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The xi function

by

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1. Introduction

Despite the fact that spectral and inverse spectral properties of one-dimensional Schrödinger operators $H=-d^2/dx^2+V$ have been extensively studied for seventy-five years, there remain large areas where our knowledge is limited. For example, while the inverse theory for operators on $L^2((-\infty,\infty))$ is well understood in case V is periodic [12], [24], [25], [35], [39]–[42], [49], it is not understood in case $\lim_{|x|\to\infty} V(x)=\infty$ and H has discrete spectrum.

Our goal here is to introduce a special function $\xi(x,\lambda)$ on $\mathbf{R}\times\mathbf{R}$ associated to H which we believe will be a valuable tool in the spectral and inverse spectral theory. In a sense we will make precise, it complements the Weyl m-functions, $m_\pm(x,\lambda)$.

A main application of ξ which we will make here concerns a generalization of the trace formula for Schrödinger operators to general V's.

Recall the well-known trace formula for periodic potentials: Let $V(x)=V(x+1)$. Then, by Floquet theory (see, e.g., [10], [37], [44]),

$$\operatorname{spec}(H)=[E_0,E_1]\cup[E_2,E_3]\cup\ldots,$$

a set of bands. If V is C^1, one can show that the sum of the gap sizes is finite, that is,

$$\sum_{n=1}^{\infty}|E_{2n}-E_{2n-1}|<\infty. \tag{1.1}$$

For a fixed y, let H_y be the operator $-d^2/dx^2+V$ on $L^2([y,y+1])$ with $u(y)=u(y+1)=0$ boundary conditions. Its spectrum is discrete, that is, there are eigenvalues $\{\mu_n(y)\}_{n=1}^{\infty}$ with

$$E_{2n-1}\leqslant\mu_n(y)\leqslant E_{2n}. \tag{1.2}$$

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The trace formula says

$$V(y)=E_0+\sum_{n=1}^{\infty}[E_{2n}+E_{2n-1}-2\mu_n(y)]. \tag{1.3}$$

By (1.2),

$$|E_{2n}+E_{2n-1}-2\mu_n(y)|\leqslant |E_{2n}-E_{2n-1}|$$

so (1.1) implies the convergence of the sum in (1.3).

The earliest trace formula for Schrödinger operators was found on a finite interval in 1953 by Gel'fand and Levitan [15] with later contributions by Dikii [8], Gel'fand [13], Halberg–Kramer [23], and Gilbert–Kramer [22]. The first trace formula for periodic V was obtained in 1965 by Hochstadt [24], who showed that for finite-gap potentials

$$V(x)-V(0)=2\sum_{n=1}^{g}[\mu_n(0)-\mu_n(x)].$$

Dubrovin [9] then proved (1.3) for finite-gap potentials. The general formula (1.3) under the hypothesis that V is periodic and C^∞ was proven in 1975 by McKean–van Moerbeke [41], and Flaschka [12], and later for general C^3 potentials by Trubowitz [49]. Formula (1.3) is a key element of the solution of inverse spectral problems for periodic potentials [9], [12], [24], [35], [39], [41], [42], [49].

There have been two classes of potentials for which (1.3) has been extended. Certain almost-periodic potentials are studied in Levitan [34], [35], Kotani–Krishna [31], and Craig [5].

In 1979, Deift–Trubowitz [7] proved that if $V(x)$ decays sufficiently rapidly at infinity and $-d^2/dx^2+V$ has no negative eigenvalues, then

$$V(x)=\frac{2i}{\pi}\int_{-\infty}^{\infty}dk\,k\ln\left[1+R(k)\frac{f_+(x,k)}{f_-(x,k)}\right] \tag{1.4}$$

(where $f_\pm(x,k)$ are the Jost functions at energy $E=k^2$ and $R(k)$ is a reflection coefficient) which, as we will see, is an analog of (1.3). Recently, Venakides [50] studied a trace formula for V, a positive smooth potential of compact support, by writing (1.3) for the periodic potential

$$V_L(x)=\sum_{n=-\infty}^{\infty}V(x+nL)$$

and then taking L to ∞. He found an integral formula which, although he didn't realize it, is precisely (1.4)!

The basic definition of ξ depends on the theory of the Krein spectral shift [32]. If A and B are self-adjoint operators with $A\geqslant\eta$, $B\geqslant\eta$ for some real η and so that

$[(A+i)^{-1}-(B+i)^{-1}]$ is trace class, then there exists a measurable function $\xi(\lambda)$ associated with the pair (B,A) so that

$$\mathrm{Tr}[f(A)-f(B)] = -\int_{\mathbf{R}} f'(\lambda)\xi(\lambda)\,d\lambda \tag{1.5}$$

for f's which are sufficiently smooth and which decay sufficiently rapidly at infinity, and, in particular for $f(\lambda)=e^{-t\lambda}$ for any $t>0$; and so that

$$\xi(\lambda)=0 \quad \text{if } \lambda<\eta. \tag{1.6}$$

Moreover, (1.5), (1.6) uniquely determine $\xi(\lambda)$ for a.e. λ, and if $[(A+i)^{-1}-(B+i)^{-1}]$ is rank n, then

$$|\xi(\lambda)|\leqslant n$$

and if $B\geqslant A$, then $\xi(\lambda)\geqslant 0$.

For the rank one case of importance in this paper, an extensive study of ξ can be found in [48] and a brief discussion in the appendix to this paper.

Let V be a continuous function on $\mathbf{R}$ which is bounded from below. Let $H=-d^2/dx^2+V$ which is essentially self-adjoint on $C_0^\infty(\mathbf{R})$ (see, e.g., [43]) and let $H_{D;x}$ be the operator on $L^2((-\infty,x))\oplus L^2((x,\infty))$ with $u(x)=0$ Dirichlet boundary conditions. Then $[(H_{D;x}+i)^{-1}-(H+i)^{-1}]$ is rank one, so there results a Krein spectral shift $\xi(x,\lambda)$ for the pair $(H_{D;x},H)$ which in particular obeys:

$$\mathrm{Tr}(e^{-tH}-e^{-tH_{D;x}}) = t\int_0^\infty e^{-t\lambda}\xi(x,\lambda)\,d\lambda. \tag{1.7}$$

While ξ is defined in terms of H and $H_{D;x}$, there is a formula that only involves H, or more precisely, the Green's function $G(x,y;z)$ defined by

$$((H-z)^{-1}f)(x) = \int_{\mathbf{R}} G(x,y,z)f(y)\,dy \tag{1.8}$$

for $\operatorname{Im} z\neq 0$. Then by general principles, $\lim_{\varepsilon\downarrow 0} G(x,y;\lambda+i\varepsilon)$ exists for a.e. $\lambda\in\mathbf{R}$, and

THEOREM 1.1.
$$\xi(x,\lambda) = \frac{1}{\pi}\operatorname{Arg}\big(\lim_{\varepsilon\downarrow 0} G(x,x,\lambda+i\varepsilon)\big).$$

This is *formally* equivalent to formulae that Krein [32] has for ξ but in a singular setting (i.e., corresponding to an infinite coupling constant). It follows from equations (A.8)–(A.10) in the appendix. With this definition out of the way, we can state the general trace formula:

$$V(x) = \lim_{\alpha\downarrow 0}\left[E_0+\int_{E_0}^\infty e^{-\alpha\lambda}[1-2\xi(x,\lambda)]\,d\lambda\right], \tag{1.9}$$

where $E_0 \leqslant \inf \operatorname{spec}(H)$. In particular, if $\int_{E_0}^{\infty} |1-2\xi(x,\lambda)|\, d\lambda < \infty$, then

$$V(x) = E_0 + \int_{E_0}^{\infty} [1-2\xi(x,\lambda)]\, d\lambda. \tag{1.10}$$

For certain almost-periodic potentials, Craig [5] used a regularization similar to the α-regularization in (1.9).

We will prove (1.9) in §3 if V is continuous, bounded below, and obeys a bound

$$|V(x)| \leqslant C_1 e^{C_2 x^2}. \tag{1.11}$$

In a subsequent paper [17], we allowed any V which is bounded below and even dropped the continuity property ((1.9) then holds at points, x, of Lebesgue continuity for V). That paper also discusses "higher order trace formulae", familiar from the context of the Korteweg–de Vries hierarchy, that is, formulae where the left side has suitable polynomials in derivatives of V at x. Basically, (1.9) will follow from (1.7) and an asymptotic formula,

$$\operatorname{Tr}(e^{-tH} - e^{-tH_{D;x}}) = \tfrac{1}{2}[1 - tV(x) + o(t)]. \tag{1.12}$$

Examples of the trace formula can be found in §3 including the case $V(x) \to \infty$ as $|x| \to \infty$. In [16], we proved that (1.4) is a special case of (1.9).

The proof in §3 depends on technical preliminaries in §2. We discuss the case of Jacobi matrices (discrete Schrödinger operators) in §4 including a result for $\mathbf{Z}^n$. A general $\mathbf{R}^n$ result that is a kind of analog of (1.12) can be found in [18].

In §5 we turn to some continuity properties of $\xi(x,\lambda)$ in the potential V and use them to find a new proof (and generalization) of a recent striking result of Last [33]. In particular, we establish $\xi(x,\lambda)$ as a new tool in spectral theory and derive a novel criterion for the essential support of the absolutely continuous spectrum of one-dimensional Schrödinger operators and (multi-dimensional) Jacobi matrices. In §6, we discuss an overview of the connection of the function ξ to inverse problems, including a generalized trace formula that shows how to recover the diagonal Green's function $g(x,z) := G(x,x,z)$ (a Herglotz function with respect to z) from $\xi(x,\lambda)$.

2. First order asymptotics of the heat kernel trace

As we have seen, a basic role is played by the asymptotics of

$$\operatorname{Tr}(e^{-tH} - e^{-tH_{D;x}}) \quad \text{as } t \downarrow 0.$$

In this section we will prove:

THEOREM 2.1. *Let V be a continuous function which is bounded from below and which obeys*

$$|V(x)|\leqslant C_1e^{C_2x^2}. \tag{2.1}$$

Then

$$\mathrm{Tr}(e^{-tH}-e^{-tH_{D;x}})=\tfrac{1}{2}[1-tV(x)+o(t)]. \tag{2.2}$$

Under hypothesis (2.1), one can prove this result using the method of images and a DuHamel expansion of e^{-tH} in terms of e^{-tH_0}, $H_0=-d^2/dx^2$. We will instead use a path integral expansion. The advantage of this approach is that by a more detailed analysis of the path space measure, one can automate higher order expansions in t as $t\downarrow 0$ and can drop the growth condition (2.1). This is described in a subsequent paper [17]. By translation invariance, we henceforth set the point x in (2.2) to $x=0$.

So, our first step in proving Theorem 2.1 is to define a process we will call the xi process, that is, a probablity measure on paths ω: $[0,1]\to\mathbf{R}$. Recall [46] that the Brownian bridge is the Gaussian process $\{\alpha(s)\,|\,0\leqslant s\leqslant 1\}$ with $E(\alpha(s))=0$, $E(\alpha(s)\alpha(t))=s(1-t)$ if $0\leqslant s\leqslant t\leqslant 1$. The Brownian bridge is of interest because of the following Feynman–Kac formula [46]:

$$e^{-tH}(x,x)=(4\pi t)^{-1/2}E\biggl(\exp\biggl(-t\int_0^1 V\bigl(x+\sqrt{2t}\,\alpha(s)\bigr)\,ds\biggr)\biggr), \tag{2.3}$$

$$\begin{aligned}e^{-tH_{D;0}}(x,x)&=(4\pi t)^{-1/2}\\&\quad\times E\biggl(\exp\biggl(-t\int_0^1 V\bigl(x+\sqrt{2t}\,\alpha(s)\bigr)\,ds\biggr)\chi\bigl(\alpha\,|\,x+\sqrt{2t}\,\alpha(s)\neq 0 \text{ for all } s\bigr)\biggr),\end{aligned} \tag{2.4}$$

where $\chi(\alpha\,|\,x+\sqrt{2t}\,\alpha(s)\neq 0$ for all $s)$ is the characteristic function of those α for which $x+\sqrt{2t}\,\alpha(s)$ is non-vanishing for all s in $[0,1]$, so since paths are continuous, those α with $x+\sqrt{2t}\,\alpha(s)>0$ for all s if $x>0$. There is a $\sqrt{2t}$ in (2.3), (2.4) rather than the $\sqrt{t}$ in [46] because [46] considers $-\frac{1}{2}(d^2/dx^2)$ where we consider $-d^2/dx^2$.

Consider the measure $d\varkappa$ on $\Omega=\mathbf{R}\times C([0,1])$ given by $(4\pi)^{-1/2}\,dx\otimes\mathcal{D}\alpha$ where dx is Lebesgue measure, and define ω on Ω by $\omega(s)=x+\alpha(s)$. Since $\alpha(0)=\alpha(1)\equiv 0$, we have $\omega(0)=\omega(1)=x$. ω defines a natural map of Ω to $C([0,1])$ and we henceforth view everything on that space. Let $\Omega_0=\{\omega\,|\,\omega(s)=0$ for some s in $[0,1]\}$.

PROPOSITION 2.2. *The $\varkappa$ measure of Ω_0 is $\frac{1}{2}$.*

Proof. Let $\Delta=d^2/dx^2$ and Δ_D be the corresponding operator with a Dirichlet boundary condition at $x=0$. By (2.3), (2.4) with $V=0$,

$$\begin{aligned}\varkappa(\Omega_0)&=\int_{\mathbf{R}}dx\,[e^{\Delta/2}(x,x)-e^{\Delta_D/2}(x,x)]=\int_{\mathbf{R}}dx\,e^{\Delta/2}(x,-x)\\&=\int_{\mathbf{R}}dx\,e^{\Delta/2}(2x,0)=\frac{1}{2}\int_{\mathbf{R}}dx\,e^{\Delta/2}(0,x)=\frac{1}{2},\end{aligned}$$

where the second equality is by the method of images. □

We will call the probability measure $2\chi_{\Omega_0}\, d\varkappa$ on $C([0,1])$ the xi process and denote its expectations as E_ω. (2.3), (2.4) and the regularity of the integral kernel immediately imply that

PROPOSITION 2.3. *For any V which is bounded from below:*

$$\operatorname{Tr}(e^{-tH}-e^{-tH_{D;0}})=\tfrac{1}{2}E_\omega\left(\exp\left(-t\int_0^1 V(\sqrt{2t}\,\omega(s))\,ds\right)\right).$$

We note that the $t^{-1/2}$ in front of (2.3), (2.4) is absorbed in the change of variables from $x+\sqrt{2t}\,\alpha(s)$ to $\sqrt{2t}\,(x+\alpha(s))$.

LEMMA 2.4. *If $C<\frac{1}{2}$, then $E_\omega(e^{C\omega(s)^2})<\infty$ for each s with a bound uniform in s.*

Proof. Let f be a bounded even function on $\mathbf{R}$. Then

$$E_\omega(f(\omega(s))=2\int_{x>0,y>0}[e^{(1-s)\Delta/2}(x,y)f(y)\,e^{s\Delta/2}(y,x) \\ -e^{(1-s)\Delta_D/2}(x,y)f(y)\,e^{s\Delta_D/2}(y,x)]\,dx\,dy$$

and it is easy to see using the method of images that for $f(y)=\min(R,e^{Cy^2})$ the integral remains finite as $R\to\infty$. □

Proof of Theorem 2.1. It is easy to see if we prove the formula for $V(x)$, it follows for V replaced by $V(x)+C$. Thus, without loss we suppose $V\geqslant 0$. Let $a\leqslant 0$. Then by Taylor's theorem with remainder:

$$|e^a-1-a|\leqslant\tfrac{1}{2}a^2.$$

Thus, with $a=-t\int_0^1 V(\sqrt{2t}\,\omega(s))\,ds$,

$$\left|\tfrac{1}{2}E_\omega(e^a)-\tfrac{1}{2}-\tfrac{1}{2}E_\omega(a)\right|\leqslant\tfrac{1}{4}E_\omega(a^2).$$

Using (2.1) and Lemma 2.4, it is easy to see that

$$E_\omega(a^2)=O(t^2)$$

so it suffices to show that

$$E_\omega\left(\int_0^1 V(\sqrt{2t}\,\omega(s))\,ds\right)=V(0)+o(1).$$

This follows from Lemma 2.4, (2.1), continuity of V at $x=0$, and dominated convergence. □

Remark. This is crude analysis compared with the detailed path space argument in [17] but it is elementary and beyond the argument of previous authors who supposed that V is bounded.

3. The trace formula: Schrödinger case

Our main goal in this section is to prove:

THEOREM 3.1. *Suppose V is a continuous function bounded from below on* **R**. *Let $\xi(x,\lambda)$ be the Krein spectral shift for the pair $(H_{D;x}, H)$ with $H_{D;x}$ the operator on $L^2((-\infty,x))\oplus L^2((x,\infty))$ obtained from $H=-d^2/dx^2+V$ with a Dirichlet boundary condition at x. Let $E_0\leqslant\inf\operatorname{spec}(H)$. Then*

$$V(x)=\lim_{\alpha\downarrow 0}\left[E_0+\int_{E_0}^{\infty}e^{-\alpha\lambda}[1-2\xi(x,\lambda)]\,d\lambda\right]. \tag{3.1}$$

Proof. Let $E_1=\inf\operatorname{spec}(H)$. Then for $E_0\leqslant E_1$,

$$E_0+\int_{E_0}^{\infty}e^{-\alpha\lambda}(1-2\xi)\,d\lambda=E_0+\int_{E_0}^{E_1}e^{-\alpha\lambda}\,d\lambda+\int_{E_1}^{\infty}e^{-\alpha\lambda}(1-2\xi)\,d\lambda$$

and

$$\lim_{\alpha\downarrow 0}\int_{E_0}^{E_1}e^{-\alpha\lambda}\,d\lambda=E_1-E_0$$

so the formula for E_1 implies it for E_0; that is, without loss we suppose $E_0=E_1$. By Theorem 2.1 and equation (1.7),

$$\alpha\int_{E_0}^{\infty}e^{-\alpha\lambda}\xi(x,\lambda)\,d\lambda=\tfrac12[1-\alpha V(x)+o(\alpha)].$$

Moreover,

$$\tfrac12\alpha\int_{0}^{\infty}e^{-\alpha\lambda}\,d\lambda=\tfrac12 \tag{3.2}$$

so

$$\tfrac12\alpha\int_{E_0}^{\infty}e^{-\alpha\lambda}\,d\lambda=\tfrac12[1-\alpha E_0+o(\alpha)]$$

and hence

$$\alpha\int_{E_0}^{\infty}e^{-\alpha\lambda}\left(\xi-\tfrac12\right)d\lambda=-\tfrac12\alpha[V(x)-E_0]+o(\alpha)$$

which is (3.1). □

Example 3.2. $V=0$. Then $g(x,\lambda)=\frac12(-\lambda)^{-1/2}$ and so $\arg g(x,\lambda)=0$ $\left(\text{or } \frac12\pi\right)$ if $\lambda<0$ (or $\lambda>0$). Thus, by Theorem 1.1, $\xi(x,\lambda)\equiv\frac12$ on $[0,\infty)$ and (3.2) is just Theorem 2.1 for $V=0$. When $\xi=\frac12$ on a subset of $\operatorname{spec}(H)$, that set drops out of (3.1).

Example 3.3. Suppose that $V(x)\to\infty$ as $|x|\to\infty$. Then H has eigenvalues $E_0<E_1<E_2<\ldots$ and H_x^D has eigenvalues $\{\mu_j(x)\}_{j=1}^{\infty}$ with $E_{j-1}\leqslant\mu_j(x)\leqslant E_j$. We have

$$\xi(x,\lambda)=\begin{cases}1, & E_{j-1}<\lambda<\mu_j(x),\\ 0, & \lambda<E_0 \text{ or } \mu_j(x)<\lambda<E_j.\end{cases}$$

Thus (3.1) becomes:

$$V(x)=E_0+\lim_{\alpha\downarrow 0}\left[\sum_{j=1}^{\infty}\frac{2e^{-\alpha\mu_j(x)}-e^{-\alpha E_j}-e^{-\alpha E_{j-1}}}{\alpha}\right]. \tag{3.3}$$

If we could take α to zero inside the sum, we would get

$$V(x)=E_0+\sum_{j=1}^{\infty}[E_j+E_{j-1}-2\mu_j(x)] \quad \text{(formal)} \tag{3.4}$$

which is just a limit of the periodic formula (1.3) in the limit of vanishing band widths. (3.3) is just a kind of abelianized summation procedure applied to (3.4).

As a special case of this example, consider $V(x)=x^2-1$. Then $E_j=2j$ and $\{\mu_j(0)\}$ is the set $\{2,2,6,6,10,10,14,14,\ldots\}$ of j odd eigenvalues, each doubled. Thus (3.4) is the formal sum

$$-1=-2+2-2+2\ldots \quad \text{(formal)}$$

with (3.3),

$$-1=\lim_{\alpha\downarrow 0}\frac{1-e^{-2\alpha}}{\alpha}\{1-e^{-2\alpha}+e^{-4\alpha}\ldots\}=\lim_{\alpha\downarrow 0}\frac{1-e^{-2\alpha}}{\alpha}\cdot\frac{1}{1+e^{-2\alpha}},$$

its abelian summation.

Example 3.4. Suppose $V(x)=V(x+1)$. Let E_j, $\mu_j(x)$ be the band edges and Dirichlet eigenvalues as in (1.2), (1.3). Then it follows from results in Kotani [30] (see also Deift and Simon [6]) and the fact that $g(x,\lambda):=G(x,x,\lambda+i0)=-[m_+(x,\lambda)+m_-(x,\lambda)]^{-1}$ in terms of the Weyl m-functions, that $g(x,\lambda)$ is purely imaginary on spec(H); that is, $\xi(x,\lambda)=\frac{1}{2}$ there, so

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

It follows that

$$\int_{E_0}^{\infty}|1-2\xi(x,\lambda)|\,dx=\sum_{n=1}^{\infty}|E_{2n}-E_{2n-1}|$$

is finite if (1.1) holds. In that case one can take the limit inside the integral in (3.1) and so recover (1.3).

Example 3.5. In [16] we showed that if V is short-range, that is, $V \in H^{2,1}(\mathbf{R})$, then $\int_{E_0}^{\infty} |1-2\xi(x,\lambda)|\, d\lambda < \infty$ and we can take the limit in (3.1) inside the integral. This recovers Venakides' result [50] with an explicit form for ξ in terms of the Green's function (see Theorem 1.1). Similarly, one can treat short-range perturbations W of periodic background potentials V (modeling scattering off defects or impurities, described by W, in one-dimensional solids) and "cascading" potentials, that is, potentials approaching different spatial asymptotes sufficiently fast [16].

4. The trace formula: Jacobi case

Our goal here is the proof of an analog for Theorem 3.1 for Jacobi matrices. It will be a special case of the following:

THEOREM 4.1. *Let A be a bounded self-adjoint operator in some complex separable Hilbert space $\mathcal{H}$ with $\alpha = \inf \operatorname{spec}(A)$, $\beta = \sup \operatorname{spec}(A)$. Let $\varphi \in \mathcal{H}$ be an arbitrary unit vector and let $\xi(\lambda)$ be the Krein spectral shift for the pair (A_∞, A), $A_\infty := A + \infty(\varphi, \cdot)\varphi$ (where the infinite coupling perturbation is discussed in the appendix). Then for any $E_- \leqslant \alpha$ and $E_+ \geqslant \beta$:*

$$(\varphi, A\varphi) = E_- + \int_{E_-}^{E_+} [1-\xi(\lambda)]\, d\lambda \tag{4.1}$$

$$= E_+ - \int_{E_-}^{E_+} \xi(\lambda)\, d\lambda \tag{4.2}$$

$$= \tfrac{1}{2}(E_+ + E_-) + \tfrac{1}{2} \int_{E_-}^{E_+} [1-2\xi(\lambda)]\, d\lambda. \tag{4.3}$$

Proof. (4.1) follows from (4.2) by integrating 1 from E_- to E_+ and (4.3) is the average of (4.1) and (4.2). Moreover, since $\xi(\lambda)=1$ for $\lambda \geqslant \beta$ and $\xi(\lambda)=0$ for $\lambda \leqslant \alpha$, it is easy to see that it suffices to prove the result for $E_- = \alpha$ and $E_+ = \beta$. Thus, we are reduced to proving (4.2) for $E_+ = \beta$, $E_- = \alpha$.

Let $f \in C_0^\infty(\mathbf{R})$ with $f = x$ on $[\alpha, \beta]$. Then $f(A) = A$, $f(A_\infty) = QAQ$ and with $Q = 1 - (\varphi, \cdot)\varphi$, $\operatorname{Tr}[f(A) - f(A_\infty)] = (\varphi, A\varphi)$ (see the appendix). Thus

$$(\varphi, A\varphi) = \int_{-\infty}^{\alpha} (-f'(\lambda))\xi(\lambda)\, d\lambda + \int_{\alpha}^{\beta} (-f'(\lambda))\xi(\lambda)\, d\lambda + \int_{\beta}^{\infty} (-f'(\lambda))\xi(\lambda)\, d\lambda.$$

Since $\xi(\lambda)=0$ on $(-\infty, \alpha)$, the first integral is zero. Since $f'(\lambda)=1$ on $[\alpha, \beta]$, the second integral is $-\int_\alpha^\beta \xi(\lambda)\, d\lambda$. Since $f \equiv 0$ near infinity and $\xi(\lambda) \equiv 1$ on (β, ∞), the third integral is $f(\beta) = \beta$. □

COROLLARY 4.2. *Let H be a Jacobi matrix on $l^2(\mathbf{Z}^\nu)$, that is, for a bounded function V on $\mathbf{Z}^\nu$:*

$$(Hu)(n)=\sum_{|n-m|=1} u(m)+V(n)u(n), \quad n\in\mathbf{Z}^\nu. \tag{4.4}$$

For $r\in\mathbf{Z}^\nu$, let H_r^D be the operator on $L^2(\mathbf{Z}^\nu\backslash\{r\})$ given by (4.4) with $u(r)=0$ boundary conditions. Let $\xi(r,\lambda)$ be the spectral shift for the pair (H_r^D,H). Then

$$V(r)=E_-+\int_{E_-}^{E_+}[1-\xi(r,\lambda)]\,d\lambda \tag{4.5}$$

$$=E_+-\int_{E_-}^{E_+}\xi(r,\lambda)\,d\lambda \tag{4.6}$$

$$=\tfrac{1}{2}(E_++E_-)+\tfrac{1}{2}\int_{E_-}^{E_+}[1-2\xi(r,\lambda)]\,d\lambda \tag{4.7}$$

for any $E_-\leqslant\inf\operatorname{spec}(H)$, $E_+\geqslant\sup\operatorname{spec}(H)$.

Remark. Only when $\nu=1$ does this have an interpretation as a formula using Dirichlet problems on the half-line.

5. Absolutely continuous spectrum

We will also show that the $\xi(x,\lambda)$ function for a single fixed $x\in\mathbf{R}$ determines the absolutely continuous spectrum of a one-dimensional Schrödinger operator or Jacobi matrix. We begin with a result that holds for a higher-dimensional Jacobi matrix as well:

PROPOSITION 5.1. (i) *For an arbitrary Jacobi matrix, H, on $\mathbf{Z}^\nu$, $\bigcup_{j\in\mathbf{Z}^\nu}\{\lambda\in\mathbf{R}\mid 0<\xi(j,\lambda)<1\}$ is an essential support for the absolutely continuous spectrum of H.*

(ii) *For a one-dimensional Schrödinger operator, $H=-d^2/dx^2+V$ (with V continuous and bounded from below), $\bigcup_{x\in\mathbf{Q}}\{\lambda\in\mathbf{R}\mid 0<\xi(x,\lambda)<1\}$ is an essential support for the absolutely continuous spectrum of H.*

Remark. Recall that every absolutely continuous measure, $d\mu$, has the form $f(E)\,dE$. $S\equiv\{E\mid f(E)\neq 0\}$ is called an essential support of $d\mu$. Any Borel set which differs from S by sets of zero Lebesgue measure is also called an essential support of $d\mu$. If A is a self-adjoint operator on $\mathcal{H}$ and φ_n an orthonormal basis for $\mathcal{H}$, and $d\mu_n$ the spectral measure for the pair, A,φ_n (i.e., $(\varphi_n,e^{isA}\varphi_n)=\int_{\mathbf{R}}e^{isE}\,d\mu_n(E)$), and if $d\mu_n^{\mathrm{ac}}$ is the absolutely continuous component of $d\mu_n$ with S_n its essential support, then $\bigcup_n S_n$ is an essential support of the absolutely continuous spectrum for A.

Proof. (i) Let $g(j,z)$ be the diagonal Green's function $(\delta_j,(A-z)^{-1}\delta_j)$ for $\operatorname{Im} z\neq 0$. Thus $g(j,z)=\int_{\mathbf{R}}d\mu_j(E)(E-z)^{-1}$. By general properties of Borel transforms of measures (see, e.g., [28], [48]), for a.e. $\lambda \in \mathbf{R}$, $\lim_{\varepsilon\downarrow 0} g(j,\lambda+i\varepsilon)$ exists and is non-zero; and S_j, the essential support of $d\mu_{j,\mathrm{ac}}$, is given by

$$S_j = \{\lambda \in \mathbf{R} \mid \operatorname{Im} g(j,\lambda+i0) \neq 0\}.$$

But if $g(j,\lambda+i0)\neq 0$, then $\operatorname{Im} g(j,\lambda+i0)\neq 0$ is equivalent to $0<\operatorname{Arg}(g(j,\lambda+i0))<\pi$, so, up to sets of measure 0,

$$S_j = \{\lambda \in \mathbf{R} \mid 0 < \xi(j,\lambda) < 1\}.$$

Since $\{\delta_j\}_{j\in\mathbf{Z}^\nu}$ are an orthonormal basis for $\mathbf{Z}^\nu$, the result is proven.

(ii) Let $\mathcal{H}_{-1}$ be the minus one space in the scale of spaces associated to H (see, e.g., [43]). Then, δ_x, the delta function supported at x is in $\mathcal{H}_{-1}$ and the diagonal Green's function $g(x,z)$ is just $(\delta_x,(H-z)^{-1}\delta_x)$. Since $\{\delta_x\}_{x\in\mathbf{Q}}$ are total in $\mathcal{H}_{-1}$, the argument is essentially the same as in (i). □

In one dimension though, a single x suffices:

THEOREM 5.2. *For one-dimensional Schrödinger operators or Jacobi matrices, respectively,* $\{\lambda\in\mathbf{R} \mid 0<\xi(x,\lambda)<1\}$ *is an essential support for the absolutely continuous measure for* any *fixed* $x\in\mathbf{R}$ *or* $\mathbf{Z}$, *respectively.*

Proof. Consider the Schrödinger case first. Let $m_\pm(x,z)$ be the Weyl m-functions (see, e.g., [48]) for $-d^2/dx^2+V$ and let $H_{\pm,x}$ be the Dirichlet operators on $L^2((x,\pm\infty))$. Then

$$g(x,z) = -\frac{1}{m_+(x,z)+m_-(x,z)} \tag{5.1}$$

and $H_{\pm,x}$ is unitarily equivalent to multiplication by λ on $L^2(\mathbf{R};d\mu_{x,\pm})$, where $d\mu_{x,\pm}$ is a limit of the measures $(1/\pi)\operatorname{Im} m_\pm(x,\lambda+i\varepsilon)\,d\lambda$ as $\varepsilon\downarrow 0$. Thus, up to sets of measure zero:

$$\begin{aligned}\{\lambda \in \mathbf{R} \mid 0 < \xi(x,\lambda) < 1\} &= \{\lambda \in \mathbf{R} \mid \operatorname{Im} g(x,\lambda+i0) \neq 0\} \\ &= \{\lambda \in \mathbf{R} \mid \operatorname{Im} m_+(x,\lambda+i0) \neq 0\} \cup \{\lambda \in \mathbf{R} \mid \operatorname{Im} m_-(x,\lambda+i0) \neq 0\} \\ &= S_{x,+} \cup S_{x,-}\end{aligned}$$

with $S_{x,\pm}$ the essential support of the a.c. part of $d\mu_{\pm,x}$. Thus, $\{\lambda\in\mathbf{R} \mid 0<\xi(x,\lambda)<1\}$ is an essential support for the a.c. spectrum of $H_{+,x}\oplus H_{-,x}$. But H and $H_{+,x}\oplus H_{-,x}$ have resolvents differing by a rank one perturbation and so equivalent absolutely continuous spectrum by the theory of trace class perturbations [27], [47].

The Jacobi case is similar but requires (5.1) to be replaced by

$$g(j,z) = -\frac{1}{m_+(j,z)+m_-(j,z)+z-V(j)}.$$ □

These results are of particular interest because of their implications for a special kind of semi-continuity of the spectrum. We begin by noting a lemma (that requires a preliminary definition).

Definition. Let $\{V_n\}, V$ be continuous potentials on $\mathbf{R}$ (or $\mathbf{Z}$). We say that V_n converges to V locally as $n\to\infty$ if and only if

(i) $\inf_{(n,x)\in\mathbf{N}\times\mathbf{R}} V_n(x)>-\infty$ ($\mathbf{R}$ case) or $\sup_{(n,j)\in\mathbf{N}\times\mathbf{Z}} |V_n(j)|<\infty$ ($\mathbf{Z}$ case),

(ii) for each $R<\infty$, $\sup_{|x|\leqslant R} |V_n(x)-V(x)|\to 0$ as $n\to\infty$.

LEMMA 5.3. *If $V_n\to V$ locally as $n\to\infty$ and H_n, H are the corresponding Schrödinger operators (or Jacobi matrices), then $(H_n-z)^{-1}\to(H-z)^{-1}$ strongly for* $\operatorname{Im} z\neq 0$ *as $n\to\infty$.*

Proof. Let $\varphi\in C_0^\infty(\mathbf{R})$ or a finite sequence in $l^2(\mathbf{Z})$. Then

$$[(H_n-z)^{-1}-(H-z)^{-1}](H-z)\varphi=(H_n-z)^{-1}(V-V_n)\varphi\to 0 \quad \text{as } n\to\infty.$$

But $\{(H-z)\varphi\}$ is a dense set (since H is essentially self-adjoint on $C_0^\infty(\mathbf{R})$ or on finite sequences, respectively). □

THEOREM 5.4. *If $V_n\to V$ locally as $n\to\infty$ and $\xi_n(x,\lambda)$, $\xi(x,\lambda)$ are the corresponding xi functions for fixed x, then $\xi_n(x,\lambda)\,d\lambda$ converges to $\xi(x,\lambda)\,d\lambda$ weakly in the sense that*

$$\int_{\mathbf{R}} f(\lambda)\xi_n(x,\lambda)\,d\lambda\to\int_{\mathbf{R}} f(\lambda)\xi(x,\lambda)\,d\lambda \quad \text{as } n\to\infty \tag{5.2}$$

for any $f\in L^1(\mathbf{R};d\lambda)$.

Proof. By a simple density argument (using $|\xi(x,\lambda)|\leqslant 1$), it suffices to prove this for $f(\lambda)=(\lambda-z)^{-2}$ and all $z\in\mathbf{C}\setminus\mathbf{R}$. But by (A.7′):

$$\int_{\mathbf{R}}(\lambda-z)^{-2}\xi_n(x,\lambda)\,d\lambda=\frac{d}{dz}F_n(x,z),$$

where $F_n(x,z)=\ln g_n(x,z)$. Since the F's are analytic and uniformly bounded, pointwise convergence of the F's implies convergence of the derivatives dF_n/dz. Thus we need only show

$$g_n(x,z)\to g(x,z) \quad \text{as } n\to\infty.$$

This follows from Lemma 5.3 (and, in the Schrödinger case, some elliptic estimates to turn convergence of the operators to pointwise convergence of the integral kernels). □

Definition. For any H, let $|S_{\mathrm{ac}}(H)|$ denote the Lebesgue measure of the essential support of the absolutely continuous spectrum of H.

THEOREM 5.5 (for one-dimensional Schrödinger operators or Jacobi matrices). *Suppose $V_n \to V$ locally as $n\to\infty$ and each V_n is periodic. Then for any interval $(a,b)\subset\mathbf{R}$:*

$$|(a,b)\cap S_{\mathrm{ac}}| \geqslant \overline{\lim_{n\to\infty}}\, |(a,b)\cap S_{\mathrm{ac}}(H_n)|.$$

Remark. The periods of V_n need *not* be fixed; indeed, almost-periodic V's are allowed.

Proof. By periodicity, $\xi_n(x,\lambda)$ is 0, $\frac{1}{2}$, 1 for a.e. $\lambda\in\mathbf{R}$. Let

$$A_n = \{\lambda\in(a,b) \mid \xi_n(x,\lambda)=0\} \quad \text{and} \quad A=\{\lambda\in(a,b)\mid \xi(x,\lambda)=0\}.$$

Then, $\xi_n(x,\lambda)\geqslant\frac{1}{2}$ on $A\backslash A_n$, so for any a,b:

$$\int_A \xi_n(x,\lambda)\,d\lambda \geqslant \tfrac{1}{2}|(A\backslash A_n)|.$$

But by Theorem 5.4, $\int_A \xi_n(x,\lambda)\,d\lambda \to \int_A \xi(x,\lambda)\,d\lambda=0$ as $n\to\infty$. Thus, $\frac{1}{2}|A\backslash A_n|\to 0$, so $|A|\leqslant \underline{\lim}_{n\to\infty}|A_n|$. Similarly, using $1-\xi$, we get an inequality on

$$|\{\lambda\in(a,b)\mid \xi(x,\lambda)=1\}| \leqslant \underline{\lim_{n\to\infty}}\, |\{\lambda\in(a,b)\mid\xi(x,\lambda)=1\}|.$$

This implies the result. □

Example 5.6. Let α_n be a sequence of rationals and $\alpha=\lim_{n\to\infty}\alpha_n$. Let H_n be the Jacobi matrix with potential $\lambda\cos(2\pi\alpha_n+\theta)$ for λ,θ fixed. Then [2] have shown for $|\lambda|\leqslant 2$, $|S_n|\geqslant 4-2|\lambda|$. It follows from the last theorem that $|S|\geqslant 4-2|\lambda|$. This provides a new proof (and a strengthening) of an important result of Last [33].

Example 5.7. Let $\{a_m\}_{m\in\mathbf{N}}$ be a sequence with $s=\sum_{m=1}^{\infty}2^m|a_m|<2$. Let $V(n)=\sum_{m=1}^{\infty}a_m\cos(2\pi n/2^m)$, a limit periodic potential on $\mathbf{Z}$. Let h be the corresponding Jacobi matrix. We claim that

$$|\sigma_{\mathrm{ac}}(h)|\geqslant 2(2-s). \tag{5.31}$$

For let $V_M(n)=\sum_{m=1}^{M}a_m\cos(2\pi n/2^m)$ with h_M the associated Jacobi matrix. Then the external edges of the spectrum move in at most by $\|V_M\|_\infty\leqslant\sum_{m=1}^{M}|a_m|$. V_{M-1} has at most $2^{M-1}-1$ gaps. They increase in size in going from V_{M-1} to V_M by $2|a_M|$. In addition, V_M has 2^{M-1} new gaps. Thus, $\sigma(h_M)\geqslant 4-2\|V\|_\infty-\sum_{m=1}^{M}(2^m-1)|a_m|\geqslant 4-2s$, which yields (5.31) on account of Theorem 5.5. Knill–Last [29] have shown how to use our Theorem 5.5 to treat more general limit periodic potentials, including Schrödinger operators of the form studied by Chulaevsky [4], and have also treated quasi-periodic potentials of the form $V(n)=\sum_{m=1}^{\infty}\lambda_m\cos([2\pi\alpha n+\theta]m)$ where they show $|\sigma_{\mathrm{ac}}|\geqslant 4-6\sum_{m=1}^{\infty}m|\lambda_m|$.

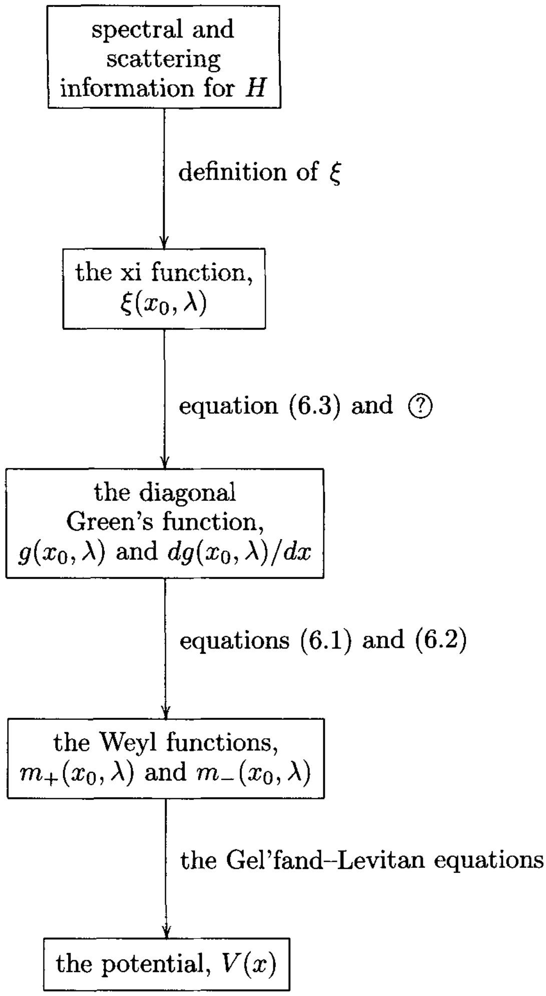

Fig. 1. An inverse spectral philosophy

6. Inverse problems

We want to give an overview of how we believe $\xi(x, \lambda)$ can be an important tool in the study of inverse problems and apply the philosophy in a few cases. Roles are played by $\xi(x_0, \lambda)$, the diagonal Green's function $g(x_0, \lambda)$, and the Weyl m-functions $m_\pm(x_0, z)$ (corresponding to the Dirichlet boundary condition at $x = x_0$). The relationship is that ξ is closest to spectral and scattering information and, under proper circumstances, it determines $g(x_0, \lambda)$ and the derivative $g'(x_0, \lambda)$. They determine $m_\pm(x_0, \lambda)$, which in turn determine $V(x)$ for a.e. $x \in \mathbf{R}$ by the Gel'fand–Levitan method [14], [36]. The scheme underlying our philosophy is illustrated in Figure 1.

That $m_\pm(y,\lambda)$ for all λ and a single y determine $V(x)$ on $(-\infty,y)$ and (y,∞) is well known [38]. That $g(x,\lambda)$ and $dg(x,\lambda)/dx$ at a single point x determine $m_\pm(x,\lambda)$ follows from the pair of formulae,

$$g(x,\lambda) = -[m_+(x,\lambda)+m_-(x,\lambda)]^{-1}, \tag{6.1}$$

$$g'(x,\lambda) = -\frac{m_+(x,\lambda)-m_-(x,\lambda)}{m_+(x,\lambda)+m_-(x,\lambda)}. \tag{6.2}$$

(6.2) follows from (6.1) and the Riccati equations

$$m'_\pm(x,\lambda) = \mp[m_\pm^2(x,\lambda)-V(x)+\lambda].$$

(6.2) is not new; it can be found, for example, in Johnson–Moser [26].

Thus, to recover $V(x)$ for all $x\in\mathbf{R}$ from $\xi(x_0,\lambda)$ for a fixed x_0 and all λ, we only need a method to compute $g(x_0,\lambda)$ and $g'(x_0,\lambda)$ from $\xi(x_0,\lambda)$. One can get g in general from the following formula which follows from Theorem A.2 in the appendix and the proposition below:

$$\begin{gathered} g(x,z) = (E_0-z)^{-1/2} \lim_{\gamma\to\infty} \exp\left(\int_{E_0}^\infty \frac{\xi(x,\lambda)-\frac{1}{2}}{\lambda-z}\cdot\frac{\gamma}{\gamma+\lambda}\,d\lambda\right), \\ E_0 = \inf \operatorname{spec}(H). \end{gathered} \tag{6.3}$$

The proposition we need is

PROPOSITION 6.1. *Let V be continuous and bounded from below and let $g(x,z) = G(x,x,z)$ be the diagonal Green's function for $H=-d^2/dx^2+V$. Then*

$$\lim_{\lambda\to\infty} \lambda^{1/2} g(x,-\lambda) = 1. \tag{6.4}$$

Proof. Let $p(x,t)$ be the diagonal heat kernel for H. By the Feynman–Kac formula [46],

$$p(x,t) = (4\pi t)^{-1/2} E\left(\exp\left(-t\int_0^1 V(x+\sqrt{2t}\,\alpha(s))\,ds\right)\right),$$

where α is the Brownian bridge. It follows by the dominated convergence theorem that

$$(4\pi t)^{1/2} p(x,t) \to 1 \quad \text{as } t\downarrow 0. \tag{6.5}$$

Since

$$g(x,-\lambda) = \int_0^\infty e^{-\lambda t} p(x,t)\,dt$$

we obtain (6.4). □

Remarks. (i) (6.4) can also be read off of asymptotics of $m_\pm$ found in [1], [11].

(ii) (6.5) can be used to prove the following stronger version of (6.3):

$$g(x,z)=(E_0-z)^{-1/2}\lim_{\alpha\downarrow 0}\exp\left(\int_{E_0}^{\infty}\frac{\xi(x,\lambda)-\frac{1}{2}}{\lambda-z}e^{-\alpha\lambda}\,d\lambda\right).$$

Thus, the solution of the inverse problem for going from $\xi(x_0,\cdot\,)$ at a single x_0 to $V(x)$ for all $x\in\mathbf{R}$ is connected to finding $g'(x_0,z)$ from $\xi(x_0,\lambda)$. In absolute generality, we are unsure how to proceed with this because we have no general theory for a differential equation that $\xi(x,\lambda)$ obeys for λ in the essential spectrum of H. Indeed, for random V's where typically spec$(H)=[\alpha,\infty)$ for some α, $\xi(x,\lambda)=1$ or 0 on $\mathbf{R}$ and

$$\overline{\{\lambda\in\mathbf{R}\mid\xi(x,\lambda)=1\}}=[\alpha,\infty),\quad \overline{\{\lambda\in\mathbf{R}\mid\xi(x,\lambda)=0\}}=\mathbf{R}$$

and the x dependence must be very complex. However, one class of potentials does allow some progress:

Definition. We say that V is discretely dominated if for all $x\in\mathbf{R}$, $\xi(x,\lambda)=\frac{1}{2}$ for a.e. $\lambda\in\sigma_{\text{ess}}(H)$.

Examples include reflectionless (soliton) potentials in the short-range case, the periodic case, algebro-geometric finite-gap potentials and limiting cases thereof (such as solitons relative to finite-gap backgrounds), certain almost-periodic potentials, and potentials with $V(x)\to\infty$ as $|x|\to\infty$. In this case if $E_0=\inf\operatorname{spec}(H)$, $[E_0,\infty)\backslash\operatorname{spec}(H)=\bigcup_{n=1}^{N}(\alpha_n,\beta_n)$ where N is finite or infinite. For each x, there is at most one eigenvalue for $H_{D;x}$ in each (α_n,β_n); call it $\mu_n(x)$. If there is no eigenvalue in (α_n,β_n), then $\xi(x,\lambda)$ is either 1 on (α_n,β_n) or 0, and then we set $\mu_n(x)$ equal to β_n or to α_n. Thus

$$\xi(x,\lambda)=\begin{cases}\frac{1}{2}, & \lambda\in\operatorname{spec}(H),\\ 0, & \mu_n(x)<\lambda<\beta_n,\\ 1, & \alpha_n<\lambda<\mu_n(x),\end{cases}$$

and the inverse formulae at a fixed x say that

$$V(x)=\lim_{t\downarrow 0}\sum_{n=1}^{N}\frac{2e^{-t\mu_n(x)}-e^{-t\alpha_n}-e^{-t\beta_n}}{t},\tag{6.6}$$

$$g(x,z)=(E_0-z)^{-1/2}\lim_{\gamma\to\infty}\left[\prod_{n=1}^{N}\left\{\frac{[z-\mu_n(x)]^2}{(z-\alpha_n)(z-\beta_n)}\cdot\frac{(\gamma+\alpha_n)(\gamma+\beta_n)}{[\gamma+\mu_n(x)]^2}\right\}\right]^{1/2}.\tag{6.7}$$

If $\sum_n|\beta_n-\alpha_n|<\infty$, then

$$g(x,z)=(E_0-z)^{-1/2}\left[\prod_{n=1}^{N}\frac{[z-\mu_n(x)]^2}{(z-\alpha_n)(z-\beta_n)}\right]^{1/2}\tag{6.8}$$

(with an absolutely convergent product if $N=\infty$).

The μ's obey a differential equation essentially that was found by Dubrovin [9] in 1975 for the finite-gap periodic case and extended later by McKean–Trubowitz [42], Trubowitz [49], Levitan [34], [35], Kotani–Krishna [31], and Craig [5]. The form we give is the one in Kotani–Krishna [31]. Previous authors only considered the periodic or almost-periodic case, so, in particular, our result is new in the case $|V(x)|\to\infty$ where the regularization (6.6) is needed since $\sum_{n\in\mathbf{N}}|\beta_n-\alpha_n|=\infty$:

THEOREM 6.2. *Let $\alpha_n<\mu_n(x_0)<\beta_n$. Then μ_n is C^1 near x_0 and*

$$\frac{d}{dx}\mu_n(x)\Big|_{x=x_0}=\frac{\pm 1}{\partial g(x_0,\lambda)/\partial\lambda}\Big|_{\lambda=\mu_n(x_0)}, \tag{6.9}$$

where g is given by (6.7) or (6.8). In (6.9), the ± 1 is $+1$ (or -1) if $\mu_n(x_0)$ is an eigenvalue of $H_{x_0;D}$ on (x_0,∞) (or $(-\infty,x_0)$).

Proof. The number $\mu_n(x)$ obeys

$$g(x,\mu_n(x))=0.$$

It is easy to see that g is strictly monotone; indeed, $\partial g/\partial\lambda>0$ on each (α_n,β_n) and so by the implicit function theorem, $\mu_n(x)$ is C^1 and

$$\frac{d\mu_n}{dx}=-\frac{\partial g/\partial x}{\partial g/\partial\lambda}$$

so (6.9) is equivalent to $\partial g/\partial x=\mp 1$ if the eigenvalue corresponds to the half-line (x,∞) (or $(-\infty,x)$). But the associated eigenvector lies in $L^2((x_0,\infty))$ (or $L^2((-\infty,x_0))$) if and only if $m_+(x,\lambda)$ (or $m_-(x,\lambda)$) is ∞ at $x=x_0$, $\lambda=\mu_n(x_0)$. By (6.2), $\partial g/\partial x=\mp 1$ if $m_\pm=\infty$. □

The simple example of the unique discretely dominated potential with $\sigma(H)=\{-1\}\cup[0,\infty)$ (the one-soliton potential) is discussed in [48]. (6.8) and (6.9) become an elementary differential equation and V is then given by (6.6). This is further explored in [20] and [21].

Analogs of ξ in the related inverse cases are also useful. For example, we have shown that the ξ function relating to half-line problems on $[0,\infty)$ with different boundary conditions at 0 determines the potential uniquely a.e. This result was previously obtained independently by Borg [3] and Marchenko [38] in 1952 under the strong additional hypothesis that the corresponding spectra were purely discrete. Our approach allows us to dispense with the discrete spectrum hypothesis and applies to arbitrary spectra.

Appendix: Rank one perturbations and the Krein spectral shift

In this appendix, we will give a self-contained approach to the Krein spectral shift in a slightly more general setting than usual and using more streamlined calculations. The lecture notes [48] contain more about this approach. Let $A\geqslant 0$ be a positive self-adjoint operator in some complex separable Hilbert space $\mathcal{H}$ and let $\mathcal{H}_k(A)$ $(-\infty<k<\infty)$ be the usual scale of spaces associated to A [43]. Let $\varphi\in\mathcal{H}_{-1}(A)$.

Then $(\varphi,\cdot)\varphi$ defines a form bounded perturbation of A with relative bound zero, so for any $\alpha\in\mathbf{R}$, we can define

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

as a closed form on $\mathcal{H}_{+1}(A)$ with an associated self-adjoint operator also denoted by A_α. For $\operatorname{Im} z\neq 0$ define

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

By the second resolvent formula

$$(A_\alpha-z)^{-1}=(A-z)^{-1}-\alpha((A_\alpha-\bar{z})^{-1}\varphi,\cdot)(A-z)^{-1}\varphi \tag{A.3}$$

so taking expectations in φ and solving for F_α, we find

$$F_\alpha(z)=\frac{F(z)}{1+\alpha F(z)} \tag{A.4}$$

and then applying (A.3) to φ:

$$(A_\alpha-z)^{-1}\varphi=[1+\alpha F(z)]^{-1}(A-z)^{-1}\varphi \tag{A.5}$$

so by (A.3) again,

$$(A_\alpha-z)^{-1}=(A-z)^{-1}-\frac{\alpha}{1+\alpha F(z)}((A-\bar{z})^{-1}\varphi,\cdot)(A-z)^{-1}\varphi. \tag{A.6}$$

In particular,

$$\begin{aligned}\operatorname{Tr}\big[(A-z)^{-1}-(A_\alpha-z)^{-1}\big] &= \frac{\alpha}{1+\alpha F(z)}(\varphi,(A-z)^{-2}\varphi)\\ &= \frac{d}{dz}\ln(1+\alpha F(z)).\end{aligned} \tag{A.7}$$

By (A.6), $\lim_{\alpha\to\infty}(A_\alpha-z)^{-1}$ exists in norm. Since A_α is a monotone increasing sequence of forms we can identify the limit, which we will call A_∞, explicitly [27], [45]. If $\varphi\notin\mathcal{H}$, then A_∞ is the self-adjoint operator associated to the densely defined closed form

A restricted to $\{\eta\in\mathcal{H}_{+1}(A)\,|\,(\varphi,\eta)=0\}$ and $\lim(A_\alpha-z)^{-1}=(A_\infty-z)^{-1}$. If $\varphi\in\mathcal{H}$, then one looks at the self-adjoint operator A_∞ on $\mathcal{H}(A_\infty)\equiv\{\eta\in\mathcal{H}\,|\,(\varphi,\eta)=0\}$ whose quadratic form is A restricted to $\mathcal{H}(A_\infty)$. Extend $(A_\infty-z)^{-1}$ to all of $\mathcal{H}$ by setting it to 0 on $\mathcal{H}(A_\infty)^\perp=\{c\varphi\,|\,c\in\mathbf{C}\}$. Then $\lim_{\alpha\to\infty}(A_\alpha-z)^{-1}=(A_\infty-z)^{-1}$ still holds. Convergence properties of $d\mu_\alpha$, the spectral measure for φ associated to A_α (i.e., $F_\alpha(z)=\int_{\mathbf{R}}(x-z)^{-1}\,d\mu_\alpha(x)$) are studied in detail in [19].

Taking α to infinity in (A.6) and repeating the proof of (A.7), we get

$$\operatorname{Tr}[(A-z)^{-1}-(A_\infty-z)^{-1}]=\frac{d}{dz}\ln F(z). \tag{A.7$'$}$$

$F(z)$ is the Borel transform of a measure, so by general principles ([28], [48]), there exist boundary values $F(\lambda+i0)$ for a.e. $\lambda\in\mathbf{R}$ and $F(\lambda+i0)$ takes any given value $-1/\beta$ on a set of measure zero. Thus we can define

$$\xi_\alpha(\lambda)=\begin{cases}(1/\pi)\operatorname{Arg}(1+\alpha F(\lambda+i0)), & \alpha \text{ finite}, \qquad \text{(A.8)}\\ (1/\pi)\operatorname{Arg}(F(\lambda+i0)), & \alpha=\infty, \qquad \text{(A.8$'$)}\end{cases}$$

for each $\alpha\in\mathbf{R}$ and a.e. $\lambda\in\mathbf{R}$. For $\alpha>0$ we have $0\leqslant\operatorname{Arg}(\,\cdot\,)\leqslant\pi$ (and $\operatorname{Im}F(z)>0$ if $\operatorname{Im}z>0$) and thus

$$0\leqslant\xi_\alpha(\lambda)\leqslant 1$$

in this case.

Since $\operatorname{Arg}(F(\lambda+i0))=\operatorname{Im}\ln(F(\lambda+i0))$, an elementary contour integral argument ([48]) shows that (A.7) becomes

$$\operatorname{Tr}[(A-z)^{-1}-(A_\alpha-z)^{-1}]=\int_{E_\alpha}^\infty\frac{\xi_\alpha(\lambda)\,d\lambda}{(\lambda-z)^2},\quad E_\alpha=\inf\operatorname{spec}(A_\alpha). \tag{A.9}$$

(A.9) is a special case of

$$\operatorname{Tr}[f(A)-f(A_\alpha)]=-\int_{E_\alpha}^\infty f'(\lambda)\xi_\alpha(\lambda)\,d\lambda \tag{A.10}$$

for the functions $f_z(\lambda)=(\lambda-z)^{-1}$. By analyticity in z, one sees immediately that $[(A-z)^{-n}-(A_\alpha-z)^{-n}]$ is trace class and (A.10) holds for $f_{z,n}(\lambda)=(\lambda-z)^{-n}$. A straightforward limiting argument lets one prove ([48]) that if f is C^2 on $\mathbf{R}$ with

$$(1+|x|)^2\frac{d^jf}{dx^j}\in L^2((0,\infty))\quad\text{for } j=1,2,$$

then $[f(A)-f(A_\alpha)]$ is trace class and (A.10) holds. In particular,

$$\operatorname{Tr}(e^{-At}-e^{-tA_\alpha})=t\int_{E_\alpha}^\infty e^{-t\lambda}\xi_\alpha(\lambda)\,d\lambda. \tag{A.11}$$

For the case where $\alpha=\infty$ and $\varphi\in\mathcal{H}$, $f(A_\alpha)$ is interpreted as the operator on $\mathcal{H}(A_\infty)$ extended to $\mathcal{H}$ by setting it equal to zero on $\mathcal{H}(A_\infty)^\perp$. This follows from the approximation argument since that is the meaning of $(A_\infty-z)^{-1}$. In particular, THEOREM A.1. *Let A be a bounded operator and φ a unit vector in $\mathcal{H}$. Let $Q=I-(\varphi,\cdot)\varphi$. Then $A-QAQ$ is finite rank and*

$$\operatorname{Tr}(A-QAQ)=-\int_{-\infty}^{\infty} f'(\lambda)\xi_\infty(\lambda)\,d\lambda,$$

where $\xi_\infty(\lambda)=(1/\pi)\operatorname{Arg}(\varphi,(A-\lambda-i0)^{-1}\varphi)$ and f is any function in C_0^∞ with $f(x)=x$ for $x\in[-\|A\|_\infty,\|A\|_\infty]$.

One cannot recover $F(z)$ from $\xi_\infty(A)$ without some additional information. For by (A.7′), ξ_∞ determines $d\ln F(z)/dz$. There is then a constant needed to get F by integration. However, asymptotics of F at $-\infty$ are often enough to recover F from ξ_∞. This is what is needed in §6. For generalizations, see [48].

THEOREM A.2. *Let $A\geqslant 0$. Suppose $(-z)^{1/2}F(z)\to 1$ as $z\to-\infty$ along the real axis. Then*

$$F(z)=(-z)^{-1/2}\lim_{\gamma\to\infty}\exp\left[\int_0^\infty \frac{\xi_\infty(\lambda)-\frac{1}{2}}{z-\lambda}\cdot\frac{\gamma}{\lambda+\gamma}\,d\lambda\right].$$

Proof. Let $F^{(0)}(z)=(-z)^{-1/2}$. Then

$$\frac{d}{dz}\ln F^{(0)}(z)=\frac{1}{2}\int_0^\infty\frac{d\lambda}{(z-\lambda)^2}$$

so by (A.7′):

$$\frac{d}{dz}\left(\frac{F(z)}{F^{(0)}(z)}\right)=\int_0^\infty\frac{\xi_\infty(\lambda)-\frac{1}{2}}{(z-\lambda)^2}\,d\lambda,$$

hence integrating,

$$\ln\frac{F(z)}{F^{(0)}(z)}-\ln\frac{F(-\gamma)}{F^{(0)}(-\gamma)}=\int_0^\infty\frac{\xi_\infty(\lambda)-\frac{1}{2}}{(\lambda-z)(\lambda+\gamma)}(\gamma+z)\,d\lambda.$$

By hypothesis,

$$\lim_{\gamma\to\infty}\ln\frac{F(-\gamma)}{F^{(0)}(-\gamma)}=0$$

and by dominated convergence for any fixed z,

$$\lim_{\gamma\to\infty}\int_0^\infty\frac{\xi_\infty(\lambda)-\frac{1}{2}}{(\lambda-z)(\lambda+\gamma)}\,d\lambda=0,$$

proving the theorem. □

As an example of the abstract theory, fix V, a continuous function on $\mathbf{R}$ which is bounded from below, and $x_0\in\mathbf{R}$. Let $A=-d^2/dx^2+V$. Let $\Phi\colon Q(A)\to\mathbf{C}$ by $\Phi(f)=f(x_0)$.

By a Sobolev estimate and using $\mathcal{H}_1(A)\subset\mathcal{H}_1(-d^2/dx^2)$, Φ is a functional in $\mathcal{H}_{-1}$, so we write $\Phi(f)=\langle\varphi,f\rangle$ with $\varphi(x)=\delta(x-x_0)$. The form domain of A_∞ is thus $f\in\mathcal{H}_1(A)$ with $f(x_0)=0$; thus A_∞ is exactly the operator $H_{x_0;D}$ with a Dirichlet boundary condition at x_0 that we discuss in the body of the paper.

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