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TRACE FORMULAE AND INVERSE SPECTRAL THEORY FOR SCHRÖDINGER OPERATORS

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ABSTRACT. We extend the well-known trace formula for Hill's equation to general one-dimensional Schrödinger operators. The new function ξ, which we introduce, is used to study absolutely continuous spectrum and inverse problems.

In this note we will consider one-dimensional Schrödinger operators

$$H = -\frac{d^2}{dx^2} + V(x) \quad \text{on } L^2(\mathbb{R}; dx) \tag{1S}$$

and Jacobi matrices

$$(hu)(n) = u(n+1) + u(n-1) + v(n)u(n) \quad \text{on } l^2(\mathbb{Z}). \tag{1J}$$

We will suppose that $V(x)$ is continuous and bounded below and $v(n)$ is bounded.

In the analysis of the inverse problem for H when V is periodic ($V(x+L) = V(x)$), a crucial role is played by a trace formula [5, 13, 15]. H then has as its spectrum an infinite set of bands: $\operatorname{spec}(H) = [E_0, E_1] \cup [E_2, E_3] \cup \cdots$. Let $\{\mu_n(x)\}_{n=1}^{\infty}$ be the eigenvalues of the Dirichlet Schrödinger operator in $L^2(x, x+L)$ (w.r.t. Lebesgue measure) with $u(x) = u(x+L) = 0$ boundary conditions ($E_{2n-1} \le \mu_n(x) \le E_{2n}$). The trace formula says that if V is in $H^{1,2}([0, L])$, where $H^{m,p}$ is the Sobolev space of distributions with derivatives up to order m in L^p, then

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

One of our main goals here is to prove a version of this trace formula for arbitrary Schrödinger and Jacobi operators.

We will need the paired half-line Dirichlet operator H_{D}^x defined on $L^2(-\infty, x) \oplus L^2(x, \infty)$ and h_{D}^n on $l^2(\mathbb{Z}|m < n) \oplus l^2(\mathbb{Z}|m > n)$ with $u(x)$ (or $u(n)$) vanishing boundary conditions. In the periodic case, it can be shown that $\mu_n(x)$ are precisely the eigenvalues of H_{D}^x (as long as $E_{2n-1} < \mu_n(x) < E_{2n}$, i.e., no equality).

The difference $(H-i)^{-1} - (H_{\mathrm{D}}^x - i)^{-1}$ is rank 1 (and similarly in the case of h_{D}^n if we define $(h_{\mathrm{D}}^n - i)^{-1}(n, m) \equiv 0$)) and so trace class. As a result, the Krein

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spectral shift [11] exists; i.e., there is a function $\xi(x, \lambda)$ uniquely determined a.e. in λ w.r.t. Lebesgue measure by

$$\text{(3)} \qquad \operatorname{Tr}(f(H) - f(H_{\mathrm{D}}^{x})) = -\int_{-\infty}^{\infty} f'(\lambda)\xi(x, \lambda)\, d\lambda,$$

$$\text{(4)} \qquad 0 \le \xi(x, \lambda) \le 1, \qquad \xi(x, \lambda) = 0 \quad \text{if } \lambda < \inf(\operatorname{spec}(H))$$

for any C^1 function, f, with $\sup_\lambda |(1+\lambda^2)\, df/d\lambda| < \infty$.

ξ is a remarkable function which we claim is central to the proper understanding of inverse problems; it will be discussed in detail in three forthcoming papers which include detailed proofs of the theorems that we present here [6–8]. Our general trace formula is

Theorem 1S [6]. *Let V be continuous at x and $E_0 \le \inf(\operatorname{spec}(H))$. Then*

$$\text{(5S)} \qquad V(x) = E_0 + \lim_{\alpha \downarrow 0} \int_{E_0}^{\infty} e^{-\alpha\lambda}(1 - 2\xi(x, \lambda))\, d\lambda.$$

Theorem 1J [6]. *Let $E_- \le \inf(\operatorname{spec}(h))$ and $E_+ \ge \sup(\operatorname{spec}(h))$. Then*

$$\text{(5J)} \qquad v(n) = \frac{1}{2}(E_- + E_+) + \int_{E_-}^{E_+} \left(\frac{1}{2} - \xi(n, \lambda)\right) d\lambda.$$

Remarks. 1. If V is smooth, there are higher-order trace relations including KdV invariants [7].

2. In the Jacobi case, $\xi(n, \lambda) = 1$ if $\lambda > \sup(\operatorname{spec}(h))$, which is needed for consistency in (5J).

3. While we have singled out the Dirichlet boundary condition at $x \in \mathbb{R}$, any other selfadjoint boundary condition of the type $\psi'(x) + \beta\psi(x) = 0$, $\beta \in \mathbb{R}$, has been worked out as well in [7].

4. Besides the motivating equation (2), two other special cases are in the literature. Kotani and Krishna [10] and Craig [3] discuss the case where V is bounded and continuous and (in our language) $\xi = \frac{1}{2}$ a.e. on $\operatorname{spec}(H)$; and Venakides [16] has a trace formula when V is positive of compact support. In [6] we will discuss the relation of our work to these in more detail.

Sketch of Proof. For simplicity, we consider only the Schrödinger case and suppose $H \ge 0$ and take $E_0 = 0$. By (3)

$$\operatorname{Tr}(e^{-\alpha H} - e^{-\alpha H_{\mathrm{D}}^{x}}) = \alpha \int_0^{\infty} e^{-\alpha\lambda}\xi(x, \lambda)\, d\lambda.$$

Moreover, a path integral argument shows that

$$\operatorname{Tr}(e^{-\alpha H} - e^{-\alpha H_{\mathrm{D}}^{x}}) = \frac{1}{2}(1 - \alpha V(x) + o(\alpha)).$$

Given that

$$\text{(6)} \qquad \frac{1}{2} = \alpha \int_0^{\infty} e^{-\alpha\lambda} \frac{1}{2}\, d\lambda,$$

we get (5S) for $E_0 = 0$.

A second critical result that we prove is

Theorem 2 [6]. *For each* $x \in \mathbb{R}$ *and a.e.* λ *in* $\mathbb{R}$,

$$\xi(x, \lambda) = \frac{1}{\pi} \arg(G(x, x; \lambda + i0)).$$

Remark. G is the integral kernel (resp. matrix elements) of $(H - \lambda)^{-1}$ (resp. $(h - \lambda)^{-1}$). By general principles for each x, $\lim_{\varepsilon \downarrow 0} G(x, x; \lambda + i\varepsilon)$ exists for a.e. λ.

Examples. 1. $V = 0$. In the H case, $G(x, x; \lambda) = (-\lambda)^{-1/2}$ for $\lambda \in \mathbb{C}\backslash[0, \infty)$ with the branch of square root, so $G > 0$ for $\lambda \in (-\infty, 0)$. Thus, for $\lambda \in (0, \infty)$, $G(x, x; \lambda + i0) = i|\lambda|^{-1/2}$ and $\xi(x, \lambda) \equiv \frac{1}{2}$. Equation (6) is then an expression of the known fact that $\operatorname{Tr}(e^{-\alpha H_0} - e^{-\alpha H^x_{\mathrm{D},0}}) = \frac{1}{2}$ for all α.

2. Let V be periodic and in $H^{1,2}([0, L])$ with $V(x + L) = V(x)$. The spectrum of H is $\bigcup_{n=0}^{\infty}[E_{2n}, E_{2n+1}]$ as noted already. Because V is in $H^{1,2}([0, L])$,

$$\sum_{n=0}^{\infty} |E_{2n} - E_{2n-1}| < \infty. \tag{7}$$

It can be shown (see, e.g., Kotani [9], Simon [14], and Deift and Simon [4]) that $G(x, x; \lambda + i0)$ is pure imaginary on $\operatorname{spec}(H)$, so $\xi = \frac{1}{2}$ there. Thus we claim (here and below, we do not give a value to ξ at points of discontinuity; the real-valued function ξ is only determined a.e.):

$$\xi(x, \lambda) = \begin{cases} \dfrac{1}{2}, & E_{2n} < \lambda < E_{2n+1}, \\ 1, & E_{2n+1} < \lambda < \mu_{n+1}(x), \\ 0, & \mu_{n+1}(x) < \lambda < E_{2n+2}, \end{cases}$$

for $0 \le \xi \le 1$, and ξ jumps by -1 at $\mu_{n+1}(x)$. Because of (7), $\int_{E_0}^{\infty} |1 - 2\xi(x, \lambda)| \, d\lambda < \infty$ and (5S) becomes (2).

3. Let $V(x) \to \infty$ as $|x| \to \infty$. Then H has eigenvalues $E_0 < E_1 < E_2 < \cdots$ and H^x_{D} eigenvalues $\mu_1(x) < \mu_2(x) < \cdots$ with $E_{n-1} \le \mu_n(x) \le E_n$. $|1 - 2\xi| = 1$, so the integral in (5S) is not absolutely convergent if α is set equal to zero and (5S) becomes a summability result; explicitly

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

For an explicit case, let $V(x) = x^2 - 1$ and place the Dirichlet condition at $x = 0$. Then

$$E_n = 2n, \qquad \mu_n(0) = \begin{cases} 2n & (n \text{ odd}) \\ 2(n-1) & (n \text{ even}, \ n \ge 2), \end{cases}$$

so $\xi(0, \lambda) = 1$ on $(0, 2) \cup (4, 6) \cup \cdots$ and $\xi(0, \lambda) = 0$ on $(2, 4) \cup (6, 8) \cup \cdots$ and formally

$$\int_0^{\infty} (1 - 2\xi(0, \lambda)) \, d\lambda = -2 + 2 - 2 \cdots.$$

The regularization (5S) is just the Abelian sum which is -1, which is exactly $V(0)$.

4. Let $V(x)$ be short range in the sense that V is $L^1(\mathbb{R})$. Then one can write down $\xi(x, \lambda)$ in terms of the reflection coefficients $R(\lambda)$ and Jost functions $f_+(x, \lambda)$ $(\lim_{x\to\infty} e^{-i\lambda^{1/2}x} f_+(x, \lambda) = 1)$, viz [8]

$$\xi(x, \lambda) = \frac{1}{2} + \frac{1}{\pi} \arg\left[\frac{1 + R(\lambda) f_+(x, \lambda)^2}{|f_+(x, \lambda)|^2}\right], \qquad \lambda > 0. \tag{8}$$

In particular, $|\xi(x, \lambda) - \frac{1}{2}| \le \frac{1}{2}|R(\lambda)|$, and if $V \in H^{2,1}(\mathbb{R})$, we have that

$$\int_{E_0}^{\infty} \left|\xi(x, \lambda) - \frac{1}{2}\right| d\lambda < \infty, \tag{9}$$

so

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

without a need for regularization.

5. There is a general summability result [8] like (9) also for the sum of a smooth periodic potential and a sufficiently short-range potential modeling impurity scattering in one-dimensional crystals.

The Krein spectral shift has rather strong continuity properties:

Lemma 3a. *Let $V_m(x)$ (resp. $v_m(n)$) converge to $V(x)$ uniformly for $x \in [-L, L]$ for each L (resp. to $v(n)$ for each n) and so that $\inf_{x,m} V_m(x) < -\infty$ (resp. $\sup_{n,m} |v_m(n)| < \infty$). Then as measures in λ, $\xi_m(x, \lambda)\, d\lambda$ converges weakly to $\xi(x, \lambda)\, d\lambda$ for each fixed x.*

It follows from Theorem 2 that

Lemma 3b. *For each fixed x, $\operatorname{spec}_{ac}(H) = \{\lambda | 0 < \xi(\lambda, x) < 1\}^{-\text{ess}}$ where $^{-\text{ess}}$ is the essential closure.*

Third, it follows from results of Kotani [9] in the Schrödinger case and Simon [14] in the Jacobi case:

Lemma 3c. *If V (resp. v) is periodic, then $\xi(x, \lambda) \equiv \frac{1}{2}$ on $\operatorname{spec}(H)$ (resp. $\operatorname{spec}(h)$).*

These three lemmas imply

Theorem 3 [6]. *Suppose V_m (resp. v_m) converge to V (resp. v) in the sense of Lemma 3a and each V_m (resp. v_m) is periodic. Then for any measurable set $S \subset \mathbb{R}$*

$$|S \cap \operatorname{spec}_{ac}(H)| \ge \overline{\lim}\, |S \cap \operatorname{spec}(H_m)|$$

(resp. replacing H by h) where $|\cdot| =$ Lebesgue measure.

Example. Consider the Jacobi matrix with $v(n) = \lambda \cos(\pi\alpha n)$ (almost Mathieu or Harper's model). Avron et al. [1] have proven that if α is rational, then $|\operatorname{spec}(h_\alpha)| \ge 4 - 2|\lambda|$. Theorem 3 then implies (by approximating any α by rationals) that $|\operatorname{spec}_{ac}(h_\alpha)| \ge 4 - 2|\lambda|$, slightly strengthening a recent result of Last [12]. In particular, we have a new proof of Last's spectacular result that $\operatorname{spec}_{ac}(h_\alpha) \ne \varnothing$ if $|\lambda| < 2$ and α is a Liouville number.

Finally, [6] will use ξ to study the inverse problem. Typical of our results is the following:

Let $V(x) \to \infty$ as $x \to \pm\infty$. Let $E_n(V)$ be the eigenvalues of $H = -d^2/dx^2 + V$. We claim that when V is even, $\{E_n\}$ are a complete set of spectral data in the sense that

Theorem 4. *If V, W are continuous functions on $\mathbb{R}$ bounded from below, going to infinity at $\pm\infty$, and obeying $V(x) = V(-x)$ and $W(x) = W(-x)$ so that $E_n(V) = E_n(W)$ for all n, then $V = W$.*

Borg [2] proved this result over forty years ago. The ξ function proof is natural, and we have an extension to the nonsymmetric case. When V is not symmetric, the Dirichlet eigenvalues and the information about whether each is a Dirichlet eigenvalue on $(-\infty, 0)$ or $(0, \infty)$ also needs to be supplied.

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