

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

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

and Jacobi matrices

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

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: $\text{spec}(H) = [E_0, E_1] \cup [E_2, E_3] \cup \dots$. 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

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

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 $H_{\mathbb{D}}^x$ defined on $L^2(-\infty, x) \oplus L^2(x, \infty)$ and $h_{\mathbb{D}}^n$ 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 $H_{\mathbb{D}}^x$ (as long as $E_{2n-1} < \mu_n(x) < E_{2n}$, i.e., no equality).

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The difference $(H - i)^{-1} - (H_D^x - i)^{-1}$ is rank 1 (and similarly in the case of h_D^n if we define $(h_D^n - i)^{-1}(n, m) \equiv 0$) 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

$$(3) \quad \text{Tr}(f(H) - f(H_D^x)) = - \int_{-\infty}^{\infty} f'(\lambda) \xi(x, \lambda) d\lambda,$$

$$(4) \quad \begin{aligned} 0 &\leq \xi(x, \lambda) \leq 1, \\ \xi(x, \lambda) &= 0 \quad \text{if } \lambda < \inf(\text{spec}(H)) \end{aligned}$$

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 $E_0 \leq \inf(\text{spec}(H))$. Then*

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

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

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

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 $\lambda > \sup(\text{spec}(h))$, 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 $\text{spec}(H)$; 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 $H \geq 0$ and take $E_0 = 0$. By (3)

$$\text{Tr}(e^{-\alpha H} - e^{-\alpha H_D^x}) = \alpha \int_0^{\infty} e^{-\alpha\lambda} \xi(x, \lambda) d\lambda.$$

Moreover, a path integral argument shows that

$$\text{Tr}(e^{-\alpha H} - e^{-\alpha H_D^x}) = \frac{1}{2}(1 - \alpha V(x) + o(\alpha)).$$

Given that

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

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 $\lambda \in \mathbb{C} \setminus [0, \infty)$ 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 $\text{Tr}(e^{-\alpha H_0} - e^{-\alpha H_{\mathbb{D}, 0}^x}) = \frac{1}{2}$ 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 $H^{1,2}([0, L])$,

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

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 $\text{spec}(H)$, 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.):

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

for $0 \leq \xi \leq 1$, 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 $V(x) \rightarrow \infty$ as $|x| \rightarrow \infty$. Then H has eigenvalues $E_0 < E_1 < E_2 < \dots$ and $H_{\mathbb{D}}^x$ eigenvalues $\mu_1(x) < \mu_2(x) < \dots$ with $E_{n-1} \leq \mu_n(x) \leq E_n$. $|1 - 2\xi| = 1$, 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

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

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

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

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 $f_+(x, \lambda)$ ($\lim_{x \rightarrow \infty} e^{-i\lambda^{1/2}x} f_+(x, \lambda) = 1$), viz [8]

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

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

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

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 , $\text{spec}_{ac}(H) = \{\lambda | 0 < \xi(\lambda, x) < 1\}^{-\text{ess}}$ 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 $\text{spec}(H)$ (resp. $\text{spec}(h)$).*

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 $S \subset \mathbb{R}$*

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

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

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

1. J. Avron, P. H. M. van Mouche, and B. Simon, *On the measure of the spectrum for the almost Mathieu operator*, Comm. Math. Phys. **132** (1990), 103–118.
2. G. Borg, *Uniqueness theorems in the spectral theory of $y'' + (\lambda - q(x))y = 0$* , Proc. 11th Scandinavian Congress of Mathematicians, Johan Grundt Tanums Forlag, Oslo, 1952, pp. 276–287.
3. W. Craig, *The trace formula for Schrödinger operators on the line*, Comm. Math. Phys. **126** (1989), 379–407.
4. P. Deift and B. Simon, *Almost periodic Schrödinger operators, III. The absolutely continuous spectrum in one dimension*, Comm. Math. Phys. **90** (1983), 389–411.
5. H. Flaschka, *On the inverse problem for Hill's operator*, Arch. Rational Mech. Anal. **59** (1975), 293–309.
6. F. Gesztesy and B. Simon, *The ξ function*, Ann. of Math (2), to be submitted.
7. F. Gesztesy, H. Holden, B. Simon, and Z. Zhao, *Higher order trace relations for Schrödinger operators*, Comm. Pure Appl. Math. (to appear).
8. F. Gesztesy, H. Holden, and B. Simon, *Absolute summability of the trace relation for certain Schrödinger operators*, Comm. Math. Phys., to be submitted.
9. S. Kotani, *Ljapunov indices determine absolutely continuous spectra of stationary random one-dimensional Schrödinger operators*, Stochastic Analysis (K. Ito, ed.), North-Holland, Amsterdam, 1984, pp. 225–247.
10. S. Kotani and M. Krishna, *Almost periodicity of some random potentials*, J. Funct. Anal. **78** (1988), 390–405.
11. M. G. Krein, *Perturbation determinants and a formula for the traces of unitary and self-adjoint operators*, Soviet Math. Dokl. **3** (1962), 707–710.
12. Y. Last, *A relation between a.c. spectrum of ergodic Jacobi matrices and the spectra of periodic approximants*, Comm. Math. Phys. **151** (1993), 183–192.
13. H. P. McKean and P. van Moerbeke, *The spectrum of Hill's equation*, Invent. Math. **30** (1975), 217–274.
14. B. Simon, *Kotani theory for one-dimensional stochastic Jacobi matrices*, Comm. Math. Phys. **89** (1983), 227–234.
15. E. Trubowitz, *The inverse problem for periodic potentials*, Comm. Pure Appl. Math. **30** (1977), 321–337.
16. S. Venakides, *The infinite period limit of the inverse formalism for periodic potentials*, Comm. Pure Appl. Math. **41** (1988), 3–17.

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