\infty(x)=1$ for $x>\|A\|$ so the integral diverges logarithmically exactly as $\ln x$. This is typical of the case when $\|\varphi\|<\infty$.

THEOREM I.17 ([25]). *If $\|\varphi\|<\infty$, then $\int(1+|x|)^{-1}[1-\xi_\infty(x)]\,dx<\infty$ and*

$$\ln\left[(-z)F(z)/\|\varphi\|^2\right] = \int_0^\infty \frac{[\xi_\infty(x)-1]}{x-z}\,dx. \tag{I.30}$$

PROOF. We have that

$$\frac{d}{dz}\ln F(z) = \int \frac{\xi_\infty(x)}{(x-z)^2}\,dx \tag{I.31}$$

while clearly

$$\frac{d}{dz}\ln(-z^{-1}) = \int_0^\infty \frac{1}{(x-z)^2}\,dx \tag{I.32}$$

since for $z<0$, both sides are just $(-z)^{-1}$. (I.32) is a direct calculation but can also be regarded as (I.31) for the case $F(z)=-1/z$.

By (I.31–32):

$$\frac{d}{dz}\ln((-z)F(z)/\|\varphi\|^2) = \int_0^\infty \frac{(\xi_\infty(x)-1)}{(x-z)^2}\,dx.$$

By Theorem I.1(iv), $\ln((-z)F(z)/\|\varphi\|^2) \to 0$ as $z \to -\infty$ along the real axis. The same monotone convergence theorem argument that we used in the proof of Theorem I.13(i) and the fact that $1-\xi_\alpha(x) \geq 0$ implies that $(1+|x|)^{-1}(1-\xi_\infty)$ is in L^1 and that (I.30) holds. $\square$

In §IV.1, we will extend this idea to some cases where $\|\varphi\| = \infty$.

How can one get a handle on a spectral measure for A_∞? At first sight, it seems a hard job since

$$\lim_{\alpha\to\infty}\int \frac{d\mu_\alpha(x)}{x-z} = \lim_{\alpha\to\infty}\frac{F(z)}{1+\alpha F(z)} = 0$$

so $d\mu_\alpha(x) \to 0$ weakly. The key is to renormalize! Define

$$d\rho_\alpha(x) = (1+\alpha^2)\,d\mu_\alpha(x).$$

One can prove the following

Theorem I.18 ([25]). (i) *There exists a measure $d\rho_\infty$ (which is non-zero except for the trivial case where φ is an eigenvector of A) so that*

$$\int \frac{d\rho_\infty(x)}{(1+|x|)^2} < \infty$$

and

$$\lim_{\alpha\to\infty}\int f(x)\,d\rho_\alpha(x) = \int f(x)\,d\rho_\infty(x) \tag{I.33}$$

for any $f \in C_0^\infty(\mathbb{R})$.

(ii) *There exists a vector $\eta \in \mathcal{H}_{-2}(A_\infty)$ so that $d\rho_\infty$ is the spectral measure $d\mu^\eta_{A_\infty}$. If φ is cylic for A, then η is cyclic for A_∞.*

(iii) (I.33) *holds for $f(x) = (x-z)^{-3}$ but it only holds for $f(x) = (x-z)^{-2}$ if $\|\varphi\| = \infty$; explicitly,*

$$\lim_{\alpha\to\infty}\int \frac{d\rho_\alpha(x)}{(x-z)^2} = \|\varphi\|^{-2} + \int \frac{d\rho_\infty(x)}{(x-z)^2}.$$

(iv) *$d\rho_\infty$ is the boundary value of $-F(z)^{-1}$ in the sense that for $f \in C_0^\infty(\mathbb{R})$*

$$\int f(x)\,d\rho_\infty(x) = \lim_{\epsilon\downarrow 0}\frac{1}{\pi}\int f(x)\,\operatorname{Im}[-F(x+i\epsilon)^{-1}]\,dx.$$

We refer the reader to [25] for a complete proof but will make a series of remarks that illuminate the result and partly prove it.

REMARKS. 1. Notice that η is only stated to be in $\mathcal{H}_{-2}(A_\infty)$, not $\mathcal{H}_{-1}(A_\infty)$. Indeed, the differential equation case of the next section when $V = 0$ is one where $d\rho_\infty(x) \sim cx^{1/2}\,dx$ and $\eta \notin \mathcal{H}_{-1}(A_\infty)$. Indeed [25], for any $\theta < 2$, there are examples where $\int d\rho_\infty(x)/(1+|x|)^\theta = \infty$.

2. If A is bounded, $\eta = (1-P)A\varphi$. Otherwise, one has that η obeys

$$(A_\infty - z)^{-1}\eta = (1-P)F(z)^{-1}(A-z)^{-1}\varphi$$

(with the convention that $P = 0$ if $\|\varphi\| = \infty$).

3.
$$\int \frac{d\mu_\alpha(x)}{(x-z)^2} = \frac{d}{dz}\,\frac{F(z)}{1+\alpha F(z)} = \frac{F'(z)}{(1+\alpha F(z))^2}$$

so

$$\lim_{\alpha\to\infty} \int \frac{d\rho_\alpha(x)}{(x-z)^2} = \frac{F'}{F^2} \tag{I.34}$$

so the $\|\varphi\|^{-2}$ term in (iii) is related to Theorem I.1(v).

4. Notice that the right side of (I.34) is $\frac{d}{dz}(-1/F)$. This is the key to proving (iv).

There is an interesting reparametrization of the ρ's that is exactly what is used in the differential equation case. For $\theta \in (0,\pi)$, we can define $\alpha = -\cot(\theta)$ so α runs from $-\infty$ to ∞ as θ runs from 0 to π. Let

$$d\tilde\rho_\theta(x) = d\rho_{-\cot(\theta)}(x) = [\sin^2(\theta)]^{-1}\,d\mu_{-\cot(\theta)}(x).$$

Then, $d\tilde\rho_\theta$ has a limit as $\theta \to 0, \pi$ which is just what we called $d\rho_\infty(x)$. Moreover, we claim that

$$\int_\theta^\pi (d\tilde\rho_\theta(E))\,d\theta = dE \tag{I.35}$$

for

$$\int_0^\pi d\tilde\rho_\theta(E)\,d\theta = \int_{-\infty}^\infty (1+\alpha^2)\,d\mu_\alpha(E)\,\frac{d\alpha}{1+\alpha^2} = dE.$$

I.6 Boundary Condition Variation of ODE's

For applications to Schrödinger operators, there are two main categories of the general theory: variation of potential in the discrete (Jacobi) case, which we'll discuss in the next section, and the subject of this section, variation of boundary condition.

We begin with a lightning review of the standard Weyl m-function approach (see [48]) and then rephrase the set-up into the context of these lectures. We will consider a Schrödinger operator on $(0,\infty)$ (and later on $(-\infty,\infty)$) of the form

$$H_\theta u = -u''(x) + V(x)\,u(x) \tag{I.36}$$

where, for simplicity, we suppose that $V(x)$ is bounded from below but continuous. This makes H limit point at infinity so we only need a boundary condition at zero, which is where the parameter θ enters. The boundary condition at 0 is

$$u(0)\cos\theta + u'(0)\sin\theta = 0 \qquad 0 \le \theta < \pi \tag{I.37}$$

so that $\theta = 0$ is the Dirichlet boundary condition and $\theta = \pi/2$ is the Neumann boundary condition.

Explicitly, H_θ defines a self-adjoint operator with domain

$$\begin{aligned} D(H_\theta) = \{u \in L^2(0,\infty) \mid u, u' &\text{ are locally absolutely continuous functions,} \\ u \text{ obeys (I.37) and } H_\theta u \in L^2\}. \end{aligned}$$

We will often be interested in solutions of the differential equation

$$-u'' + Vu = zu \tag{I.38}$$

and will consider the Wronskian $W(f,g)$ of two functions

$$W(f,g)(x) = f(x)g'(x) - f'(x)g(x).$$

As usual, if f, g solve (I.38) for the same z, then $W(f,g)(x)$ is independent of x.

Given θ, three solutions of (I.38) will concern us: ϕ which obeys the boundary condition (I.37), η defined with a "dual" boundary condition, and ψ_+ for Im $z \neq 0$, the solution which is L^2 near $x = \infty$. Explicitly, ϕ, η are defined by boundary values at $x = 0$:

$$\begin{aligned} &\phi_\theta(z,0) = -\sin(\theta) \qquad && \phi'_\theta(z,0) = \cos(\theta) \\ &\eta_\theta(z,0) = \cos\theta && \eta'_\theta(z,0) = \sin(\theta) \end{aligned}$$

so

$$W(\eta_\theta, \phi_\theta)(x) = 1. \tag{I.39}$$

The third solution ψ_+ is defined with mixed boundary conditions; it is in $L^2((0,\infty))$, which determines it up to a multiplicative constant, and it is normalized by

$$W(\psi_{+,\theta}, \phi_\theta) = \psi_{+,\theta}(0)\cos\theta + \psi'_{+,\theta}(0)\sin\theta = 1. \tag{I.40}$$

Since ϕ, η are independent solutions of (I.38), we have $\psi_+ = a\eta + b\phi$. By (I.39/40), $a = 1$. We therefore define the Weyl m-function, $m_\theta(z)$, by

$$\psi_{+,\theta}(z,x) = \eta_\theta(z,x) + m_\theta(z)\phi_\theta(z,x) \tag{I.41a}$$

or equivalently:

$$m_\theta(z) = W(\eta_\theta, \psi_{+,\theta}) \tag{I.41b}$$

or

$$m_\theta(z) = -\lim_{R\to\infty} \frac{\eta_\theta(z,R)}{\phi_\theta(z,R)}. \tag{I.41c}$$

The last (which follows from $\psi_+ \to 0$ at infinity) is the usual definition in the limit point case because it is what Weyl used, although the first two are more useful.

It can be seen that

$$\text{Im } z > 0 \Longrightarrow \text{Im } m_\theta(z) > 0. \tag{I.42}$$

We won't prove this now, since it will follow from the general theory of Borel transforms once we have set up the connection. The spectral measure $d\rho_\theta$ is defined by

$$d\rho_\theta(x) = \lim_{\epsilon \downarrow 0} \frac{1}{\pi} [\text{Im } m_\theta(x + i\epsilon)] \, dx.$$

For $\theta \neq 0$, as we'll see

$$m_\theta(z) = \cot(\theta) + \int \frac{d\rho_\theta(x)}{x - z}. \tag{I.43}$$

The Green's function, $G_\theta(x, x'; z)$ is the integral kernel of $(H_\theta - z)^{-1}$, that is

$$((H_\theta - z)^{-1} u(x) = \int G_\theta(x, x'; z) u(x') \, dx'.$$

Because of the normalization (I.40), one has

$$G_\theta(x, x'; z) = \phi_\theta(z, x_<) \psi_{+,\theta}(z, x_>)$$

where $x_< = \min(x, x'), x_> = \max(x, x')$. In particular, by (I.41a)

$$G_\theta(0, 0; z) = + \sin^2 \theta(-\cot \theta + m_\theta(z)). \tag{I.44}$$

As a final general formula, we note that Wronskian gymnastics (we'll get it other ways below) shows that

$$m_\kappa(z) = \frac{-\sin(\kappa - \theta) + \cos(\kappa - \theta) m_\theta(z)}{\cos(\kappa - \theta) + \sin(\kappa - \theta) m_\theta(z)}. \tag{I.45a}$$

In particular,

$$m_0(z) = -\frac{1}{m_{\pi/2}(z)}. \tag{I.45b}$$

We want to show how to think of this in terms of rank one perturbations. Let $u \in D(H_\theta)$ be real-valued. Then, integrating by parts

$$\begin{aligned} (u, H_\theta u) &= \int_0^\infty (u(x))[-u'' + Vu](x) \, dx \\ &= \int_0^\infty [u'(x)^2 + V(x) u^2(x)] \, dx + u'(0) u(0) \\ &\equiv \tau(u, u) - \cot(\theta) u(0)^2 \end{aligned} \tag{I.46}$$

because of the boundary condition.

Let A be the $\theta = \pi/2$ Neumann boundary condition operator. A simple Sobolev estimate shows that for any $u \in \mathcal{H}_{+1}(A)$ is continuous in x and

$$|u(0)|^2 \leq c(u, (A+1)u),$$

that is, $\delta(x)$, the Dirac delta function, lies in $\mathcal{H}_{-1}(A)$. We can form

$$A_\alpha = A + \alpha\delta(x).$$

(I.46) says that $H_\theta = A_{-\cot(\theta)}$. Moreover,

$$F_\alpha(z) = (\delta, (A_\alpha - z)^{-1}\delta)$$

is exactly $G_\theta(0, 0; z)$. Since G is related to m by (I.44), equation (I.45) is just the relation $F_\alpha(z) = F(z)/[1 + \alpha F(z)]$.

In addition, because of (I.44) and (I.43), we have

$$d\rho_\theta(E) = \sin^2\theta \, d\mu_{-\cot(\theta)}(E),$$

that is, the spectral measure $d\rho$ is precisely the measure we called $d\tilde{\rho}_\theta$ in the last section. The Dirichlet spectral measure, $d\tilde{\rho}_0$, is an example of a $d\rho_\infty$ with $\int d\rho_\alpha(E)/[|E| + 1] = \infty$. (I.45b) is just Theorem I.18(iv). The vector η of §I.5 is just δ'; see [25].

The point of this section is the spectral analysis of rank one perturbations in the next chapter will apply to boundary condition variation directly (rather than by analogy).

I.7 Jacobi Matrices

Jacobi matrices are operators on $\ell^2(\mathbb{Z}^\nu)$ which are discrete analogs of Schrödinger operators. We write $u \in \ell^2(\mathbb{Z}^\nu)$ as a function on $\mathbb{Z}^\nu$. Given a function, V, on $\mathbb{Z}^\nu$, we define the associated Jacobi matrix, h, by

$$(hu)(n) = \sum_{|j|=1} u(n+j) + V(n)u(n) \tag{I.47a}$$

which we write as

$$h = h_0 + V. \tag{I.47b}$$

Let δ_0 be the vector in ℓ^2 which is given by

$$\delta_0(n) = \delta_{n0}.$$

Let P be the projection on $\delta_0 : (\delta_0, \cdot)\delta_0$. Fix V and let A be the Jacobi matrix associated to $V - \delta_{\cdot 0}(V(0))$. Then

$$h = A + V(0)P$$

and variations of V are precisely rank one perturbations.

As an application of this idea, let $V_\omega(n)$ be a random process where the $V_\omega(n)$ are independent, identically distributed random variables with distribution $p(v)\,dv$ where p is bounded. There is a fundamental quality called the integrated density of states, $k(\lambda)$, which is given by the following: Let $d\mu_\omega^{(0)}$ be the spectral measure for $h_0 + V_\omega$ with vector δ_0. Then

$$k(\lambda) = E_\omega(\mu_\omega^{(0)}(-\infty, \lambda)). \tag{I.48}$$

This is not the basic definition but a derived formula for k (see, e.g., [6,9]). We claim

Theorem I.19 (Wegner's Estimate [49]).

$$|k(\lambda) - k(\lambda')| \leq c|\lambda - \lambda'|$$

where $c = \sup_\gamma p(\gamma)$.

Proof. The result is equivalent to saying that dk is absolutely continuous with respect to $d\lambda$ with $dk = q(\lambda)\,d\lambda$ with $\|q\|_\infty \leq c$. Fix $(V_\omega(n))_{n\neq 0}$. Then, by Theorem I.8

$$\int [d\mu_\omega^{(0)}(\lambda)]p(v(0))\,dv(0) \leq c \int d\mu_\omega^{(0)}(\lambda)\,dv(0) = c\,d\lambda.$$

Averaging over $(V_\omega(n))_{n\neq 0}$, we get

$$E_\omega(d\mu_\omega) \leq c\,d\lambda$$

which is exactly what we want. $\square$

CHAPTER II

SPECTRAL THEORY OF RANK ONE PERTURBATIONS

II.0 Introduction

We begin our analysis with the study of the absolutely continuous spectrum, obtaining a result that also follows from the trace class theory of scattering, but without wave operators. We next discuss the fundamental work of Aronszajn [3] and Donoghue [4], which identifies spectral information for A_α in terms of $F(z)$. Next, we discuss the Simon-Wolff [47] work on localization and apply it to one-dimensional random Jacobi matrices. Finally, we discuss recent results of Gordon [27] and del Rio, et al. [12] on singular spectrum.

Henceforth, we assume that φ is a cyclic vector for A, that is, $\{(A-z)^{-1}\varphi \mid z \in \mathbb{C}\}$ is a total set for $\mathcal{H}$. In general, if $\mathcal{H}_0$ is the closed subspace generated by these vectors, then $\mathcal{H}_0^\perp$ is an invariant space for each A_α and $A_\alpha = A$ on $\mathcal{H}_0^\perp$. Thus, the extension from the cylic to general case is trivial. We make the assumption to be able to focus on the real issues and not have to state the theorems in convoluted forms to give the general case.

II.1 Invariance of the Absolutely Continuous Spectrum

Let $f(x)\,dx$ and $g(x)\,dx$ be two absolutely continuous (positive) measures on $\mathbb{R}$. Recall these measures are equivalent if and only if $\{x \mid f(x) \neq 0\}$ and $\{x \mid g(x) \neq 0\}$ agree up to sets of Lebesgue measure zero. Moreover, if A is multiplication by x on $L^2(\mathbb{R}, f\,dx)$ and C is multiplication by x on $L^2(\mathbb{R}, g\,dx)$, then A and C are unitarily equivalent if and only if $f\,dx$ and $g\,dx$ are equivalent. With these preliminaries

Theorem II.1. *For all $\alpha \neq \beta$, $(A_\alpha)_{\rm ac}$ and $(A_\beta)_{\rm ac}$, the absolutely continous parts of A_α and A_β are unitarily equivalent.*

Proof. Since $A_\alpha = A_\beta + (\alpha-\beta)(\varphi,\cdot)\varphi$, we can suppose for $\beta = 0$ w.l.o.g. By the above discussion and Theorem I.6(iv), it suffices to show that $S_1 \equiv \{E \mid \text{Im } F(E+i0) \neq 0\}$ and $S_2 \equiv \{E \mid \text{Im } F_\alpha(E+i0) \neq 0\}$ agree up to sets of measure zero. By the Aronszajn-Krein formula $F_\alpha = \frac{F}{1+\alpha F}$, which implies that

$$\text{Im } F_\alpha(z) = \frac{\text{Im } F(z)}{|1+\alpha F(z)|^2}. \tag{II.1}$$

It follows that S_1 and S_2 agree up to the sets where $F(E+i0)$ fails to exist, the set where $F(E+i0)=\infty$, and the set where $F(E+i0)=-\alpha^{-1}$. These sets all have measure zero, so S_1 and S_2 agree up to sets of measure zero. $\square$

REMARKS. 1. The result extends to the non-cyclic case and so extends to the finite rank case. It should be possible to accommodate the trace class case. This is an area under present study.

2. Since $(A_\infty+1)^{-1}-(A_0+1)^{-1}$ is rank one in the usual sense, we can apply the theorem to $(A_\infty-1)^{-1}$ and $(A_0+1)^{-1}$ and so, by a spectral mappping theorem, extend the result to allow $\alpha=\infty$. One can also get $\alpha=\infty$ by using $d\rho_\infty$ and $\text{Im }(-1/F)=\text{Im }F/|F|^2$.

II.2 The Aronszajn-Donoghue Theory

Recall that $G(x)=\int\frac{d\mu(y)}{(x-y)^2}$. The following basic theorem was proven by Aronszajn [3] for boundary condition dependence of spectrum for Sturm-Liouville operators and then extended to (bounded) rank one perturbations by Donoghue [14].

THEOREM II.2. *For $\alpha\neq 0$ ($\alpha=$ infinity allowed with $\infty^{-1}=0$), define*

$$\begin{aligned} S_\alpha &= \{x\in\mathbb{R}\mid F(x+i0)=-\alpha^{-1}; G(x)=\infty\}\\ P_\alpha &= \{x\in\mathbb{R}\mid F(x+i0)=-\alpha^{-1}; G(x)<\infty\}\\ L &= \{x\in\mathbb{R}\mid \mathit{Im}\ F(x+i0)\neq 0\}.\end{aligned}$$

Then (i) $\{S_\alpha\}_{\alpha\neq 0;|\alpha|\leq\infty}$, $\{P_\alpha\}_{\alpha\neq 0;|\alpha|\leq\infty}$ *and L are mutually disjoint.*

(ii) *P_α is the set of eigenvalues of A_α. In fact*

$$(d\mu_\alpha)_{\text{pp}}(x)=\sum_{x_n\in P_\alpha}\frac{1}{\alpha^2G(x_n)}\,\delta(x-x_n)\qquad \alpha<\infty$$

$$(d\rho_\infty)_{\text{pp}}(x)=\sum_{x_n\in P_\infty}\frac{1}{G(x_n)}\,\delta(x-x_n)\qquad \alpha=\infty.$$

(iii) *$(d\mu_\alpha)_{\text{ac}}$ is supported on L, $(d\mu_\alpha)_{\text{sc}}$ is supported on S_α.*

(iv) *For $\alpha\neq\beta$, $(d\mu_\alpha)_{\text{sing}}$ and $(d\mu_\beta)_{\text{sing}}$ are mutually singular.*

REMARK. We say that a set S "supports" a measure $d\nu$ if $\nu(\mathbb{R}\backslash S)=0$.

PROOF. (i) is trivial and (iv) follows from (i), given (ii) and (iii). That L supports $(d\mu_\alpha)_{\text{ac}}$ is proven in the last section.

By Theorem I.6(iv), $(d\mu_\alpha)_{\text{sing}}$ is supported by $\{E\mid \lim_{\epsilon\downarrow 0}|F_\alpha(E+i\epsilon)|=\infty\}$. But

$$F_\alpha(z)=\frac{F(z)}{1+\alpha F(z)}$$

says that $|F_\alpha(E+i\epsilon)|\to\infty$ if and only if $F(E+i\epsilon)\to -1/\alpha$.

(ii), (iii) thus follow by Theorem I.6(iii) and the claim that when $F(E+i\epsilon) \to -1/\alpha$ (even if $G(E) = \infty$):

$$\lim_{\epsilon \downarrow 0} \epsilon \text{ Im } F_\alpha(E+i\epsilon) = 1/[\alpha^2 G(E)] \qquad (0 < \alpha < \infty) \tag{II.2a}$$

$$\lim_{\epsilon \downarrow 0} \epsilon \text{ Im } (-F(E+i\epsilon))^{-1} = 1/G(E) \qquad (\alpha = \infty). \tag{II.2b}$$

If $G(E) < \infty$, (II.2) follows from Theorem I.2(v) which implies that $F(E+i\epsilon) = -1/\alpha + i\epsilon G(x) + o(\epsilon)$ and the formula for F_α. If $G(E) = \infty$ and $\alpha = \infty$, Theorem I.2(iv) implies $\epsilon^{-1}|F(x+i\epsilon)| \to \infty$ so $\left|\frac{\epsilon}{F(x+i\epsilon)}\right| \to 0$ proving II.2b in that case. If $G(E) = \infty$ and $0 < \alpha < \infty$, by Theorem I.2(iv) again, ϵ^{-1} Im$(1+\alpha F) \to \infty$ so $\epsilon|1+\alpha F|^{-1} \to 0$. Thus, since $F \to -1/\alpha$, $\epsilon|F/1+\alpha F| \to 0$. $\square$

This theorem has interesting consequences for one-dimensional Schrödinger operators and Jacobi matrices:

THEOREM II.3. *Let A be a Schrödinger operator on $[0,\infty)$ with Neumann boundary conditions at $x = 0$ as in §I.6. Then $G(E) < \infty$ if and only if both of the following hold:*

(i) *E is not an eigenvalue of A;*
(ii) *(I.38) (with $E = z$) has a solution which is L^2 at $+\infty$.*

PROOF. Since $G(E)$ finite implies that $F(E+i0)$ exists and is real and finite, Theorem II.2 implies that $G(E) < \infty$ if and only if E is an eigenvalue of $A + \alpha\delta$ for some $\alpha \neq 0$ in $\mathbb{R} \cup \{\infty\}$. But this is equivalent to (i), (ii). $\square$

THEOREM II.4. *Let A be a Jacobi matrix on $\ell^2(\mathbb{Z})$ and $\varphi = \delta_0$ as in §I.7. Then $G(E) < \infty$ if and only if*

(i) *E is not an eigenvalue of A;*
(ii) *One of the following holds:*
(a) *The equation*

$$u(n+1) + u(n-1) + V(n)u(n) = Eu(n) \tag{II.3}$$

has an ℓ^2 solution on $(0,\infty)$ with $u(0) = 0$;

(b) *(II.3) has an ℓ^2 solution on $(-\infty,0)$ with $u(0) = 0$;*
(c) *(II.3) has ℓ^2 solutions $u_\pm$ on both $(0,\infty)$ and $(-\infty,0)$ with both $u_+(0) \neq 0$ and $u_-(0) \neq 0$.*

REMARKS. 1. To say u is a solution on $(0,\infty)$ means u is defined on $[0,\infty)$ but (II.3) holds for $n = 1, 2, \ldots$.

2. In particular, if (II.3) has ℓ^2 solutions on both $(0,\infty)$ and $(-\infty,0)$, then either E is an eigenvalue of A or $G(E) < \infty$.

PROOF. (a), (b) of (ii) hold if and only if E is an eigenvalue of A_∞. (c) holds if and only if E is an eigenvalue of some A_α with $|\alpha| < \infty$. Given these, the proof is the same as for the last two theorems. $\square$

II.3 The Simon-Wolff Criterion

The following is useful in discussing localization for random Jacobi matrices:

THEOREM II.5 ([47]). *Fix an interval $[a, b]$. Then the following are equivalent:*

(a) $G(E) < \infty$ *for a.e.* E *in* $[a, b]$ *(w.r.t. Lebesgue measure).*
(b) *For a.e.* α *(w.r.t. Lebesgue measure),* A_α *has only pure point spectrum in* $[a, b]$.

PROOF. Let $S = \{E \in [a, b] \mid G(E) = \infty\}$. Suppose (a) holds. Then $|S| = 0$ by hypothesis. By Theorem I.8 that means $\int \mu_\alpha(S)\, d\alpha = 0$ so $\mu_\alpha(S) = 0$ for a.e. α. But if $\mu_\alpha(S) = 0$, then in the language of Theorem II.2, $\mu_\alpha(L \cap [a, b]) = \mu_\alpha(S_\alpha \cap [a, b]) = 0$. It follows by that theorem that μ_α has only point spectrum, so (b) holds.

Conversely, if A_α has only point spectrum on $[a, b]$, then $\mu_\alpha(S) = 0$. If (b) holds, $\int \mu_\alpha(S)\, d\alpha = 0$, so by Theorem I.8, $|S| = 0$ and (a) holds. $\square$

As an example of how to apply this theorem, we want to prove localization for the Anderson model in one dimension following [45]. We'll use various facts about that model proven elsewhere.

THEOREM II.6. *Let* $\{v_\omega(x)\}_{n \in \mathbb{Z}}$ *be bounded i.i.d.s. with distribution* $p(\lambda)\, d\lambda$. *Let* $h_\omega = h_0 + v_\omega$ *as in §I.7. Then for a.e.* ω, h_ω *has only point spectrum.*

REMARKS. 1. The general proof following the steps below requires a lot less than bounded or independent random variables; see [45].

2. The proofs show that the eigenfunctions decay exponentially.

3. If $\operatorname{supp} p = [a, b]$, then $\operatorname{spec}(h_\omega) = [a - 2, b + 2]$ with probability one, so this is point spectrum dense in an interval.

PROOF. 1. The transfer matrix, $A_n(E, \omega)$, is the two by two matrix defined by $\binom{u(n+1)}{u(n)} = A_n(E, \omega)\binom{u(1)}{u(0)}$ where u obeys (II.3) for v_ω. General principles (the subadditive ergodic theorem; see [45]) imply that for each fixed E,

$$\lim_{|n| \to \infty} \frac{1}{|n|} \ln \|A_n(\omega, E)\| = \gamma(E) \tag{II.4}$$

for a.e. ω and a fixed γ. Obviously, whether the limit in (II.4) holds only depends on v_ω in a neighborhood of infinity.

2. It can be proven that $\gamma(E) > 0$ for almost all E. In the i.i.d. case under discussion, this follows from Furstenberg's theorem ([19]) for *all* E, but under much weaker conditions (v-non-deterministic), one gets the result for a.e. E from Kotani's theory [32,44].

3. The theorem of Ruelle-Oseledec [39,37] implies that when (II.4) holds, with $\gamma(E) > 0$, then there exist initial values $u_\pm(0), u_\pm(1)$ so that the corresponding solutions $u_\pm$ of (II.3) are ℓ^2 at $\pm\infty$. (In fact, the solutions decay exponentially.)

4. Theorem II.4 then implies that if $\gamma(E) > 0$ and (II.4) holds, then either E is an eigenvalue of h_ω or $G(E, \omega) < \infty$ (with $G(E, \omega)$ associated to h_ω and δ_0).

5. By Fubini's theorem, for a.e. $\{v_\omega(n)\}_{n\neq 0}$, (II.4) holds for a.e. E with $\gamma > 0$. Since h_ω has only countably many eigenvalues, we conclude that $G(E,\omega) < \infty$ for a.e. E (for this typical set of ω). Thus, by Theorem II.5, $h_\omega + \alpha\delta_0$ has pure point spectrum for a.e. α.

6. By the hypothesis on the absolute continuity of the distribution of $v_\omega(0)$, h_ω has point spectrum for a.e. ω. $\square$

Essentially, the identical argument proves

THEOREM II.7. *Let $\{V_\omega(x)\}_{-\infty<x<\infty}$ be a non-deterministic bounded ergodic process on $\mathbb{R}$. Then for a.e. ω and a.e. $\theta \in [0,\pi)$,*

$$-\frac{d^2}{dx^2} + V_\omega(x)$$

on $L^2((0,\infty); dx)$ with θ the boundary condition at 0 has only pure point spectrum.

In Chapter III, we'll need the following formula of Simon-Wolff [47]:

THEOREM II.8. *Suppose $\|\varphi\| = 1$. Let δ_n be an orthonormal basis for $\mathcal{H}$ with $\delta_0 = \varphi$. Then for each $E \in \mathbb{R}$, $\sum_n |(\delta_n, (A - E - i\epsilon)^{-1}\delta_0)|^2$ is monotone increasing as $\epsilon \downarrow 0$ and*

$$G(E) = \lim_{\epsilon\downarrow 0} \sum_n |(\delta_n, (A - E - i\epsilon)^{-1}\delta_0)|^2.$$

PROOF. By the Plancherel theorem, the sum is $\|(A-E-i\epsilon)^{-1}\varphi\|^2 = \int \frac{d\mu_0(x)}{(x-E)^2+\epsilon^2}$. The monotonicity and identification of the limit are immediate. $\square$

II.4 Instability of Point Spectrum

Random potentials have point spectrum embedded in the essential spectrum of h_ω. One of our results in this section is that there are locally uncountably many values of $v_\omega(0)$ which turn that point spectrum into singular continuous spectrum. These are ideas obtained by Gordon [26,27], and then independently by del Rio, et al. [11,12], whose presentation we follow.

The key in many ways is Theorem I.2(iv) which says that $\{x \mid G(x) = \infty\}$ is a dense G_δ. As an example of what this implies, we prove the following (first proven in a slightly weaker form by del Rio [10]):

THEOREM II.9. *Let V be a bounded potential on $[0,\infty)$. Let S be the set of non-isolated points of $\sigma_{\mathrm{ess}}\big(-\frac{d^2}{dx^2} + V\big)$ (this set is independent of boundary conditions at 0). Then, there exists $T \subset S$, a dense G_δ in S so that*

(i) *$E \in T$ is not an eigenvalue of $-\frac{d^2}{dx^2} + V$ for any boundary condition θ at $x = 0$.*

(ii) *If $E \in T$, $\big(-\frac{d^2}{dx^2} + V\big)u = Eu$ does not have a solution ℓ^2 at infinity and, in particular, there is no Lyapunov behavior with $\gamma(E) > 0$ for $E \in T$.*

PROOF. By Theorem I.2(iv), the $G(E)$ associated to the Neumann operator with $\varphi = \delta(x)$ has $G(E) = \infty$ on T_0, a dense G_δ in S. Let T be T_0 minus any eigenvalues for $\theta = \pi/2$. (i), (ii) follow by the results earlier in this chapter. $\square$

EXAMPLE. If V is random with $\operatorname{spec}(H) = [0, \infty)$, this implies non-Lyapunov behavior for a dense G_δ on $[0, \infty)$, even though we know there is such behavior for a.e. E. Dense G_δ sets are sometimes called Baire generic while complements of sets of measure zero are called Lebesgue generic. Both kinds of sets are locally uncountable. The theorem says the sets where one does/does not have Lyapunov behavior with $\gamma > 0$ are intertwined, locally uncountable sets!

We want to turn the $G(E) = \infty$ result into one about α values.

THEOREM II.10 ([12]). *Let $d\mu$ be any measure on $\mathbb{R}$ obeying (I.4). Then the set of values $\{F(E + i0) \mid E \in \operatorname{supp}(d\mu)$ and $G(E) < \infty\}$ is the complement of a dense G_δ.*

PROOF. There is a general argument that the complement is a G_δ [46], so we focus on the fact that the set, S, is a countable union of nowhere dense sets. We sketch the idea behind the proof in [12], leaving the details for that paper.

Write $\{E \mid \in \operatorname{supp}(d\mu)$ and $G(E) < \infty\}$ as a countable union of sets A_n so that

(i) $G(E)$ is close to the constant, γ_n, on A_n.

(ii) For some δ_n and all $x \in A_n$, $\int_{|x-y|<\delta_n} |x - y|^{-2}\, d\mu(y)$ is small compared to the variation of G over A_n.

(iii) For each $x \in A_n$, consider the equilateral triangle, T_x, in $\mathbb{C}$ with one vertex at x and base on the line Im $z = a\delta_n$ with a fixed number, a, (fixed in the proof in [12]). Then $\bigcup_{x \in A_n} T_x$ is connected.

By (i), (ii) $F'(E)$ is very close to the constant γ_n on each T_x so $|F(z) - F(y) - \gamma_n(z - y)| \le \frac{1}{3}\gamma_n |y - z|$ on T_x. By a simple geometric argument using (iii), $|F(z) - F(y) - \gamma_n(z - y)| \le \frac{2}{3}\gamma_n |y - z|$ for $y, z \in \bigcup_{x \in A_n} T_x$ and so in A_n. Since A_n is nowhere dense and this inequality says that F on A_n is the restriction of a homeomorphism from $\mathbb{R}$ to $\mathbb{R}$, we see that $F[A_n]$ is nowhere dense. $\square$

Combining this with Theorem II.2, we immediately get

THEOREM II.11. *In the general context of rank one perturbations, suppose that $[a, b] \subset \operatorname{spec}(A)$ and $\operatorname{spec}_{\mathrm{ac}}(A) \cap (a, b) = \emptyset$. Then for a dense G_δ of α's, A_α has purely singular continuous spectrum on (a, b).*

We emphasize that there is a distinction between singular and point spectrum. If $\operatorname{spec}_{\mathrm{ac}}(A) \cap (a, b) = \emptyset$ and $(a, b) \subset \operatorname{spec}(A)$, there are *always* many α's for which A_α has singular continuous spectrum. There may or may not be α's when there is point spectrum there. The Simon-Wolff criterion gives cases where there is point spectrum for many α's, but the criterion may or may not hold.

REMARK. This result on singular continuous spectrum for dense G_δ's is one of many recently discovered [27,46,11,29]. For example, in [46], it is proven that in $C_\infty(\mathbb{R}^n)$, the continuous functions vanishing at infinity, there is a dense G_δ, S, so that if $V \in S$, then $-\Delta + V$ has purely singular continuous spectrum on $[0, \infty)$.

COROLLARY II.12. *Let $V_\omega(x)$ be a non-deterministic ergodic random process for $x \in \mathbb{R}$ so that* $\operatorname{spec}\big(-\frac{d^2}{dx^2}+V\big) = [a,\infty)$ *for some a. Let H_θ be $-\frac{d^2}{dx^2}+V$ on $L^2(0,\infty)$ with θ boundary condition at $x=0$. Then for a dense G_δ of θ's, H_θ has purely singular continuous spectrum on $[0,\infty)$ (while for Lebesgue almost all, it has only point spectrum there).*

COROLLARY II.13. *Let $\{V_\omega(n)\}_{n\in\mathbb{Z}^\nu}$ be independent, identically distributed random variables with uniform distribution in $[a,b]$ and let H_ω be the corresponding Jacobi matrix on $\ell^2(\mathbb{Z}^\nu)$. Let $|b-a|$ be so large that H_ω has only point spectrum for a.e. ω (see Chapter III). Then for a.e. ω, there is a dense G_δ, S in $[a,b]$, so that for $\alpha \in S$*

$$\begin{aligned} W(n) &= V_\omega(n) \qquad && n \neq 0 \\ &= \alpha && n = 0 \end{aligned}$$

yields a Jacobi matrix with only singular continuous spectrum.

Both corollaries follow immediately from the theorem and earlier discussions of the examples.

II.5 Examples

The astute reader may have noticed that $d\mu_0$ completely determines the spectral properties of the family A_α (assuming cyclicity, of course). Moreover, given μ_0, let A be multiplication by x on $L^2(\mathbb{R}, d\mu_0)$ and let $\varphi(x) \equiv 1$. Then $F(z)$ is just the Borel transform of $d\mu_0$. So we can describe examples by giving the measure $d\mu_0$, which we'll denote by $d\mu$.

EXAMPLE 1 (THE FRIEDRICHS MODEL). Let $d\mu = dx \restriction [0,1] + \delta_{1/2}$ be the sum of Lebesgue measure on $[0,1]$ and a point mass at $1/2$. Then $G(x) = \infty$ on $[0,1]$, and

$$\begin{aligned} \frac{1}{\pi} \operatorname{Im} F(x+i0) &= 1 \qquad && 0 < x < 1; x \neq \frac{1}{2} \\ &= \frac{1}{2} && x = 0, 1. \end{aligned}$$

Thus, A_α has only a.c. spectrum on $[0,1]$ for $\alpha \neq 0$ (there is a single eigenvalue on $(-\infty,0)$ for $\alpha < 0$ and on $(1,\infty)$ for $\alpha > 0$). The embedded eigenvalue dissolves.

EXAMPLE 2. Let $\{q_n\}_{n=1}^\infty$ be a counting of the rationals on $[0,1]$. Let

$$d\mu = dx \restriction [0,1] + \sum_{n=1}^\infty 2^{-n} \delta_{q_n}.$$

As above, all eigenvalues disappear for $\alpha \neq 0$. The interesting case is to take $d\mu = d\mu_{-1}$. The new A has no eigenvalues on $[0,1]$ but $A + (\varphi,\cdot)\varphi$ suddenly has dense point spectrum embedded in the a.c. spectrum.

EXAMPLE 3. Let $d\mu$ be conventional Cantor measure. We claim that $G(x) = \infty$ on C, the Cantor set. In fact,

$$\text{Im } F(x + i\epsilon) \to \infty \tag{II.5}$$

for $x \in C$, which implies that $G(x) = \infty$. This fact about Im F implies that A_α has neither point nor singular spectrum on C. In fact, each A_α has one eigenvalue $e_j(\alpha)$ in each interval, I_j in $[0,1]\backslash C$. The corresponding eigenvectors, together with one, $e_0(\alpha)$, in $I_0 \equiv \mathbb{R}\backslash[0,1]$, are complete. $\text{Spec}(A_\alpha) = \bigcup\limits_{j=0}^{\infty}\{e_j(\alpha)\} \cup C$ since the limit points of the e's are precisely C. To prove (II.5), we claim first that

$$\text{Im } F(x_0 + i\epsilon) \geq \frac{1}{2\epsilon}\,\mu(\{y \mid |x - y| \leq \epsilon\}) \tag{II.6}$$

for any measure μ. Moreover, if $x \in C$, then

$$\mu(\{y \mid |x - y| \leq 2(3^{-n})\}) \geq 2^{-n}$$

so (II.6) implies (II.5).

EXAMPLE 4 ([47]). Let $d\mu_n = \frac{1}{2^n}\sum\limits_{j=1}^{2^n}\delta_{j/2^n}$ and $\mu = \sum a_n\, d\mu_n$ where $\sum a_n < \infty$. If $x \in [0,1]$, then clearly, since there is a j with $|x - (j/2^n)| \leq 2^{-n}$, we have

$$\int |x - y|^{-2}\, d\mu_n(y) \geq (2^{-n})^{-2}2^{-n} = 2^n$$

so if $\sum 2^n a_n = \infty$, then $G(x) = \infty$ on $[0,1]$ and thus A_α has no point spectrum $[0,1]$. So A has dense point spectrum on $[0,1]$ which turns into purely singular continuous spectrum on $[0,1]$ for all $\alpha \neq 0$.

EXAMPLE 5. Let $d\nu$ be Cantor measures and let

$$d\mu(x) = \chi_{[0,1]}\sum_{n=1}^{\infty} n^{-2}\Bigl[\sum_{j=1}^{2^n} d\nu\bigl(x - (j/2^n)\bigr)\Bigr].$$

Then $\mu\{y \mid |y - x| \leq 2^{-n+1}\} \geq 3^{-n}n^{-2}$ for any $\chi \in [0,1]$ so $G(x) \geq \frac{1}{4}(2^{-n})^{-2}3^{-n}$ $n^{-2} = \frac{1}{4}(\frac{4}{3})^n n^{-2}$ for any n and so $G = \infty$ on $[0,1]$. This yields an example with $\sigma(A_\alpha)$ purely singular continuous on $[0,1]$ for all α. As noted, this cannot happen for point spectrum.

EXAMPLE 6 ([47]). Let x_n be arbitrary points in $[0,1]$. Let a_n be a sequence with $0 \leq a_n \leq C_0\alpha^n$ for some $\alpha < 1$. Let

$$d\mu = \sum a_n\delta_{x_n}.$$

We claim $G(x) < \infty$ for a.e. x. For if $|x - x_n| > D^{1/2}\alpha^{n/4}$ for *all* n, then

$$G(x) < \sum_n C_0\alpha^n D^{-1}\alpha^{-n/2} = (1 - \alpha^{1/2})^{-1}C_0/D.$$

Thus

$$\{x \mid G(x) > (1-\alpha^{1/2})^{-1}C_0/D\} \leq \sum 2D^{1/2}\alpha^{n/4} = 2D^{1/2}(1-\alpha^{1/2})^{-1}$$

goes to zero as $D \to 0$ proving that $G(x) < \infty$ for a.e. x. In this case, by the Simon-Wolff criterion, A_α has only pure point spectrum for a.e. α, but for a dense G_δ of α, it has singular continuous spectrum, of course.

Let x_n be the counting of the dyadic rationals. Let $d\mu = \sum b_n \delta_{x_n}$. Examples 4 and 6 say that depending on the b's, A_α can have dense point or singular continuous spectrum for Lebesgue typical α. Spectral properties depend heavily on φ as well as A!

Example 7 ([13]). Let $\{q_n\}_{n=1}^\infty$ be a counting of the rationals in $(0,1)$. Define $a_n = \min(3^{-n-1}, q_n, 1-q_n)$ and let $S = \bigcup_n (q_n - a_n, q_n + a_n)$ so $|S| \leq 2\sum a_n \leq \frac{1}{3}$. Let $d\mu_0 = \chi_S\, dx$ so $\operatorname{spec}(A_0) = [0,1]$ since S is dense in $[0,1]$. Since $|[0,1]\backslash S| \geq \frac{2}{3}$ and $d\mu_{\alpha,\mathrm{ac}}([0,1]\backslash S) = 0$, there must be a positive measure set of α's with point and/or singular spectrum embedded in $\operatorname{spec}(A_\alpha)$. As in the last example, if $|x - q_n| \geq a_n + \sqrt{\epsilon}\, 3^{-n/4}$ for all n, then $G(x) \leq \epsilon^{-1}(1-\sqrt{1/3})^{-1}$. Thus, $\{x \in S \mid G(x) > \epsilon^{-1}(1-\sqrt{1/3})^{-1}\} = \sqrt{\epsilon}\,(1-\sqrt{1/3})^{-1}$ so $G(x) < \infty$ for a.e. $x \in [0,1]\backslash S$. We conclude that for a.e. α, A_α has no singular spectrum on S but it has some point spectrum there for a positive measure set of α's.

Example 8 ([13]). Let $S_n = \bigcup_{j=1}^{n-1} \left(\frac{j}{2^n} - \frac{1}{4n^2 2^n}, \frac{j}{2^n} + \frac{1}{4n^2 2^n}\right)$ and $S = \bigcup_n S_n$, so $|S_n| \leq \frac{1}{2n^2}$ and $|S| \leq \frac{\pi^2}{12} < 1$. Let $d\mu_0 = \chi_S\, dx$. Then, $\operatorname{spec}(A_0) = [0,1]$ but since $|[0,1]\backslash S| > 0$, there must be a positive measure set of α's with point and/or singular spectrum embedded in $\operatorname{spec}(A_\alpha)$. As in Example 4, $G(x) = \infty$ on $[0,1]$ since for any n

$$G(x) \geq (2^{-n-1})^{-2} 2^{-n-1} n^{-2} = 2^n/8n^2 \to \infty.$$

Thus, for all α we have no point spectrum in $[0,1]$ but we have singular continuous spectrum embedded in the a.c. spectrum for a set of positive measure α's.

CHAPTER III

LOCALIZATION IN THE ANDERSON MODEL FOLLOWING AIZENMAN-MOLCHANOV

In this chapter we'll present the approach of Aizenman-Molchanov [2] to the proof of localization for the large coupling Anderson model in arbitrary dimension. The proof is so simple, we won't even put it in separate sections. Results on exponential decay of Green's functions were first obtained by Fröhlich-Spencer [18], with later extensions and simplifications by [17,15]. Even taking into account the fact that we have already developed some of the facts we need, this proof is something like a factor of ten shorter and has smaller constants.

We will prove:

Theorem III.1. *Let* $\{V_\omega(n)\}_{n\in\mathbb{Z}^\nu}$ *be independent identically distributed random variables with uniform density on* $[0,1]$. *Then, there is a fixed constant,* K, *so that if* $|\lambda| > K\nu^2$, *then the Jacobi matrix,* $h_0 + \lambda V_\omega$, *has only pure point spectrum* (*and it is dense in* $[-2\nu, 2\nu+\lambda]$).

Remark. I believe that $K = 32$ is what comes out of the minimization problem below.

Suppose for a moment that we could prove that $E_\omega\bigl(\sum\limits_n |G(n,0;E+i0)|^2\bigr) \le Ce^{-D|n|}$. Then, by Fubini's theorem, we'd get that for a.e. pair (E,ω), $\sum\limits_n |(\delta_n,(A-E-i0)^{-1}\delta_0)|^2 < \infty$, so by Theorems II.8 and II.5, we'd have localization. The problem with this idea is that there is no chance that even $E_\omega(|G(0,0;E+i0)|^2)$ is finite, since after all, $G(0,0;E+i0)$ is precisely $F_\alpha(E+i0)$ for $\alpha = V_\omega(0)$ and that is $F/[1+\alpha F]$ and has a first order zero at $\alpha = -1/F$ if there is to be an eigenvalue. But then, $\int dv(0)(v(0)-a)^{-2}$ is infinite if $a \in \operatorname{supp} v(0)$. So the first key idea of [2] is to look at powers of $(G)^s$ with $0 < s < 1$. For simplicity, we will take $s = \frac{1}{2}$. The following lemma will be useful:

Lemma III.2. *If* $s > 1$, *then for* $\{x_n\}_{n=1}^N$ *all positive* $(N = 1,2,\dots,\infty)$*:*

$$\sum_{n=1}^N {x_n}^s \le \left(\sum_{n=1}^N x_n\right)^s.$$

If $s < 1$, *then*

$$\sum_{n=1}^N {x_n}^s \ge \left(\sum_{n=1}^N x_n\right)^s.$$

PROOF. If $s > 1$, ${x_n}^{s-1} \leq \big(\sum_{m=1}^{N} x_m\big)^{s-1}$

$$ {x_n}^s = x_n {x_n}^{s-1} \leq x_n \left(\sum_{m=1}^{N} x_m\right)^{s-1}. $$

Now sum over n. If $s < 1$, ${x_n}^{s-1} \geq \big(\sum_{m=1}^{N} x_m\big)^{s-1}$ and the proof is identical. $\square$

In particular,

$$ \left(\sum_n |G(n,0;E+i\epsilon)|^2\right)^{1/4} \leq \sum_n |G(n,0;E+i\epsilon)|^{1/2}. \tag{III.1} $$

So we need only control $\sum_n E_\omega(|G(n,0;E+i\epsilon)|^{1/2})$.

A key lemma that we will need is

LEMMA III.3. *There is a universal constant, C_0 so that for all complex numbers, α, β:*

$$ \int_0^1 |x-\alpha|^{1/2} |x-\beta|^{-1/2}\, dx \geq C_0 \int_0^1 |x-\beta|^{-1/2}\, dx. \tag{III.2} $$

REMARK. I believe $\alpha = \beta = \frac{1}{2}$ is the extreme point, in which case $C_0 = 1/\sqrt{8}$.

PROOF. It is easy to see the integral on the left side of (III.2) only decreases if α is replaced by $\operatorname{Re}\alpha$ or if $\alpha \notin [0,1]$ and is replaced by the nearest point in $[0,1]$. So we can suppose that $\alpha \in [0,1]$. By $x \to \frac{1}{2} - x$ symmetry, we can suppose $\alpha \in [0, \frac{1}{2}]$. But then

$$ \int_0^1 |x-\alpha|^{1/2} |x-\beta|^{-1/2}\, dx \geq \sqrt{1/4} \int_{3/4}^1 |x-\beta|^{-1/2}\, dx $$

so we need only show that

$$ \inf_{\beta \in \mathbb{C}} \left[\int_{3/4}^1 |x-\beta|^{-1/2}\, dx \Big/ \int_0^1 |x-\beta|^{-1/2}\, dx \right] > 0. $$

Let $h(\beta)$ be the function in $[\,\cdot\,]$. It is clearly continuous on $\mathbb{C}$, non-vanishing and $\lim_{\beta\to\infty} h(\beta) = \frac{1}{4}$ so the inf is strictly positive. $\square$

One last lemma we will need concerns the free Laplacian, h_0.

LEMMA III.4. (a) *Let $f, g \in \ell^\infty(\mathbb{Z}^\nu)$ be non-negative functions and suppose that*

$$ (1 - a h_0) f \leq g $$

for some $0 < a < \frac{1}{2\nu}$. *Then*

$$f \leq (1 - ah_0)^{-1} g.$$

(b) *If* $0 < a < (2\nu)^{-1}$, *then*

$$(1 - ah_0)^{-1}(i,j) \leq (2\nu a)^{|j-i|}(1 - 2\nu a)^{-1}.$$

PROOF. h_0 has norm 2ν so $(1 - ah_0)^{-1} = \sum_{m=0}^{\infty} (ah_0)^m$ if $2\nu a < 1$. This is a positivity preserving operator, so it preserves inequalities which proves (a). Moreover, by the above expression and $(ah_0)^m(i,j) = 0$ if $m < |i - j|$, we see that

$$(1 - ah_0)^{-1}(i,j) = \sum_{m=|i-j|}^{\infty} (ah_0)^m(i,j) \leq \sum_{m=|i-j|}^{\infty} (2\nu a)^m$$

proving (b). □

PROOF OF THEOREM III.1. Fix $z \in \mathbb{C} \backslash \mathbb{R}$ and let $g_\omega(n) = G_\omega(0, n; z)$ and

$$k(n) = E_\omega(|g_\omega(n)|^{1/2}).$$

We claim that (with C_0 the constant in Lemma III.3):

$$k(n) \leq (C_0 \lambda^{1/2})^{-1} \left[\left(\sum_{|j|=1} k(n+j) \right) + \delta_{n0} \right] \tag{III.3}$$

For g_ω obeys

$$\sum_{|j|=1} g_\omega(n+j) + (\lambda v_\omega(n) - z) g_\omega(n) = \delta_{n0}.$$

Using Lemma III.2,

$$E_\omega\big(|\lambda v_\omega(n) - z|^{1/2} |g_\omega(n)|^{1/2}\big) \leq \delta_{n0} + \sum_{|j|=1} k(n+j). \tag{III.4}$$

Fix $\{v_\omega(\ell)\}_{\ell \neq n}$. Then, by (I.14), $g_\omega(n) = C/(\lambda v_\omega(n) + d)$ with $C \neq 0$ and C, d are functions of $\{v_\omega(\ell)\}_{\ell \neq n}$. Thus averaging only over $v_\omega(n)$:

$$\begin{aligned}
\int_0^1 |\lambda v - z|^{1/2} |C/(\lambda v_\omega + d)|^{1/2}\, dv &= \lambda^{1/2}(C/\lambda)^{1/2} \int_0^1 |v - z\lambda^{-1}|^{1/2} |1/v + d\lambda^{-1}|^{1/2}\, dv \\
&\geq C_0 \lambda^{1/2} (C/\lambda)^{1/2} \int_0^1 |1/v + d\lambda^{-1}|^{1/2}\, dv \\
&= C_0 \lambda^{1/2} \int_0^1 |C/\lambda v + d|^{1/2}\, dv
\end{aligned}$$

where C_0 is the constant in Lemma III.3. Averaging over $\{v_\omega(\ell)\}_{\ell\neq n}$, we get

$$E_\omega\big(|\lambda v_\omega - z|^{1/2}|g_\omega(n)|^{1/2}\big) \geq C_0\lambda^{1/2}k(n). \tag{III.5}$$

Obviously, (III.4/5) imply (III.3).

(III.3) can be rewritten to say

$$(1 - C_0\lambda^{1/2}h_0)k \leq \delta_{n0}.$$

Because $z \notin \mathbb{R}$, $|g_\omega(n)| \leq (1/|\mathrm{Im}\ z|)^{1/2}$, so $k \in \ell^\infty$. We can therefore apply Lemma III.4 to conclude that if $(C\lambda^{1/2})^{-1} < (2\nu)^{-1}$ (or $\lambda > 4C^{-2}\nu^2$)

$$\begin{aligned} k(n) &\leq (C_0\lambda^{1/2})^{-1}(1 - (C\lambda^{1/2})^{-1}h_0)^{-1}(0,n) \\ &\leq (C_0\lambda^{1/2})^{-1}[(2\nu)(C_0\lambda^{1/2})^{-1}]^{|n|}(1 - 2\nu(C_0\lambda^{1/2})^{-1})^{-1}. \end{aligned}$$

Thus, $\sum\limits_n k(n)$ is bounded uniformly in z, so by (III.1):

$$\sup_z E_\omega\bigg(\Big(\sum_n |G(n,0;z)|^2\Big)^{1/4}\bigg)$$

is bounded uniformly in z. Using Theorem II.8, this implies that for $A = h_\omega$, $\varphi = \delta_0$, we have

$$E_\omega(G(E)^{1/4}) < \infty$$

for all $E \in \mathbb{R}$. Thus for a.e. pairs, (V,E), $G(E) < \infty$. Now apply Theorem II.5 to get localization. $\square$

Actually, the proof shows that $E_\omega\big((e^{\delta|n|}\sum\limits_n |G(n,0;z)|^2)^{1/4}\big) < \infty$ for some $\delta > 0$ and this implies exponential decay of eigenfunctions (essentially by (I.14)). Indeed, one easily sees that each eigenvector φ obeys $|\varphi(n)| \leq C_{\varphi,\epsilon}\big[\frac{\nu^2}{k|\lambda|}\big]^{(1-\epsilon)|n|/2}$ for each $\epsilon > 0$. For extensions of these ideas, see [2,1].

CHAPTER IV

THE XI FUNCTION

IV.0 Introduction: The Trace Formula

In this chapter, I'll discuss a program of F. Gesztesy and mine (in part with Holden and Zhao) that deals with inverse spectral theory for one-dimensional Schrödinger and Jacobi matrices [22]. In the study of the inverse problem for periodic potentials, an important role is played by the trace formula originally proven by Gelfand-Levitan and exploited/refined by many authors subsequently; see [24] for a history.

Let me describe this formula: let $V(x+L) = V(x)$. Then $\operatorname{spec}\bigl(-\frac{d^2}{dx^2} + V(x)\bigr) = [E_0, E_1] \cup [E_2, E_3], \dots$ where $E_0, E_3, E_4, \dots, E_{4n-1}, E_{4n}, \dots$ are periodic eigenvalues, and $E_1, E_2, \dots, E_{4n+1}, E_{4n+2}, \dots$ are antiperiodic eigenvalues. Let $\{\mu_j(x)\}_{j=1}^\infty$ be the eigenvalues on $L^2(x, x+L)$ with $u(x) = u(x+L) = 0$ Dirichlet boundary conditions. It can be shown that $E_{2j-1} \le \mu_j(x) \le E_{2j}$. The trace formula says that, at least when V is smooth enough (C^1 will do)

$$V(x) = E_0 + \sum_{j=1}^\infty (E_{2j} + E_{2j-1} - 2\mu_j(x)). \tag{IV.1}$$

One of our goals in this chapter is to extend this formula to more general V's than periodic. One issue to consider immediately is a case like $V(x) = x^2 - 1$ where $V(x) \to \infty$ as $|x| \to \infty$. Then the bands, $[E_{2j}, E_{2j+1}]$ collapse to a point and we have eigenvalues $E_0 < E_1 < \cdots$ and Dirichlet eigenvalues $\{\mu_j(x)\}_{j=1}^\infty$ (with $u(x) = 0$ boundary conditions) and $E_{j-1} \le \mu_j(x) \le E_j(x)$. The formal analog of (IV.1) is

$$V(x) = E_0 + \sum_{j=1}^\infty (E_{j-1} + E_j - 2\mu_j(x)). \tag{IV.2}$$

As an example, take $V(x) = x^2 - 1$ and look at $\mu_j(x=0)$: $E_n = 2n, n = 0, 1, 2, \dots$ and $\{\mu_j(0)\}_{j=1}^\infty$ are $\{2, 2, 6, 6, 10, 10, \dots\}$. It follows that (IV.2) says

$$-1 = -2 + 2 - 2 \dots.$$

Since the Abelian sum $1 - 1 + 1 - \cdots$ is $1/2$, this is promising but it is clear that the final result will need a summability method to accommodate the formula. Indeed, our trace formula (when $V > 0$) will read: Let $\xi(x,\lambda)$ be the Krein spectral shift for infinite coupling with $A = -\frac{d^2}{dx^2} + V(x)$ and $\varphi = \delta(x)$. Then

$$V(x) = \lim_{\gamma\to\infty} \int_0^\infty \frac{\gamma^2}{(\lambda+\gamma)^2}\,(1-2\xi(x,\lambda))\,dx. \tag{IV.3}$$

Note that $|1 - 2\xi(x,\lambda)| = 1$ in all discrete spectrum cases, clearly illustrating the need for a summability method.

IV.1 Abstract Trace Formula

We recall some facts from §I.5,6. As usual, let $A \geq 0$, $A_\alpha = A + \alpha(\varphi,\cdot)\varphi$ with A_∞ defined as the strong resolvent limit of A_α as $\alpha \to \infty$. Define

$$F(z) = (\varphi, (A-z)^{-1}\varphi) \tag{IV.4}$$

and ξ_∞ by

$$\xi_\infty(\lambda) = \frac{1}{\pi}\ \mathrm{Arg}\ F(\lambda + i0). \tag{IV.5}$$

Then

$$\mathrm{Tr}(f(A) - f(A_\infty)) = -\int f'(\lambda)\xi_\infty(\lambda)\,dx \tag{IV.6}$$

and

$$\int_0^\infty \frac{\xi_\infty(\lambda)\,d\lambda}{(\lambda-z)^2}\,dx = \frac{d}{dz}\ \ln F(z). \tag{IV.7}$$

We also will consider a second problem with $A^{(0)}$, $\xi_\infty^{(0)}$ and $F^{(0)}$. The point of a comparison is that with great generality, Green's functions, $G(0,0;z)$, have the same behavior, viz $(2(-z)^{1/2})^{-1}$ at $z = -\infty$.

Theorem IV.1 ([24]). *Suppose that* $\lim_{\gamma\to\infty} F(-\gamma)/F^{(0)}(-\gamma) = 1$. *Then for* $z \in \mathbb{C}\backslash[0,\infty)$

$$F(z) = F^{(0)}(z)\exp\biggl(\lim_{\gamma\to\infty}\int \frac{\gamma}{\lambda+\gamma}\ \frac{1}{\lambda-z}\,(\xi_\infty - \xi_\infty^{(0)})(x)\,dx\biggr). \tag{IV.8}$$

Proof. (IV.7) for $F, F^{(0)}$ integrated says that

$$\ln(F(z)/F^{(0)}(z)) - \ln(F(-\gamma)/F^{(0)}(-\gamma)) = \int\biggl(\frac{1}{\lambda-z} - \frac{1}{\lambda+\gamma}\biggr)(\xi_\infty - \xi_\infty^{(0)})(\lambda)\,d\lambda. \tag{IV.9}$$

Moreover, by dominated convergence, for z fixed

$$\lim_{\gamma\to\infty}\int \frac{|z|}{|\lambda-z|}\ \frac{1}{\lambda+\gamma}\,|(\xi_\infty - \xi_\infty^{(0)}(\lambda)|\,d\lambda = 0. \tag{IV.10}$$

(IV.9,10) and $\lim_{\gamma\to\infty} \ln(F(-\gamma)/F^{(0)}(-\gamma)) = 0$ imply (IV.8). $\square$

Theorem IV.2: The Abstract Trace Formula ([24]). *Supose that for some $\epsilon > 0$, $\lim_{\substack{|\gamma|\to\infty \\ |\text{Arg }\gamma|<\epsilon}} \gamma\left(\frac{F(-\gamma)}{F^{(0)}(-\gamma)} - 1\right) = a$. Then*

$$a = \lim_{\substack{\gamma\to\infty \\ \gamma \text{ real}}} \int \frac{\gamma^2}{(\lambda+\gamma)^2}(\xi_\infty - \xi_\infty^{(0)})(\lambda)\, d\lambda.$$

Proof. By hypothesis

$$\lim_{\substack{|\gamma|\to\infty \\ |\text{Arg }\gamma|<\epsilon}} \gamma \ln\left[\frac{F(-\gamma)}{F^{(0)}(-\gamma)}\right] = a.$$

By a simple contour argument

$$\lim_{\substack{\gamma\to\infty \\ \gamma \text{ real}}} \gamma^2 \left(\frac{d}{dz} \ln\left[\frac{F(z)}{F^{(0)}(z)}\right]\right)_{z=-\gamma} = a.$$

This plus (IV.7) implies the result. $\square$

IV.2 The Trace Formula for Schrödinger Operators

We'll postpone the proof of the following until later in this section:

Lemma IV.3. *Suppose that V is bounded from below and is continuous at x. Let G be the Green's function for $-\frac{d^2}{dx^2} + V(x)$ on $L^2(-\infty,\infty)$. Then as $|\gamma| \to \infty$ with $|\text{Arg }\gamma| < \pi/2$:*

$$G(x,x;-\gamma) = \frac{1}{2}(\gamma)^{-1/2}\left(1 - \frac{1}{2}\gamma^{-1}V(x) + 0(\gamma)^{-1}\right) \tag{IV.11}$$

Example. This will be the comparison $F^{(0)}$ so it is a critical example: Let $A^{(0)} = -\frac{d^2}{dx^2}$ on $L^2(\mathbb{R}, dx)$. Let $\varphi = \delta_x$. Then $F^{(0)}(z) = G^{(0)}(x,x;z) = \frac{1}{2}(-z)^{-1/2}$. Thus $F^{(0)}(x+i0) = \frac{1}{2}(x)^{-1/2}i$ and $\xi_\infty^{(0)}(x) = \frac{1}{2}, x > 0$.

We now apply the abstract theory of the last section:

Theorem IV.4. *Suppose that V is non-negative and is continuous at x. Let $\xi(x,\lambda)$ be $\xi_\infty(x)$ for $A = -\frac{d^2}{dx^2} + V; \varphi = \delta_x$. Then*

$$V(x) = \lim_{\gamma\to\infty} \int_0^\infty \frac{\gamma^2}{(\lambda+\gamma)^2}\left[1 - 2\xi(x,\lambda)\right] d\lambda \tag{IV.12}$$

and

$$G(x,x;z)=\frac{1}{2}\,(-z)^{-1/2}\exp\biggl(\lim_{\gamma\to\infty}\int_0^\infty \frac{\gamma}{\gamma+\lambda}\,\frac{1}{\lambda-z}\biggl[\xi(x,\lambda)-\frac{1}{2}\biggr]\,dx\biggr) \tag{IV.13}$$

PROOF OF LEMMA IV.3 WHEN V IS BOUNDED. W.l.o.g. suppose $x=0$. Let $\psi(x)=(H_0+\gamma)^{-1}\delta_0(x)=\frac{1}{2}\gamma^{-1/2}e^{-\gamma^{1/2}|x|}$, so $\|\psi_\gamma\|=0(\gamma^{-3/4})$. By the second resolvent equation, since V is bounded

$$(\delta_0,(H_0+V+\gamma)^{-1}\delta_0)=(\delta_0,(H_0+\gamma)^{-1}\delta_0)-(\psi_\gamma,V\psi_\gamma)+R \tag{IV.14}$$

where $\|R\|\le\|\psi_\gamma\|^2\gamma^{-1}=0(\gamma^{-5/2})$. The first term in (IV.14) is $\frac{1}{2}\gamma^{-1/2}$ and the second is

$$-\frac{1}{4}\,\gamma^{-1}\int_{-\infty}^{\infty} e^{-2\gamma^{1/2}|x|}V(x)\,dx=-\frac{1}{4}\,\gamma^{-3/2}[V(0)+o(1)]$$

since $\int_{-\infty}^{\infty} e^{-2\alpha|x|}\,dx=\alpha^{-1},\alpha>0$. □

PROOF OF LEMMA IV.3 IN THE GENERAL CASE. We will prove with $H=H_0+V$ that

$$e^{-tH}(x,x)=(4\pi t)^{-1/2}(1-tV(x)+o(t)). \tag{IV.15}$$

(IV.11) then follows from

$$G(x,x;-\gamma)=\int_0^\infty e^{-\gamma s}e^{-sH}(x,x)\,ds$$

and

$$\int_0^\infty t^{-1/2}e^{-t}\,dt=\sqrt{\pi}\quad\text{and}\quad\int_0^\infty t^{1/2}e^{-t}\,dt=\frac{1}{2}\sqrt{\pi}.$$

To prove (IV.15), let $\{\omega(s)\}_{0\le s\le 1}$ be the Brownian bridge [43] so the Feynman-Kac formula has the form [43]

$$e^{-tH}(x,x)=(4\pi t)^{-1/2}E_\omega\biggl(\exp\biggl[-t\int_0^1 V(x+2\sqrt{2t}\,\omega(s))\,ds\biggr]\biggr). \tag{IV.16}$$

A Levy-type estimate implies that

$$E_\omega\biggl(\sup_{0\le s\le 1}\omega(s)\ge\alpha\biggr)\le C_1e^{-C_2\alpha^2}.$$

Changing V outside $(x-\delta,x+\delta)$ changes the right side of (IV.16) by $0(e^{-C/t})$, so in proving (IV.15), we can suppose that V is bounded. But if V is bounded, it is easy to see that the integral is $1-tV(x)+o(t)$. □

Since we controlled $e^{-tH}(x,x)$, we can prove the slightly stronger version of (IV.12), viz [24]:

$$V(x) = \lim_{\gamma\downarrow\infty} \int_0^\infty e^{-\gamma\lambda}(1-2\xi(x,\lambda))\,d\lambda.$$

This is all with V positive. If it is only bounded below and $E_0 \le \inf\ \mathrm{spec}(H)$, then

$$V(x) = E_0 + \lim_{\gamma\downarrow 0} \int_{E_0}^\infty e^{-\gamma\lambda}(1-2\xi(x,\lambda))\,d\lambda.$$

See [23] for higher order asymptotic formula involving moments of ξ.

IV.3 Examples

EXAMPLE 1 (PERIODIC POTENTIALS). We begin with the motivating case of periodic potentials, $V(x) = V(x+L)$. The spectrum of H is $[E_0,E_1]\cup[E_2,E_3]\cup\cdots$. General principles imply that $\xi(x,\lambda)$ obeys

$$\xi(x,\lambda) = \begin{cases} \frac{1}{2}, & E_{2n} < \lambda < E_{2n+1} \\ 1, & E_{2n-1} < \lambda < \mu_n(x) \\ 0, & \mu_n(x) < \lambda < E_{2n} \text{ or } \lambda < E_0. \end{cases}$$

If V is smooth enough (e.g., $V \in C^1$), $\sum |E_{2n}-E_{2n-1}| < \infty$ so $\int |2-2\xi(x,\lambda)|\,d\lambda < \infty$ and the summability method is not needed. Clearly,

$$\int_{E_{2n-1}}^{E_{2n}} (1-2\xi)\,d\lambda = -(\mu_n - E_{2n-1}) + (E_{2n}-\mu_n) = E_{2n}+E_{2n-1}-2\mu_n$$

$$\int_0^{E_0} (1-2\xi)\,d\lambda = E_0$$

and we get

$$V(x) = E_0 + \sum_{n=1}^\infty (E_{2n}+E_{2n-1}-2\mu_n(x)).$$

EXAMPLE 2 (HARMONIC OSCILLATOR). $V(x) = x^2-1$; the eigenvalues are $0,2,4\ldots$ and

$$\xi(0,\lambda) = \begin{cases} 1, & 0<\lambda<2;\ 4<\lambda<6,\ldots \\ 0, & 2<\lambda<4;\ 6<\lambda<8,\ldots \end{cases}$$

$$\begin{aligned} \int_0^\infty e^{-\alpha\lambda}((-2\xi(0,\lambda))\,d\lambda &= \alpha^{-1}(1-e^{-2\alpha})\sum_{n=0}^\infty (-1)^{n+1}e^{-2n\alpha} \\ &= \alpha^{-1}(1-e^{-2\alpha})(-1)/[1+e^{-2\alpha}] \end{aligned}$$

converges to -1 as $\alpha\downarrow 0$. Thus the summability method yields $V(0)$. In general, THEOREM IV.5. *Let $V(x) \to \infty$ as $|x| \to \infty$. Let $E_0 \le \mu_1(x) \le E_1 \le \cdots$ be the eigenvalues of $-\frac{d^2}{dx^2} + V$ on all of $L^2(\mathbb{R}, dx)$ and with a Dirichlet boundary condition at x. Then*

$$V(x) = E_0 + \lim_{\gamma \downarrow 0} \sum_{n=1}^{\infty} [2e^{-\gamma\mu_n(x)} - e^{-\gamma E_n} - e^{-\gamma E_{n-1}}]\gamma^{-1}.$$

EXAMPLE 3 (SHORT RANGE POTENTIALS). Suppose $|V(x)| \le C(1+|x|)^{-1-\epsilon}$. Let $R_\ell(\lambda)$ be the usual reflection coefficient and $f_\ell(x,\lambda)$ the Jost function at $-\infty$. Then [21]

$$\xi(x,\lambda) = \frac{1}{2} + \operatorname{Arg}\bigl[1 + R_\ell(\lambda) f_\ell(x,\lambda)^2 / |f_\ell(x,\lambda)|^2\bigr], \qquad \lambda > 0.$$

We see that if $\int |R_\ell(\lambda)|\, d\lambda < \infty$, then $\int |1 - 2\xi(x,\lambda)|\, dx < \infty$ and one can take the limit inside the integral. See [21] for other short range examples.

As a preliminary to the next example, we need a formula about how Dirichlet eigenvalues $\mu(x)$ move as x changes.

THEOREM IV.6. *Let (a,b) be an interval in $\mathbb{R}\backslash\operatorname{spec}(H)$ (i.e., a spectral gap of H) and suppose $\mu(x)$ is an eigenvalue of H_x, the operator with a Dirichlet boundary condition at x with $\mu(x) \in (a,b)$. Let $g(x,\lambda) \equiv G(x,x;\lambda)$.*

(i) $\frac{\partial g}{\partial x}(x,\lambda)\Big|_{\lambda=\mu(x)} = \pm 1$ *with the value equal $+1$ (resp. -1) if the eigenvalue lies on $(-\infty, 0]$ (resp. $[0,\infty)$).*

(ii) *With the same sign as in* (i)

$$\mu'(x) = \pm \left(\frac{\partial g}{\partial \mu}(x, \mu(x)) \right)^{-1}. \tag{IV.17}$$

PROOF. (i) By general principles with $\varphi_\pm$ L^2 at $\pm\infty$:

$$g(x,\lambda) \equiv \frac{\varphi_-(x)\varphi_+(x)}{\varphi_+(x)\varphi_-'(x) - \varphi_-(x)\varphi_+'(x)}$$

so

$$\frac{\partial g}{\partial x}(x,\lambda) = \frac{\varphi_+(x)\varphi_-'(x) + \varphi_-(x)\varphi_+'(x)}{\varphi_+(x)\varphi_-'(x) - \varphi_-(x)\varphi_+'(x)}.$$

At $\mu(x)$, either $\varphi_+(x) = 0$, in which case $\frac{\partial g}{\partial x} = -1$, or $\varphi_-(x) = 0$, in which case $\frac{\partial g}{\partial x} = 1$ as claimed.

(ii) Immediate from (i), given the implicit function theorem that says that $\mu' = -[\partial g/\partial x]/[\partial g/\partial \mu]$. $\square$

EXAMPLE 4 (THE SOLITON). A *reflectionless* potential is one with $\xi(x,\lambda)=\frac{1}{2}$ for *all* x and a.e. λ in $\mathrm{spec}_{\mathrm{ac}}(H)$. Let us look for reflectionless potentials with a single eigenvalue at $E=-1$. Let $\mu(x)$ be the Dirichlet eigenvalue in $(-1,0]$. Then

$$\xi(x,\lambda)=\begin{cases}0, & \lambda<-1 \text{ or } \mu(x)<\lambda<0\\ 1, & -1<\lambda<\mu(x)\\ \frac{1}{2}, & \lambda>0.\end{cases}$$

The formulae for g and V then equal

$$\begin{aligned}V(x)&=2(-1-\mu(x))\\ g(x,\lambda)&=\frac{1}{2}\,(-\lambda)^{-1/2}\ \frac{\mu(x)-\lambda}{-1-\lambda}.\end{aligned}$$

(IV.17) reads

$$\mu'(x)=\pm 2(-\mu)^{1/2}(1+\mu). \tag{IV.18}$$

Let $c(x)=(-\mu)^{1/2}$. Then (IV.18) becomes

$$c'=\pm(1-c^2)$$

whose solution is $c(x)=\pm\tanh(x)$ so we get

$$\begin{aligned}V(x)&=-2(1-\tanh^2(x))\\ &=\frac{-2}{\cosh^2(x)},\end{aligned}$$

the familiar soliton! This arguments does *not* show this potential is reflectionless, only that it is the only candidate. However, a comparison with the formula for $\xi(x,\lambda)$ in Example 3 indeed verifies that $R_\ell(\lambda)=0, \lambda>0$ in the present case.

IV.4 The Trace Formula for Jacobi Matrices

THEOREM IV.7. *Let $H=H_0+V$ be a Jacobi matrix on $\mathbb{Z}^\nu$ with V bounded. Let $\xi(n,\lambda)$ be ξ_∞ for $A=H_0+V$ and $\varphi=\delta_n$. Let $E_\pm=\substack{\sup\\ \inf}$ spec(H). Then*

$$V(n)=\frac{1}{2}\,(E_+ + E_-)+\int_{E_-}^{E_+}\left(\xi(n,\lambda)-\frac{1}{2}\right)d\lambda. \tag{IV.19}$$

PROOF. (IV.19) is unchanged if we add a constant, c, to V (since then V, E_+, and E_- all increase by c), so w.l.o.g. we can suppose that $H\geq 0$. Since $\xi=0$ (resp. 1) for $\lambda<E_-$ (resp. $\lambda>E_+$), we need only prove (IV.19) for some $E_+>\sup\mathrm{spec}(H)$ and $E_-<\inf\mathrm{spec}(H)$.

Next we note that (IV.19) can be rewritten

$$V(n) = E_- + \int_{E_-}^{E_+} (\xi(n,\lambda) - 1)\, d\lambda = E_- + \int_{E_-}^{\infty} (\xi(n,\lambda) - 1)\, d\lambda$$
$$= E_+ + \int_{-\infty}^{E_+} \xi(n,x)\, dx$$

so it suffices to prove

$$V(n) = \int_0^\infty (\xi(n,x) - 1)\, dx$$

for $H \geq 0$.

But noting that

$$(\delta_n, (H+\gamma)^{-1}\delta_n) = \gamma^{-1} - \gamma^{-2}V(n) + O(\gamma^{-3}),$$

this follows from (I.30) (Theorem I.17). $\square$

IV.5 A Regularity Theorem for the A.C. Spectrum

In this section we'll prove the following:

THEOREM IV.8 ([24]). *Let $V_m(x)$ and $V_\infty(x)$ be functions on $\mathbb{R}$ (resp. $\mathbb{Z}$) so that*

(i) $\inf_{\substack{x\in\mathbb{R}\\ m=1,2,\dots,\infty}} V_m(x) > -\infty$ *and for each $R > 0$,* $\sup_{\substack{|x|\in R\\ m=1,2,\dots,\infty}} |V_m(x)| < \infty$ *(resp.* $\sup_{\substack{x\in\mathbb{Z}\\ m=1,2,\dots,\infty}} |V_m(x)| < \infty$*).*

(ii) *$V_m \to V_\infty$ uniformly on compacts (resp. pointwise).*

(iii) *Each V_m is periodic (but the period can be m-dependent).*

Let H_m, H_∞ be the Hamiltonians $-\frac{d^2}{dx^2} + V_m$ (resp. the Jacobi matrices on $\ell^2(\mathbb{Z})$, $h_0 + V_m$). Then (with $|\cdot|$ = Lebesgue measure):

$$|\sigma_{\text{ac}}(H_\infty)| \geq \overline{\lim}\, |\sigma_{\text{ac}}(H_m)|.$$

The most interesting application of this result is to prove a slightly strengthened version of a striking result of Last [34]:

COROLLARY IV.9. *Let $V(n) = \lambda\cos(\pi\alpha n + \theta)$ and let h be the corresponding Jacobi matrix. Then $|\sigma_{\text{ac}}(h)| \geq 4 - 2|\lambda|$.*

PROOF. If $\alpha = p/q$ is rational, this is proven in [7]. If α is arbitrary, let $p_m/q_m \to \alpha$ and let $V_m(n) = \lambda\cos(\pi_m\alpha n + \theta)$. Then V, V_m obey the hypotheses of Theorem IV.8. So, by the theorem, we can take limits. $\square$

REMARK. If α is a Liouville number (irrational but well approximated by rationals), it is known for $\lambda > 2$, that h has only singular continuous spectrum and before Last [34], some believed that was true also for $|\lambda| < 2$. Last showed that if $|\lambda| < 2$, $|\sigma_{\rm ac}(h)| > 0$.

To prove Theorem IV.8, we begin with

THEOREM IV.10. *Under the hypotheses* (i), (ii) *of Theorem* IV.8*,*

$$\xi_\infty^{(m)}(x,\lambda)\,dx \to \xi_\infty^{(\infty)}(x,\lambda)\,dx$$

weakly as measures where $\xi_\infty^{(m)}$ *is the spectral shift for* $-\frac{d^2}{dx^2} + V_m$ *with* $\varphi = \delta(x)$.

PROOF. It suffices to prove that for all $z \in \mathbb{C}\backslash\mathbb{R}$

$$\int \frac{\xi_\infty^{(m)}(x,\lambda)\,d\lambda}{(\lambda - z)^2} \longrightarrow \int \frac{\xi_\infty^{(\infty)}(x,\lambda)\,d\lambda}{(\lambda - z)^2}$$

by a standard density argument. By (I.29) and the Cauchy formula, it suffices to prove that $F_m(z) \to F_\infty(z)$ where $F_m(z) = G_{V_m}(0,0;z)$. Writing

$$\big[(H_n - z)^{-1} - (H_\infty - z)^{-1}\big](H_\infty - z)\psi = (H_n - z)^{-1}(V_\infty - V_n)\psi$$

for $\psi \in C_0^\infty(\mathbb{R})$, we see that

$$\text{s-lim }(H_n - z)^{-1} = (H_\infty - z)^{-1}. \tag{IV.20}$$

Let $H_0 = -\frac{d^2}{dx^2}$. Then $(H_\infty + 1)^{+1/2}(H_n - z)^{-1}(H_0 + 1)^{1/2}$ is uniformly bounded, so (IV.20) implies that

$$\text{s-lim }(H_\infty + 1)^{1/2}(H_n - z)^{-1}(H_0 + 1)^{1/2} = (H_0 + 1)^{1/2}(H_\infty - z)^{-1}(H_0 + 1)^{1/2}.$$

Since $(H_0 + 1)^{-1/2}\delta_0$ is in L^2, we can take matrix elements in this vector and conclude that $F_m(z) \to F_\infty(z)$ is as required. $\square$

PROOF OF THEOREM IV.8. Since V_m is periodic, $\xi_m(x,\lambda) = 0, 1$ or $\frac{1}{2}$ for a.e. λ. Fix $[a,b] \subset \mathbb{R}$ bounded and let $A_m = \{\lambda \mid \xi_m(x,\lambda) = 0\} \cap [a,b]$ for $m = 1, 2, \ldots, \infty$. Then

$$0 = \int\limits_{A_\infty} \xi_\infty(x,\lambda)\,d\lambda = \lim \int\limits_{A_\infty} \xi_m(x,\lambda)\,d\lambda \geq \lim \frac{1}{2}\,|A_\infty\backslash A_m| \geq \frac{1}{2}\,(|A_\infty| - \varliminf |A_m|).$$

We conclude that

$$|A_\infty| \leq \varliminf |A_m|.$$

A similar argument with $\xi_m = 1$ shows that

$$|\{\lambda \mid 0 < \xi_\infty(x,\lambda) < 1\} \cap [a,b]| \geq \varlimsup \left|\left\{\lambda \mid \xi_m(x,\lambda) = \frac{1}{2}\right\} \cap [a,b]\right|.$$

But $\xi_\infty(x,\lambda) = \frac{1}{\pi}\text{ Arg }(F_\infty(\lambda + i0))$ lies in $(0,1)$ if and only if $\text{Im } F_\infty > 0$ (at points with $F_\infty(\lambda + i0)$ finite). So

$$|\sigma_{\rm ac}(H_m) \cap [a,b]| \geq |\{\lambda \mid 0 < \xi_m(x,\lambda) < 1\} \cap [a,b]|$$

with equality if m is finite. $\square$

IV.6 Inverse Problems

These ideas play an important role in understanding inverse spectral theory. We'll give an example here; see [24] (and a paper in preparation) for further examples. We'll rely on the Gelfand-Levitan theory [20,35] which allows one to recover $V(x)$ from any $m_\alpha(z)$ and, in particular, from $G_{\theta=\pi/2}(0,0;z)$. In 1952 Borg [8] and Marčenko [36] proved that:

THEOREM IV.11. *Let $V(x) \to \infty$ to infinity. Let $\{E_n^{(\alpha)}\}_{n=1}^\infty$ be the eigenvalues for $-\frac{d^2}{dx^2} + V(x)$ with θ boundary conditions at $x = 0$ where $\alpha = -\cot(\theta)$. Then V can be recovered from $\{E_n^{(\alpha)}\}_{n=1}^\infty$ for any two distinct values of α.*

Actually, Marčenko [36] proved in addition that the two values of α can be recovered as well from the two sets $\{E_n^{(\alpha)}\}_{n=1}^\infty$.

We'll prove a generalization of this.

THEOREM IV.12. *Suppose that V is bounded below. Let $\xi_{\alpha,\beta}(\lambda)$ ($\alpha > \beta$) be the spectral shift for going from A_β to A_α. Then α, β, and V can be recovered from $\xi_{\alpha,\beta}(\lambda)$.*

REMARK. This implies Theorem IV.11. For in that case $E_n^{(\beta)} \leq E_n^{(\alpha)} \leq E_{n+1}^{(\beta)}$ and

$$\xi_{\alpha,\beta}(\lambda) = \begin{cases} 1 & E_n^{(\beta)} < \lambda < E_n^{(\alpha)} \\ 0 & E_n^{(\alpha)} < \lambda < E_{n+1}^{(\beta)}. \end{cases}$$

PROOF. Let $F(z)$ be the Neumann-Green's function, $G_{\theta=\pi/2}(0,0;z)$, from which $V(x)$ can be recovered by Gelfand-Levitan. We have that $\xi_{\alpha,\beta}(\lambda) = \xi_\alpha(\lambda) - \xi_\beta(\lambda)$ and

$$\int \frac{\xi_\alpha(\lambda)}{(\lambda - z)}\, d\lambda = \ln(1 + \alpha F(z)) \qquad \alpha < \infty \tag{IV.21}$$

$$\int \frac{\xi_\infty(\lambda)}{(\lambda - z)^2}\, d\lambda = \frac{F'(z)}{F(z)} \qquad \alpha = \infty \tag{IV.22}$$

and

$$F(z) = (-z)^{-1/2}(1 + O(|z|)^{-1}) \tag{IV.23}$$

by (I.16), (1.19), (1.29), and (IV.11).

Since $\int \xi_\alpha(\lambda)/(|\lambda|+1) = \infty$ if and only if $\alpha = \infty$, we see that $\int \frac{\xi_{\alpha,\beta}(\lambda)}{|\lambda|+1}\, d\lambda = \infty$ if and only if α is infinite, and we can read that fact off of knowing $\xi_{\alpha,\beta}(\lambda)$. Consider first the case with α, β finite. By (IV.23)

$$\begin{aligned}\ln(1 + \alpha F(z)) &= \alpha F(z) - \frac{1}{2}\,\alpha^2 F(z)^2 + O(F(z)^3) \\ &= \alpha(-z)^{-1/2} - \frac{1}{2}\,\alpha^2(-z)^{-1} + O(z^{-3/2}).\end{aligned}$$

Thus, by (IV.21)

$$\int \frac{\xi_{\alpha,\beta}(\lambda)}{(\lambda - z)}\, d\lambda \sim (\alpha - \beta)(-z)^{-1/2} - \frac{1}{2}\,(\alpha^2 - \beta^2)(-z)^{-1} + O(z^{-3/2})$$

so we can find $\alpha - \beta$ and $\alpha^2 - \beta^2$ and so α and β from $\xi_{\alpha,\beta}$. Moreover, since

$$\int \frac{\xi_{\alpha,\beta}(\lambda)}{\lambda - z}\, d\lambda = \ln\left(\frac{1+\alpha F(z)}{1+\beta F(z)}\right)$$

$\xi_{\alpha,\beta}$ determines $F(z)$ and so V by Gelfand-Levitan.

Now consider the case $\alpha = \infty$. Then by (IV.23) and a countour integral:

$$\begin{aligned}\frac{F'(z)}{F(z)} &= -\frac{1}{2}\,(-z)^{-1} + O(z^{-2})\\ \frac{\beta F'(z)}{1+\beta F(z)} &= -\frac{\beta}{2}\,(-z)^{-3/2} + O(z^{-2}).\end{aligned}$$

Thus by (IV.22) and the discussion of (IV.21):

$$\int \frac{[\xi_\infty(\lambda) - \xi_\beta(\lambda)]}{(x-z)^2}\, d\lambda = \frac{\beta F'(z)}{(1+\beta F(z)} - \frac{F'(z)}{F(z)} = \frac{1}{2}\,(-z)^{-1} - \frac{\beta}{2}\,(-z)^{-3/2} + O(z^{-2})$$

so we can read β off of $\xi_{\infty,\beta}(\lambda)$. By the above

$$\begin{aligned}\int \frac{\xi_{\infty,\beta}(\lambda)}{(\lambda - z)^2} &= \frac{d}{dz}\ln(\beta + F(z)^{-1})\\ &= -\frac{1}{2}\,z^{-1} + \frac{d}{dz}\ln((-z)^{1/2}[F(z)^{-1} + \beta])\\ &\equiv -\frac{1}{2}\,z^{-1} + \frac{d}{dz}\,[H_\beta(z)].\end{aligned}$$

By the above $H_\beta(-\gamma) \to 0$ as $\gamma \to \infty$. Thus

$$H_\beta(z) = \lim_{\gamma\to\infty} \int \frac{(\xi_{\infty,\beta} - 1/2)(\lambda)}{(\lambda - z)} \left(\frac{\gamma}{\gamma + \lambda}\right) d\lambda$$

and we can recover H_β and so F from $\xi_{\infty,\beta}(\lambda)$. Gelfand-Levitan completes the proof. □

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