APPEARED IN BULLETIN OF THE
AMERICAN MATHEMATICAL SOCIETY
Volume 29, Number 2, October 1993, Pages 250-255

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: $\mathrm{spec}(H) = [E_0, E_1] \cup [E_2, E_3] \cup \cdots$. 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 ($E_{2n-1} \leq \mu_n(x) \leq E_{2n}$). 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).

1991 *Mathematics Subject Classification*. Primary 34A55, 34L40.

Received by the editors February 2, 1993

The first author gratefully acknowledges support by the Norwegian Research Council for Science and the Humanities (NAVF) and by Caltech. The second author is grateful to the Norwegian Research Council for Science and the Humanities (NAVF) for support. The research of the third author was partially supported by USNSF Grant DMS-9101716

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

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

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

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*

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

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

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

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)

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

Moreover, a path integral argument shows that

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

Given that

$$\frac{1}{2} = \alpha\int_0^{\infty} e^{-\alpha\lambda}\frac{1}{2}\,d\lambda, \tag{6}$$

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 $\mathrm{Tr}(e^{-\alpha H_0} - e^{-\alpha H^x_{\mathrm{D},0}}) = \frac{1}{2}$ 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 $\mathrm{spec}(H)$, 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, $|\xi(x,\lambda)-\frac{1}{2}|\leq\frac{1}{2}|R(\lambda)|$, 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, $\mathrm{spec}_{ac}(H)=\{\lambda|0<\xi(\lambda,x)<1\}^{-\mathrm{ess}}$ where $^{-\mathrm{ess}}$ 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 $\mathrm{spec}(H)$ (resp. $\mathrm{spec}(h)$).*

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 $S\subset\mathbb{R}$*

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

(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 $|\,\mathrm{spec}(h_\alpha)|\geq 4-2|\lambda|$. Theorem 3 then implies (by approximating any α by rationals) that $|\,\mathrm{spec}_{ac}(h_\alpha)|\geq 4-2|\lambda|$, slightly strengthening a recent result of Last [12]. In particular, we have a new proof of Last's spectacular result that $\mathrm{spec}_{ac}(h_\alpha)\neq\varnothing$ 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.

Acknowledgments

We thank H. Kalf for valuable discussions. F. Gesztesy is indebted to the Department of Mathematical Sciences of the University of Trondheim, Norway, and the Department of Mathematics at Caltech for the hospitality extended to him in the summer of 1992.

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