

**ON TRACE FORMULAS FOR
SCHRÖDINGER-TYPE OPERATORS**

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ON TRACE FORMULAS FOR SCHRÖDINGER-TYPE OPERATORS

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Abstract. We review a variety of recently obtained trace formulas for one- and multi-dimensional Schrödinger operators. Some of the results are extended to Sturm-Liouville and matrix-valued Schrödinger operators. Furthermore, we recall a set of trace formulas in one, two, and three dimensions related to point interactions as well as a new uniqueness result for three-dimensional Schrödinger operators with spherically symmetric potentials.

1. Introduction. It is a well-established fact by now that trace formulas are of great importance in solving inverse spectral problems for Schrödinger operators. This is demonstrated in great detail in [7] in the context of short-range inverse scattering theory and in [9], [11], [26], [33], [38] in connections with the inverse periodic spectral problem. Historically these trace formulas originated in the works of Gelfand and Levitan [14] (see also [8], [12], [13]) for Schrödinger operators on a finite interval. Subsequent developments extended the range of validity of trace formulas in a variety of directions including algebro-geometric quasi-periodic finite gap potentials and certain classes of almost periodic potentials [6], [27], [30]–[32], [39]. Moreover, trace formulas proved to be a vital ingredient in descriptions of the isospectral manifold of quasi-periodic finite-gap potentials and some of their limiting cases as well as in the corresponding Cauchy problem for the Korteweg-de Vries equation. Due to the somewhat special nature of the potentials covered in the references cited thus far, it seemed natural to search for extensions of these trace formulas to a large class of potentials. This was the point of departure of our recent program which led to a trace formula for any continuous potential bound from below and subsequent generalizations to higher-order trace formulas in one dimension and certain multi-dimensional generalizations [15]–[19], [21]–[25],[37]. In the simplest case, the main new strategy is to compare the $L^2(\mathbb{R})$ Schrödinger operators $H = -\frac{d^2}{dx^2} + V$ and $H_y^D = -\frac{d^2}{dx^2} + V$, the corresponding operator with an additional Dirichlet boundary condition at the point $y \in \mathbb{R}$. The spectral characteristics of H and H_y^D , especially the Krein spectral shift function $\xi(\lambda, y)$ associated with the pair (H_y^D, H) , then allows one to recover the potential $V(y)$.

In Section 2 we extend the results of [22] and [24] to Sturm-Liouville operators of the type $r^{-2}[-(p^2 f')' + qf]$ in $L^2(\mathbb{R}; r^2 dx)$ and consider general self-adjoint boundary conditions $\psi'(y) + \beta\psi(y) = 0$, $\beta \in \mathbb{R}$ in addition to the Dirichlet case $\beta = \infty$. Section 3 sketches an extension of the trace formula to matrix-valued Schrödinger operators in the Dirichlet case. Section 4 briefly reviews the multi-dimensional trace formulas in [25] and illustrates a possible abstract approach to some of these trace formulas in the special noninteracting case. In Section 5 we recall a different type of trace formula first derived in [17] in dimensions one, two, and three based on point interactions. Section 6 finally describes a new uniqueness result for three-dimensional Schrödinger operators with spherically symmetric potentials originally proven in [19].

2. Trace Formulas for Sturm-Liouville Operators.

Let $p, q, r \in C^\infty(\mathbb{R})$ be real-valued, $p, r > 0$ and q bounded from below. We then define the self-adjoint Sturm-Liouville operator in $L^2(\mathbb{R}; r^2 dx)$ by

$$hf = \frac{1}{r^2}[-(p^2 f')' + qf], \quad (2.1)$$

$$f \in \mathcal{D}(h) = \{g \in L^2(\mathbb{R}; r^2 dx) | g, g' \in AC_{\text{loc}}(\mathbb{R}), hg \in L^2(\mathbb{R}; r^2 dx)\},$$

where $AC_{\text{loc}}(\Omega)$ denotes the set of locally absolutely continuous functions in $\Omega \subseteq \mathbb{R}$. In addition, we define the Dirichlet Sturm-Liouville operator

$$h_y^D f = \frac{1}{r^2}[-(p^2 f')' + qf], \quad (2.2)$$

$$f \in \mathcal{D}(h_y^D) = \{g \in L^2(\mathbb{R}; r^2 dx) | g, g' \in AC_{\text{loc}}(\mathbb{R} \setminus \{y\}), \lim_{\epsilon \downarrow 0} g(y \pm \epsilon) = 0, h_y^D g \in L^2(\mathbb{R}; r^2 dx)\}.$$

In order to derive trace formulas we will compare the resolvents of h and h_y^D . Let $g(z, x, x')$ and $g_y^D(z, x, x')$ denote the Green's functions (i.e., the integral kernels of the resolvents) of h and h_y^D respectively,

$$g(z, x, x') = (h - z)^{-1}(x, x'), \quad g_y^D(z, x, x') = (h_y^D - z)^{-1}(x, x'). \quad (2.3)$$

One verifies

$$g_y^D(z, x, x') = g(z, x, x') - \frac{g(z, x, y)g(z, y, x')}{g(z, y, y)}, \quad (2.4)$$

and hence

$$\text{Tr}[(h_x^D - z)^{-1} - (h - z)^{-1}] = -\frac{d}{dz} \ln[g(z, x, x)]. \quad (2.5)$$

To proceed further, we need a high-energy expansion, i.e., $z \rightarrow \infty$, of the diagonal Green's function $g(z, x, x)$. For that purpose we shall exploit the Liouville-Green transformation to find a Schrödinger operator H which is unitarily equivalent to h and hence use known results for Schrödinger operators derived in [21], [22],[24].

Define the change of variable

$$t = t(x) = \int_{x_0}^x dx' \frac{r(x')}{p(x')} \quad (2.6)$$

for an arbitrary but fixed point $x_0 \in \mathbb{R}$. Write

$$P(t) = p(x(t)), \quad Q(t) = q(x(t)), \quad R(t) = r(x(t)) \quad (2.7)$$

and introduce the unitary operator

$$U : L^2(\mathbb{R}; r^2 dx) \longrightarrow L^2(\mathbb{R}; dt) \quad (2.8)$$

$$(Uf)(t) = [P(t)R(t)]^{1/2} F(t), \quad F(t) = f(x(t)), \quad f \in L^2(\mathbb{R}; r^2 dx).$$

Theorem 2.1. ([10], see also [20]) The operator $H = UhU^{-1}$ in $L^2(\mathbb{R}; dt)$ explicitly reads

$$Hf = -f'' + Vf, \quad (2.9)$$

$$f \in \mathcal{D}(H) = \{g \in L^2(\mathbb{R}; dt) | g, g' \in AC_{\text{loc}}(\mathbb{R}), Hg \in L^2(\mathbb{R}; dt)\},$$

where

$$\begin{aligned}
V(t) &= \frac{Q(t)}{R(t)^2} + \frac{1}{(R(t)P(t))^2} \left[\frac{1}{2}(R(t)P(t))(R(t)P(t))_{tt} - \frac{1}{4}((R(t)P(t))_t)^2 \right] \\
&= \frac{q(x)}{r(x)} + \frac{p(x)}{2r(x)^3}(r(x)p(x))_{xx} + \frac{(r(x)p(x))_x}{2r(x)^2} \left(\frac{p(x)}{r(x)} \right)_x - \frac{1}{4r(x)^4}(r(x)p(x))_x^2 \\
&:= v(x), \quad x = x(t).
\end{aligned} \tag{2.10}$$

Furthermore,

$$g(z, x, x') = \frac{G(z, t(x), t(x'))}{[r(x)p(x)r(x')p(x')]^{1/2}}, \quad x, x' \in \mathbb{R}, z \in \mathbb{C}, \tag{2.11}$$

where G is the Green's function of H . Moreover,

$$H_u^D = U h_y^D U^{-1} = -\frac{d^2}{dt^2} + V \tag{2.12}$$

with V given by (2.10), is the Schrödinger operator with a Dirichlet boundary condition imposed at the point $u = \int_{x_0}^y dx [p(x)/r(x)]$. Let G_u^D denote the Green's function of H_u^D . Then

$$g_y^D(z, x, x') = \frac{G_u^D(z, t(x), t(x'))}{[p(x)r(x)p(x')r(x')]^{1/2}}. \tag{2.13}$$

Hence we find, using known results for H [22], [24] that

$$\mathrm{Tr}[e^{-\tau h_x^D} - e^{-\tau h}] \underset{\tau \downarrow 0}{\sim} \sum_{\ell=0}^{\infty} s_\ell(x) \tau^\ell, \tag{2.14}$$

$$\mathrm{Tr}[(h_x^D - z)^{-1} - (h - z)^{-1}] \underset{|z| \rightarrow \infty}{\sim} \sum_{\substack{z \in \mathbb{C} \setminus C_\epsilon \\ j=0}}^{\infty} r_j(x) z^{-j-1}, \tag{2.15}$$

where C_ϵ is a cone with apex at $E_0 := \inf\{\sigma(H)\}$ and opening angle $\epsilon > 0$. Recursion relations for s_ℓ and r_j are given by (cf. [22],[24])

$$s_\ell(x) = (-1)^{\ell+1} \frac{r_\ell(x)}{\ell!}, \quad \ell \in \mathbb{N}_0, \tag{2.16}$$

$$r_0(x) = \frac{1}{2}, \quad r_1(x) = \frac{1}{2}v(x), \tag{2.17}$$

$$\begin{aligned}
r_j(x) &= j\gamma_j(x) - \sum_{\ell=1}^{j-1} \gamma_{j-\ell}(x)r_\ell(x), \quad j = 2, 3, \dots, \\
\gamma_0 &= 1, \quad \gamma_1 = \frac{1}{2}v,
\end{aligned} \tag{2.18}$$

$$\gamma_{j+1} = -\frac{1}{2} \sum_{\ell=1}^j \gamma_\ell \gamma_{j+1-\ell} + \frac{1}{2} \sum_{\ell=0}^j \left[v\gamma_\ell \gamma_{j-\ell} + \frac{1}{4}\gamma_{\ell,x}\gamma_{j-\ell,x} - \frac{1}{2}\gamma_{\ell,xx}\gamma_{j-\ell} \right], \quad j = 1, 2, \dots$$

Explicitly, one computes

$$s_0 = -\frac{1}{2}, \quad s_1(x) = \frac{1}{2}v(x), \quad \text{etc.} \tag{2.19}$$

The proof of (2.17) in [22] follows from the well-known differential equation for $\Gamma(z, t) = G(z, t, t)$, namely

$$-2\Gamma_{tt}(z, t)\Gamma(z, t) + \Gamma_t(z, t)^2 + 4[V(t) - z]\Gamma(z, t)^2 = 1 \quad (2.20)$$

and the asymptotic expansion

$$\Gamma(z, t) \underset{z \in \mathbb{C} \setminus \mathbb{C}_\epsilon}{\underset{|z| \rightarrow \infty}{\sim}} \frac{i}{2} z^{-1/2} \sum_{j=0}^{\infty} \Gamma_j(t) z^{-j}, \quad (2.21)$$

with $\Gamma_j(t)$ defined in (2.18) but $v(x)$ replaced by $V(t)$.

The next ingredient concerns the fact that $g(z, x, x)$ is a Herglotz function for all $x \in \mathbb{R}$, i.e., $g(\cdot, x, x): \mathbb{C}_+ \rightarrow \mathbb{C}_+$ is analytic, $\mathbb{C}_+ = \{z \in \mathbb{C} \mid \text{Im } z > 0\}$. Hence g allows a representation [3]

$$g(z, x, x) = \exp \left\{ c(x) + \int_{\mathbb{R}} d\lambda \left[\frac{1}{\lambda - z} - \frac{\lambda}{1 + \lambda^2} \right] \xi(\lambda, x) \right\}, \quad (2.22)$$

where $\xi(\lambda, x)$ is Krein's spectral shift function for the pair (h_x^D, h) [28], satisfying $0 \leq \xi(\lambda, x) \leq 1$, $\xi(\cdot, x) \in L^1_{\text{loc}}(\mathbb{R}; d\lambda)$, and $\int_{\mathbb{R}} d\lambda (1 + \lambda^2)^{-1} \xi(\lambda, x) < \infty$. Although it will not be subsequently used, for completeness we show how to obtain an expression for $c(x)$. Let $z = i$ in (2.22). By taking realparts of (2.22) one infers that

$$c(x) = \text{Re}\{\ln[g(i, x, x)]\}. \quad (2.23)$$

Fatou's lemma permits the explicit representation

$$\xi(\lambda, x) = \frac{1}{\pi} \lim_{\epsilon \downarrow 0} \arg[g(\lambda + i\epsilon, x, x)] \text{ for a.e. } \lambda \in \mathbb{R} \quad (2.24)$$

and all $x \in \mathbb{R}$. We will normalize $\xi(\lambda, x)$ to be zero below the spectrum of h , i.e., $\xi(\lambda, x) = 0$ for $\lambda < E_0$. Using the spectral shift function, one can show that

$$\text{Tr}[F(h_x^D) - F(h)] = \int_{E_0}^{\infty} d\lambda F'(\lambda) \xi(\lambda, x) \quad (2.25)$$

whenever $F \in C^2(\mathbb{R})$, $(1 + \lambda^2)F^{(j)} \in L^2((0, \infty))$, $j = 1, 2$ and $F(\lambda) = (\lambda - z)^{-1}$, $z \in \mathbb{C} \setminus [E_0, \infty)$.

In particular,

$$\text{Tr}[e^{-\tau h_x^D} - e^{-\tau h}] = -\tau \int_{E_0}^{\infty} d\lambda e^{-\tau \lambda} \xi(\lambda, x), \quad \tau > 0, \quad (2.26)$$

$$\text{Tr}[(h_x^D - z)^{-1} - (h - z)^{-1}] = - \int_{E_0}^{\infty} d\lambda \frac{\xi(\lambda, x)}{(\lambda - z)^2}, \quad z \in \mathbb{C} \setminus \{\sigma(h_x^D) \cup \sigma(h)\}. \quad (2.27)$$

Combining (2.14) and (2.26) we obtain the general trace formula for Sturm-Liouville operators

$$2s_1(x) = v(x) = E_0 + \lim_{\tau \downarrow 0} \int_{E_0}^{\infty} d\lambda e^{-\tau \lambda} [1 - 2\xi(\lambda, x)]. \quad (2.28)$$

The Abelian regularization cannot be removed in general, see [18].

Higher-order trace formulas are given in the next theorem.

Theorem 2.2. One infers

$$s_0(x) = -\frac{1}{2}, \quad s_\ell(x) = \frac{(-1)^{\ell-1}}{\ell!} \left\{ \frac{E_0^\ell}{2} + \ell \lim_{t \downarrow 0} \int_{E_0}^{\infty} d\lambda e^{-t\lambda} \lambda^{\ell-1} \left[\frac{1}{2} - \xi(\lambda, x) \right] \right\}, \quad \ell \in \mathbb{N}. \quad (2.29)$$

From the high-energy behavior of the Green's function we find that

$$p(x)r(x) = i\left\{\lim_{z \downarrow -\infty} [\sqrt{z}g(z, x, x)]\right\}^{-1}. \quad (2.30)$$

In contrast to the Schrödinger case, the spectral shift function $\xi(\lambda, x)$ does not contain all the information necessary to construct both p and q in the Sturm-Liouville case, given the weight r . From (2.11) and (2.24) we see that in fact the spectral shift functions Ξ and ξ of H and h respectively, are identical in the sense that $\xi(\lambda, x) = \Xi(\lambda, t(x))$. For a given V we may construct $\Xi(\lambda, t)$ associated with (H_t^D, H) . By choosing *any* positive $p \in C^\infty(\mathbb{R})$ we may define the Sturm-Liouville operator h using (2.10) (or (2.11) for the Green's function). By construction, the pair (h_x^D, h) will have $\xi(\lambda, x)$ as the corresponding spectral shift function.

The behavior of $\xi(\lambda, x)$ is particularly simple in spectral gaps of h . Since p, q , and r are real-valued, $g(\lambda + i0, x, x)$ is real-valued for $\lambda \in \mathbb{R} \setminus \sigma(h)$. More precisely, suppose $(\lambda_1, \lambda_2) \subset \mathbb{R} \setminus \sigma(h)$ and assume that $\mu(x) \in (\lambda_1, \lambda_2)$ is an eigenvalue of h_x^D . Then one has

$$\xi(\lambda, x) = \begin{cases} 0, & \lambda_1 < \lambda < \mu(x) \\ 1, & \mu(x) < \lambda < \lambda_2. \end{cases} \quad (2.31)$$

Next, assume that p, q , and r are periodic, i.e.,

$$p(x+a) = p(x), \quad q(x+a) = q(x), \quad r(x+a) = r(x), \quad x \in \mathbb{R} \quad (2.32)$$

for some $a > 0$. Then Floquet theory implies that

$$\sigma(h) = \bigcup_{n=1}^{\infty} [E_{2(n-1)}, E_{2n-1}], \quad E_0 < E_1 \leq E_2 < E_3 \leq \dots \quad (2.33)$$

and

$$\sigma(h_x^D) = \sigma(h) \cup \{\mu_n(x)\}_{n \in \mathbb{N}}, \quad E_{2n-1} \leq \mu_n(x) \leq E_{2n}, \quad x \in \mathbb{R}, \quad n \in \mathbb{N}. \quad (2.34)$$

In the periodic case $g(\lambda + i0, x, x)$ is purely imaginary on the spectrum, and hence

$$\xi(\lambda, x) = \begin{cases} 0, & \lambda < E_0, \mu_n(x) < \lambda < E_{2n}, \quad n \in \mathbb{N} \\ 1, & E_{2n-1} < \lambda < \mu_n(x), \quad n \in \mathbb{N} \\ \frac{1}{2}, & E_{2(n-1)} < \lambda < E_{2n-1}, \quad n \in \mathbb{N} \end{cases}. \quad (2.35)$$

Combining (2.29) and (2.35) we obtain the following result.

Theorem 2.3. Let $p, q, r \in C^\infty(\mathbb{R})$, $p, r > 0$ be periodic, $p(x+a) = p(x)$, $q(x+a) = q(x)$, $r(x+a) = r(x)$ for some $a > 0$. Then

$$2(-1)^{\ell+1} \ell! s_\ell(x) = E_0^\ell + \sum_{n=1}^{\infty} [E_{2n-1}^\ell + E_{2n}^\ell - 2\mu_n(x)^\ell], \quad \ell \in \mathbb{N}, \quad x \in \mathbb{R}. \quad (2.36)$$

In particular,

$$2s_1(x) = v(x) = E_0 + \sum_{n=1}^{\infty} [E_{2n-1} + E_{2n} - 2\mu_n(x)]. \quad (2.37)$$

Finally, we turn to the case where the Dirichlet boundary condition is replaced by a family of (Robin-type) self-adjoint boundary conditions. Define

$$\begin{aligned} h_{\beta,y}f &= \frac{1}{r^2}[-(p^2f')' + qf], \\ f \in \mathcal{D}(h_{\beta,y}) &= \{g \in L^2(\mathbb{R}; r^2dx) \mid g, g' \in AC([y, \pm R]), \quad R > 0, \\ &\quad \lim_{\epsilon \downarrow 0} [g'(y \pm \epsilon) + \beta g(y \pm \epsilon)] = 0, \quad h_{\beta,y}g \in L^2(\mathbb{R}; r^2dx)\}. \end{aligned} \quad (2.38)$$

($\beta = 0$ corresponds to a Neumann boundary condition at y .)

$h_{\beta,y}$ is unitarily equivalent (using the operator U in (2.8)) to the Schrödinger operator

$$\begin{aligned} H_{\nu(\beta,u),u} &= -\frac{d^2}{dt^2} + V, \\ \mathcal{D}(H_{\nu(\beta,u),u}) &= \{g \in L^2(\mathbb{R}; dt) \mid g, g' \in AC([u, \pm R]), \quad R > 0, \\ &\quad \lim_{\epsilon \downarrow 0} [g'(u \pm \epsilon) + \nu(\beta, u)g(u \pm \epsilon)] = 0, \quad H_{\nu(\beta,u),u}g \in L^2(\mathbb{R}; dt)\}, \end{aligned} \quad (2.39)$$

where V is given by (2.10), the boundary condition is located at

$$u(y) = \int_{x_0}^y dx \frac{r(x)}{p(x)}, \quad (2.40)$$

and $\nu(\beta, u)$ depends on u as well as on β , viz.,

$$\nu = \nu(\beta, u) = \left[\frac{p}{r}\beta - \frac{(pr)_x}{2r^2} \right] \Big|_{x=y} = \left[\frac{P}{R}\beta - \frac{(PR)_t}{2PR} \right] \Big|_{t=u}. \quad (2.41)$$

The Green's function of $h_{\beta,y}$ is given by

$$\begin{aligned} g_{\beta,y}(z, x, x') &= (h_{\beta,y} - z)^{-1}(x, x') \\ &= g(z, x, x') - \frac{(\beta + \partial_2)g(z, x, y)(\beta + \partial_1)g(z, y, x')}{(\beta + \partial_1)(\beta + \partial_2)g(z, y, y)}, \end{aligned} \quad (2.42)$$

where we abbreviate

$$\partial_1 g(z, y, x') = \partial_x g(z, x, x') \Big|_{x=y}, \quad \partial_2 g(z, x, y) = \partial_{x'} g(z, x, x') \Big|_{x'=y}, \quad \text{etc.} \quad (2.43)$$

In this case $-(\beta + \partial_1)(\beta + \partial_2)g(z, y, y)$ is a Herglotz function such that $\text{Im}[(\beta + \partial_1)(\beta + \partial_2)g(\lambda + i0, y, y)] < 0$ for $-\lambda > 0$ large enough. Krein's spectral shift function for the pair $(h_{\beta,x}, h)$ then reads

$$\xi_\beta(\lambda, x) = \frac{1}{\pi} \lim_{\epsilon \downarrow 0} \{\arg[(\beta + \partial_1)(\beta + \partial_2)g(\lambda + i\epsilon, x, x)]\} - 1, \quad \beta \in \mathbb{R}, \quad x \in \mathbb{R}, \quad \lambda \in \mathbb{R}, \quad (2.44)$$

and it satisfies

$$\xi_\beta(\lambda, x) = 0 \quad \text{for } \lambda < \zeta_{\beta,0}(x) := \inf\{\sigma(h_{\beta,x})\}, \quad (2.45)$$

$$\text{Tr}[F(h_{\beta,x}) - F(h)] = \int_{\zeta_{\beta,0}(x)}^{\infty} d\lambda F'(\lambda) \xi_\beta(\lambda, x) \quad (2.46)$$

for functions F as in (2.25). In particular, we find

$$\text{Tr}[e^{-\tau h_{\beta,x}} - e^{-\tau h}] \underset{\tau \downarrow 0}{\sim} \sum_{\ell=0}^{\infty} s_{\beta,\ell}(x) \tau^\ell, \quad (2.47)$$

where

$$s_{\beta,\ell}(x) = (-1)^{\ell+1} \frac{r_{\beta,\ell}(x)}{\ell!}, \quad \ell \in \mathbb{N}_0, \quad (2.48)$$

with (cf. [22],[24]),

$$r_{\beta,0}(x) = -\frac{1}{2}, \quad r_{\beta,1}(x) = \nu(\beta, u(x))^2 - \frac{1}{2}v(x),$$

$$r_{\beta,j}(x) = j\gamma_{\beta,j-1}(x) - \sum_{\ell=1}^{j-1} \gamma_{\beta,j-\ell-1}(x)r_{\beta,\ell}(x), \quad j = 2, 3, \dots, \quad (2.49)$$

$$\gamma_{\beta,-1} = 1, \quad \gamma_{\beta,0} = \nu^2 - \frac{1}{2}v, \quad \gamma_{\beta,1} = \frac{1}{2}\nu^2v + \frac{1}{2}\nu v_x - \frac{1}{8}v^2 + \frac{1}{8}v_{xx},$$

$$\gamma_{\beta,2} = -\frac{1}{16}v^3 + \frac{3}{8}\nu^2v^2 + \frac{3}{16}v_x(4\nu v + v_x) + \frac{1}{8}v_{xx}(v - \nu^2) - \frac{1}{8}\nu v_{xxx} - \frac{1}{64}v_{xxxx},$$

$$\gamma_{\beta,j+1} = \frac{1}{8} \sum_{\ell=1}^j [2(v - \nu^2)\gamma_{\beta,\ell-1}\gamma_{\beta,j-\ell,xx} - (v - \nu^2)\gamma_{\beta,\ell-1,x}\gamma_{\beta,j-\ell,x}$$

$$- 4\gamma_{\beta,\ell}\gamma_{\beta,j-\ell} - 4v(v - \nu^2)\gamma_{\beta,\ell-1}\gamma_{\beta,j-\ell,x} - 2v_x\gamma_{\beta,\ell-1}\gamma_{\beta,j-\ell,x} + \gamma_{\beta,\ell-1}\gamma_{\beta,j-\ell}]$$

$$+ \frac{1}{8} \sum_{\ell=0}^j [\gamma_{\beta,\ell,x}\gamma_{\beta,j-\ell,x} - 2\gamma_{\beta,\ell}\gamma_{\beta,j-\ell,xx} - 4(\nu^2 - 2v)\gamma_{\beta,\ell}\gamma_{\beta,j-\ell}], \quad j = 2, 3, \dots \quad (2.50)$$

Explicitly, one computes

$$s_{\beta,0}(x) = \frac{1}{2}, \quad s_{\beta,1}(x) = \nu(\beta, u(x))^2 - \frac{1}{2}v(x), \quad \text{etc.} \quad (2.51)$$

The proof of (2.49) in [22] is based on the differential equation for $\Gamma_\nu(z, t) = (\nu + \partial_1)(\nu + \partial_2)G(z, t, t)$, namely

$$2[V(t) - \nu^2 - z]\Gamma_{\nu,tt}(z, t)\Gamma_\nu(z, t) - [V(t) - \nu^2 - z]\Gamma_{\nu,t}(z, t)^2 - 2V_t(t)\Gamma_{\nu,t}(z, t)\Gamma_\nu(z, t)$$

$$- 4\{[V(t) - z][V(t) - \nu^2 - z] - \nu V_t(t)\}\Gamma_\nu(z, t)^2 = -[V(t) - \nu^2 - z]^3 \quad (2.52)$$

and the asymptotic expansion

$$\Gamma_\nu(z, t) \underset{\substack{|z| \rightarrow \infty \\ z \in \mathbb{C} \setminus C_c}}{\sim} \frac{i}{2} z^{-1/2} \sum_{j=-1}^{\infty} \Gamma_{\nu,j}(t) z^{-j}, \quad (2.53)$$

with $\Gamma_{\nu,j}(t)$ defined as in (2.50) with β replaced by ν and $v(x)$ by $V(t)$.

The analog of Theorem 2.2 now reads

$$s_{\beta,\ell}(x) = \frac{(-1)^\ell}{\ell!} \left\{ \frac{\zeta_{\beta,0}(x)^\ell}{2} + \ell \lim_{\tau \downarrow 0} \int_{\zeta_{\beta,0}(x)}^{\infty} d\lambda e^{-\tau\lambda} \lambda^{\ell-1} \left[-\frac{1}{2} + \xi_\beta(\lambda, x) \right] \right\}, \quad \ell \in \mathbb{N} \quad (2.54)$$

and, in particular,

$$s_{\beta,1}(x) = \nu(\beta, u(x))^2 - \frac{1}{2}v(x)$$

$$= -\frac{1}{2}\zeta_{\beta,0}(x) - \lim_{\tau \downarrow 0} \int_{\zeta_{\beta,0}(x)}^{\infty} d\lambda e^{-\tau\lambda} \left[-\frac{1}{2} + \xi_\beta(\lambda, x) \right]. \quad (2.55)$$

Our last example in this section will be the periodic case, assuming (2.32) to hold.

In this case

$$\sigma(h_{\beta,x}) = \sigma(h) \cup \{\zeta_{\beta,n}(x)\}_{n \in \mathbb{N}_0},$$

$$\zeta_{\beta,0}(x) \leq E_0, \quad E_{2n-1} \leq \zeta_{\beta,n}(x) \leq E_{2n}, \quad x \in \mathbb{R}, \quad n \in \mathbb{N}, \quad (2.56)$$

with $\sigma(h)$ given as in (2.33). The spectral shift function now reads

$$\xi_\beta(\lambda, x) = \begin{cases} 0, & \lambda < \zeta_{\beta,0}(x), E_{2n-1} < \lambda < \zeta_{\beta,n}(x), n \in \mathbb{N} \\ -1, & \zeta_{\beta,n}(x) < \lambda < E_{2n}, n \in \mathbb{N}_0 \\ -\frac{1}{2}, & E_{2(n-1)} < \lambda < E_{2n-1}, n \in \mathbb{N} \end{cases} \quad (2.57)$$

and the trace formula (2.54) in the periodic case now equals

$$2(-1)^\ell \ell! s_{\beta,\ell}(x) = 2\zeta_{\beta,0}(x)^\ell - E_0^\ell + \sum_{n=1}^{\infty} [2\zeta_{\beta,n}(x)^\ell - E_{2n-1}^\ell - E_{2n}^\ell], \quad \ell \in \mathbb{N}, x \in \mathbb{R}. \quad (2.58)$$

In the case $\ell = 1$ we find

$$\begin{aligned} -2s_{\beta,1}(x) &= v(x) = \frac{q(x)}{r(x)} + \frac{p(x)}{2r(x)^3} (r(x)p(x))_{xx} + \frac{(r(x)p(x))_x}{2r(x)^2} \left(\frac{p(x)}{r(x)} \right)_x - \frac{(r(x)p(x))_x^2}{4r(x)^4} \\ &= 2 \left(\frac{p(x)}{r(x)} \beta - \frac{(p(x)r(x))_x^2}{2r(x)^2} \right)^2 + 2\zeta_{\beta,0}(x) - E_0 + \sum_{n=1}^{\infty} [2\zeta_{\beta,n}(x) - E_{2n-1} - E_{2n}]. \end{aligned} \quad (2.59)$$

Subtracting this equation from (2.37) yields

$$- \left(\frac{p(x)}{r(x)} \beta - \frac{(p(x)r(x))_x^2}{2r(x)^2} \right)^2 = E_0 - \zeta_{\beta,0}(x) + \sum_{n=1}^{\infty} [E_{2n-1} + E_{2n} - \mu_n(x) - \zeta_{\beta,n}(x)]. \quad (2.60)$$

3. Matrix-Valued Schrödinger Operators.

In this section we extend the trace formula (2.28) to self-adjoint matrix-valued Schrödinger operators. General background on matrix-valued differential expressions can be found, e.g., in [1], [40]. Unlike all other sections in this contribution, the material below is in a preliminary stage with more details appearing elsewhere.

Let H in $L^2(\mathbb{R})^m \cong L^2(\mathbb{R}) \otimes \mathbb{C}^m$ be a self-adjoint operator defined by

$$Hf = -I_m f'' + Qf, \quad (3.1)$$

$$f \in \mathcal{D}(H) = \{g \in L^2(\mathbb{R})^m \mid g_j, g'_j \in AC_{\text{loc}}(\mathbb{R}), 1 \leq j \leq m; Hg \in L^2(\mathbb{R})^m\},$$

where $f = (f_1, \dots, f_m)^T$, I_m denotes the identity in \mathbb{C}^m , and $Q = (Q_{j,k})_{1 \leq j, k \leq m}$ denotes a self-adjoint matrix satisfying

$$Q_{j,k} \in C(\mathbb{R}) \text{ bounded from below, } 1 \leq j, k \leq m. \quad (3.2)$$

Closely associated with the equation

$$Hf = zf \quad (3.3)$$

is the first-order $2m \times 2m$ system

$$L(z)(f, f')^T = 0, \quad (3.4)$$

where $(f, f')^T = (f_1, \dots, f_m, f'_1, \dots, f'_m)^T$ and

$$L(z) = I_{2m} \frac{d}{dx} - A(z), \quad A(z) = \begin{pmatrix} 0 & I_m \\ Q - z & 0 \end{pmatrix}, \quad (3.5)$$

with I_{2m} the identity in \mathbb{C}^{2m} . If $\Psi(z, x)$ denotes a fundamental matrix for $L(z)$, that is,

$$L(z)\Psi(z) = 0, \quad (3.6)$$

or equivalently,

$$\Psi'(z, x) = A(z, x)\Psi(z, x), \quad (3.7)$$

then $\tilde{\Psi}(z, x)$ defined by

$$\tilde{\Psi}(z, x) = \Psi(z, x)^{-1} \quad (3.8)$$

satisfies the adjoint system

$$\tilde{\Psi}'(z, x) = -\tilde{\Psi}(z, x)A(z, x). \quad (3.9)$$

Moreover, the fundamental matrices $\Psi(z, x)$ and $\tilde{\Psi}(z, x)$ are of the form

$$\Psi(z, x) = \begin{pmatrix} \psi_1(z, x) & \psi_2(z, x) \\ \psi_1'(z, x) & \psi_2'(z, x) \end{pmatrix}, \quad \tilde{\Psi}(z, x) = \begin{pmatrix} \tilde{\psi}_2'(z, x) & -\tilde{\psi}_2(z, x) \\ -\tilde{\psi}_1'(z, x) & \tilde{\psi}_1(z, x) \end{pmatrix}, \quad (3.10)$$

and one verifies that

$$-\psi_j''(z, x) + Q(x)\psi_j(z, x) = z\psi_j(z, x), \quad -\tilde{\psi}_j''(z, x) + \tilde{\psi}_j(z, x)Q(x) = z\tilde{\psi}_j(z, x), \quad j = 1, 2. \quad (3.11)$$

In particular, assuming $\psi_j(z)$, $\tilde{\psi}_j(z)$ to be unique solutions of (3.11) (up to right resp. left multiplication of matrices constant with respect to x) satisfying

$$\begin{aligned} \psi_{\pm}(z, \cdot) &:= \psi_{\pm}(z, \cdot) \in L^2([R, \pm\infty))^m, \\ \tilde{\psi}_{\pm}(z, \cdot) &:= \tilde{\psi}_{\pm}(z, \cdot) \in L^2([R, \pm\infty))^m, \quad R \in \mathbb{R}, z \in \mathbb{C} \setminus \sigma(H), \end{aligned} \quad (3.12)$$

the Green's matrix $G(z, x, x')$ of H becomes

$$G(z, x, x') = \begin{cases} \psi_+(z, x)\tilde{\psi}_-(z, x'), & x \geq x' \\ \psi_-(z, x)\tilde{\psi}_+(z, x'), & x \leq x' \end{cases} \quad (3.13)$$

and hence the resolvent of H is given by

$$((H - z)^{-1}f)(x) = \int_{\mathbb{R}} dx' G(z, x, x')f(x'), \quad f \in L^2(\mathbb{R})^m, \quad z \in \mathbb{C} \setminus \sigma(H). \quad (3.14)$$

Since

$$-\psi_j''(\bar{z}, x)^* + \psi_j(\bar{z}, x)^*Q(x) = z\psi_j(\bar{z}, x)^*, \quad j = 1, 2, \quad (3.15)$$

$\tilde{\psi}_j(z, x)$ are of the type

$$\tilde{\psi}_j(z, x) = A_{j,1}(z)\psi_1(\bar{z}, x)^* + B_{j,2}(z)\psi_2(\bar{z}, x)^*, \quad j = 1, 2 \quad (3.16)$$

for matrices $A_{j,k}(z)$, $B_{j,k}(z)$, $1 \leq j, k \leq 2$ in \mathbb{C}^m constant with respect to x . Introducing the "Wronskian" $W(\phi, \psi)(x)$ of $m \times m$ matrices ϕ and ψ by

$$W(\phi, \psi)(x) = \phi(x)\psi'(x) - \phi'(x)\psi(x), \quad (3.17)$$

one verifies that

$$\frac{d}{dx}W(\phi(\bar{z})^*, \psi(z))(x) = 0 \quad (3.18)$$

for solutions $\psi(z, x)$ and $\phi(\bar{z}, x)^*$ of

$$-\psi''(z, x) + [Q(x) - z]\psi(z, x) = 0, \quad -\phi''(\bar{z}, x)^* + \phi(\bar{z}, x)^*[Q(x) - z] = 0. \quad (3.19)$$

Relations (3.8), (3.12), (3.15), and (3.16) then yield

$$\tilde{\psi}_{\pm}(z, x) = \pm W(\psi_{\pm}(\bar{z})^*, \psi_{\mp}(z))^{-1}\psi_{\pm}(\bar{z}, x)^* \quad (3.20)$$

and hence

$$\begin{aligned} G(z, x, x) &= -\psi_+(z, x)W(\psi_-(\bar{z})^*, \psi_+(z))^{-1}\psi_-(\bar{z}, x)^* \\ &= \psi_-(z, x)W(\psi_+(\bar{z})^*, \psi_-(z))^{-1}\psi_+(\bar{z}, x)^*. \end{aligned} \quad (3.21)$$

The corresponding matrix-valued Dirichlet Schrödinger operator H_y^D in $L^2(\mathbb{R})^m$ then reads

$$\begin{aligned} H_y^D f &= -I_m f'' + Qf, \\ f \in \mathcal{D}(H_y^D) &= \{g \in L^2(\mathbb{R})^m \mid g_j \in AC_{\text{loc}}(\mathbb{R}), g'_j \in AC_{\text{loc}}(\mathbb{R} \setminus \{y\}), \\ &\quad \lim_{\epsilon \downarrow 0} g_j(y \pm \epsilon) = 0, H_y^D g \in L^2(\mathbb{R})^m\} \end{aligned} \quad (3.22)$$

and its Green's matrix $G_y^D(z, x, x')$, the analog of (2.4), is given by

$$G_y^D(z, x, x') = G(z, x, x') - G(z, x, y)G(z, y, y)^{-1}G(z, y, x'). \quad (3.23)$$

The analog of (2.5) then becomes

$$\begin{aligned} \text{Tr}[(H_x^D - z)^{-1} - (H - z)^{-1}] &= -\text{Tr}[G(z, \cdot, x)G(z, x, x)^{-1}G(z, x, \cdot)] \\ &= -\text{Tr}[G(z, x, x)^{-1}G(z, x, \cdot)G(z, \cdot, x)] = -\text{Tr}_{\mathbb{C}^m}\{G(z, x, x)^{-1}[\frac{d}{dz}G(z, x, x)]\} \\ &= -\frac{d}{dz}\text{Tr}_{\mathbb{C}^m}\{\ln[G(z, x, x)]\} = -\frac{d}{dz}\ln\{\det_{\mathbb{C}^m}[G(z, x, x)]\}, \end{aligned} \quad (3.24)$$

where we used cyclicity of the trace,

$$(H - z)^{-2}(x, x')_{j,k} = \frac{d}{dz}G(z, x, x')_{j,k} = \sum_{\ell=1}^m \int_{\mathbb{R}} dx'' G(z, x, x'')_{j,\ell} G(z, x'', x')_{\ell,k}, \quad (3.25)$$

and $\text{Tr}_{\mathbb{C}^m}[\ln(M)] = \ln[\det_{\mathbb{C}^m}(M)]$ for matrices M in \mathbb{C}^m . Moreover, $\text{Tr}(\cdot)$ and $\text{Tr}_{\mathbb{C}^m}(\cdot)$ in (3.24) denote the trace in $L^2(\mathbb{R})^m$ and \mathbb{C}^m , respectively.

Introducing the matrix-valued Green's kernel diagonal with respect to x (cf. (3.21))

$$\Gamma(z, x) = G(z, x, x), \quad (3.26)$$

the matrix analog of (2.20) reads

$$\begin{aligned} -\Gamma(z, x)\Gamma_{xx}(z, x) - \Gamma_{xx}(z, x)\Gamma(z, x) + \Gamma_x(z, x)^2 + \Gamma(z, x)^2 Q(x) \\ + Q(x)\Gamma(z, x)^2 + 2\Gamma(z, x)Q(x)\Gamma(z, x) - 4z\Gamma(z, x)^2 = I_m \end{aligned} \quad (3.27)$$

and considerations along the lines of (2.20), (2.21) then yield

$$\Gamma(z, x) \underset{z \in \mathbb{C} \setminus \mathbb{C}_\epsilon}{\underset{|z| \rightarrow \infty}{\sim}} \frac{i}{2} z^{-1/2} \sum_{j=0}^{\infty} \Gamma_j(x) z^{-j}, \quad (3.28)$$

with

$$\Gamma_0(x) = I_m, \quad \Gamma_1(x) = \frac{1}{2}Q(x), \text{ etc.} \quad (3.29)$$

Similarly,

$$-\frac{d}{dz} \ln[G(z, x, x)] \underset{z \in \mathbb{C} \setminus \mathbb{C}_\epsilon}{\underset{|z| \rightarrow \infty}{\sim}} \sum_{j=0}^{\infty} R_j(x) z^{-j-1}, \quad (3.30)$$

where

$$R_0(x) = \frac{1}{2}I_m, \quad R_1(x) = \frac{1}{2}Q(x), \text{ etc.} \quad (3.31)$$

Next, define for all $x \in \mathbb{R}$ the analog of (2.24) by

$$\begin{aligned}\Xi(\lambda, x) &= \frac{1}{\pi} \lim_{\epsilon \downarrow 0} \operatorname{Im} \{ \ln[G(\lambda + i\epsilon, x, x)] \} \text{ for a.e. } \lambda \in \mathbb{R}, \\ \Xi(\lambda, x) &= 0, \lambda < E_0 := \inf\{\sigma(H)\},\end{aligned}\tag{3.32}$$

where $\operatorname{Im}(M)$, $\operatorname{Re}(M)$, in obvious notation, abbreviate

$$\operatorname{Im}(M) = \frac{1}{2i}(M - M^*), \quad \operatorname{Re}(M) = \frac{1}{2}(M + M^*)\tag{3.33}$$

for matrices M in \mathbb{C}^m . It follows from the results in [5] that

$$0 \leq \Xi(\lambda, x) \leq I_m \quad \text{for a.e. } \lambda \in \mathbb{R}.\tag{3.34}$$

In the following denote by $C_{R,\epsilon}$ the counter-clockwise oriented contour

$$\begin{aligned}C_{R,\epsilon} &= \{z = E_0 + \epsilon e^{i\phi} \mid \frac{3\pi}{2} \geq \phi \geq \frac{\pi}{2}\} \cup \{z = E_0 + \lambda + i\epsilon \mid 0 \leq \lambda \leq R\} \\ &\cup \{z = E_0 + R e^{i\phi} \mid \arctan(\epsilon/R) \leq \phi \leq 2\pi - \arctan(\epsilon/R)\} \\ &\cup \{z = E_0 + \lambda - i\epsilon \mid 0 \leq \lambda \leq R\}, \quad R > \epsilon > 0.\end{aligned}\tag{3.35}$$

Applying the residue theorem, taking into account that $G(z, x, x)$, $x \in \mathbb{R}$, is analytic in $z \in \mathbb{C} \setminus \sigma(H)$ and $\det[G(z, x, x)] \neq 0$ for $z \in \mathbb{C} \setminus \sigma(H)$ (cf. (3.23)), then yields

$$\begin{aligned}\{\ln[G(z, x, x)]\}_{j,k} &= \frac{1}{2\pi i} \oint_{C_{R,\epsilon}} dz' \frac{\{\ln[G(z', x, x)]\}_{j,k}}{z' - z} \\ &= \frac{1}{2\pi i} \oint_{C_{R,\epsilon}} dz' \{\ln[G(z', x, x)]\}_{j,k} \frac{z'}{1 + z'^2} \\ &\quad + \frac{1}{2\pi i} \oint_{C_{R,\epsilon}} dz' \{\ln[G(z', x, x)]\}_{j,k} \left[\frac{1}{z' - z} - \frac{z'}{1 + z'^2} \right] \\ &= \operatorname{Re}\{\ln[G(i, x, x)]\}_{j,k} + \frac{1}{\pi} \int_{E_0}^R d\lambda \operatorname{Im}\{\ln[G(\lambda + i0, x, x)]\}_{j,k} \left[\frac{1}{\lambda - z} - \frac{\lambda}{1 + \lambda^2} \right] \\ &\quad + o(\epsilon) + o(R^{-1}) \\ &\xrightarrow{R \rightarrow \infty, \epsilon \downarrow 0} \operatorname{Re}\{\ln[G(i, x, x)]\}_{j,k} + \int_{E_0}^{\infty} d\lambda \Xi(\lambda, x)_{j,k} \left[\frac{1}{\lambda - z} - \frac{\lambda}{1 + \lambda^2} \right], \\ &\quad 1 \leq j, k \leq m.\end{aligned}\tag{3.36}$$

Thus

$$\frac{d}{dz} \ln[G(z, x, x)] = \int_{E_0}^{\infty} d\lambda \Xi(\lambda, x) (\lambda - z)^{-2},\tag{3.37}$$

and the matrix analog of (2.28) then reads

$$Q(x) = E_0 I_m + \lim_{z \rightarrow i\infty} \int_{E_0}^{\infty} d\lambda z^2 (\lambda - z)^{-2} [I_m - 2\Xi(\lambda, x)],\tag{3.38}$$

where we used a resolvent instead of a heat kernel regularization.

Defining

$$\xi(\lambda, x) = \operatorname{Tr}_{\mathbb{C}^m} [\Xi(\lambda, x)],\tag{3.39}$$

one infers from (3.24) that

$$\operatorname{Tr}[(H_x^D - z)^{-1} - (H - z)^{-1}] = - \int_{E_0}^{\infty} d\lambda \xi(\lambda, x) (\lambda - z)^{-2}\tag{3.40}$$

and that

$$\xi(\lambda, x) = \frac{1}{\pi} \lim_{\epsilon \downarrow 0} \arg \{ \det_{\mathbb{C}^m} [G(\lambda + i\epsilon, x, x)] \}, \quad 0 \leq \xi(\lambda, x) \leq m \quad \text{for a.e. } \lambda \in \mathbb{R}. \quad (3.41)$$

Further details and applications of this formalism to inverse spectral problems will appear elsewhere.

4. Multi-Dimensional Trace Formulas.

First, reporting on recent work in [25], we attempt to extend the leading behavior in (2.14),

$$2Tr[e^{-\tau H} - e^{-\tau H_x^D}] = 1 - \tau V(x) + o(\tau) \quad \text{as } \tau \downarrow 0 \quad (4.1)$$

to arbitrary space dimensions $\nu \in \mathbb{N}$. The key to such an extension is an appropriate combination of Dirichlet and Neumann boundary conditions on various hyperplanes through the point $x \in \mathbb{R}^\nu$ taking into account that (4.1) is equivalent to

$$Tr[e^{-\tau H_x^N} - e^{-\tau H_x^D}] = 1 - \tau V(x) + o(\tau) \quad \text{as } \tau \downarrow 0, \quad (4.2)$$

where $H_x^N = H_x^0$ denotes the operator (2.39) with a Neumann boundary condition at $x \in \mathbb{R}$. We start by introducing proper notations. In the following let V be a real-valued continuous function on \mathbb{R}^ν bounded from below and define the self-adjoint operator

$$H = -\Delta + V \quad (4.3)$$

as a form sum in $L^2(\mathbb{R}^\nu)$. Next, let $A \subseteq \{1, \dots, \nu\}$ and denote by $|A|$ the number of elements of A . Moreover, let $B_\alpha^{(x)}$, $\alpha \subseteq \{1, \dots, \nu\}$ be the 2^ν blocks obtained by removing the hyperplanes $\mathcal{P}_j^{(x)} = \{y \in \mathbb{R}^\nu \mid y_j = x_j\}$ from \mathbb{R}^ν , that is, $B_\alpha^{(x)} = \{y \in \mathbb{R}^\nu \mid y_\ell > x_\ell \text{ if } \ell \in \alpha, y_\ell < x_\ell \text{ if } \ell \notin \alpha\}$ and denote by \mathcal{P}_ν the power set of $\{1, \dots, \nu\}$. The operator $H_{A;x}$ is then defined to be $-\Delta + V$ on $\bigoplus_{\alpha \in \mathcal{P}_\nu} L^2(B_\alpha^{(x)})$ with Dirichlet boundary conditions on $\{P_j^{(x)}\}_{j \in A}$ and Neumann boundary conditions on $\{P_j^{(x)}\}_{j \notin A}$.

Theorem 4.1. [25] Define $C_\tau = \sum_{A \in \mathcal{B}_\nu} (-1)^{|A|} e^{-\tau H_{A;0}}$, $\tau > 0$. Then the integral kernel of C_τ is given by

$$C_\tau(x, x') = \begin{cases} 2^\nu e^{-\tau H}(x, -x'), & x, x' \text{ in the same orthant} \\ 0, & \text{otherwise.} \end{cases} \quad (4.4)$$

Moreover, C_τ , $\tau > 0$ is a trace class operator in $L^2(\mathbb{R}^\nu)$ and

$$Tr(C_\tau) = 2^\nu \int_{\mathbb{R}^\nu} d^\nu x e^{-\tau H}(x, -x), \quad \tau > 0. \quad (4.5)$$

The proof of (4.4) in [25] is based on the method of images while the trace class property of C_τ and (4.5) follow from the direct sum decomposition of C_τ in $\bigoplus_{\alpha \in \mathcal{P}_\nu} L^2(B_\alpha^{(x)})$.

Applying a Feynman-Kac-type analysis then yields the following ν -dimensional generalization of (4.2).

Theorem 4.2. [25]

$$Tr\left(\sum_{A \in \mathcal{P}_\nu} (-1)^{|A|} e^{-\tau H_{A;x}}\right) = 1 - \tau V(x) + o(\tau) \quad \text{as } \tau \downarrow 0. \quad (4.6)$$

While Theorem 4.2 represents a multidimensional trace formula for Schrödinger operators associated with unbounded regions in \mathbb{R}^ν , one can also prove new trace formulas for Schrödinger operators defined in boxes. One obtains, e.g.,

Theorem 4.3. [25] Let V be continuous on $[0, 1]^\nu$. For $A \subseteq \{1, \dots, \nu\}$, let H_A be $-\Delta + V$ on $L^2([0, 1]^\nu)$ with Dirichlet boundary conditions on the hyperplanes with $x_j = 0$ or 1 and $j \in A$ and Neumann boundary conditions on the hyperplanes with $x_j = 0$ or 1 and $j \notin A$. Let $\langle V \rangle$ be the average of V at the 2^ν corners of $[0, 1]^\nu$. Then

$$\sum_{A \in \mathcal{P}_\nu} (-1)^{|A|} \text{Tr}(e^{-\tau H_A}) = 1 - \tau \langle V \rangle + o(\tau) \text{ as } \tau \downarrow 0. \quad (4.7)$$

This result holds also for rectangular boxes $\times_{j=1}^\nu [a_j, b_j]$ but the rectangular symmetry is crucial in the proof of [25]. Similarly, one can prove

Theorem 4.4. [25] Let V be continuous on $[0, 1]^\nu$. For $A \subseteq \{1, \dots, \nu\}$ let \tilde{H}_A be $-\Delta + V$ on $L^2([0, 1]^\nu)$ with Dirichlet boundary conditions on the hyperplanes with $x_j = 0$ for $j \in A$ and Neumann boundary conditions on the hyperplanes with $x_j = 0$ for $j \notin A$ or $x_k = 1$ for all $k \in \{1, \dots, \nu\}$. Then

$$\sum_{A \in \mathcal{P}_\nu} (-1)^{|A|} \text{Tr}(e^{-\tau \tilde{H}_A}) = 2^{-\nu} [1 - \tau V(0) + o(\tau)] \text{ as } \tau \downarrow 0. \quad (4.8)$$

Finally, we mention an Abelianized version of a trace formula that Lax [29] derived formally in two dimensions.

Theorem 4.5. [25] Let V be a continuous periodic function on \mathbb{R}^2 with $V(x_1 + n_1, x_2 + n_2) = V(x_1, x_2)$ for all $(x_1, x_2, n_1, n_2) \in \mathbb{R}^2 \times \mathbb{Z}^2$. Let $H_P, H_A, H_{AP}, H_{PA}, H_N$, and H_D be the operators $-\Delta + V$ on $L^2([0, 1]^2)$ with periodic, antiperiodic, AP, PA , Neumann, and Dirichlet boundary conditions respectively, where AP (resp. PA) means antiperiodic in the x_1 (resp. x_2) direction and periodic in the x_2 (resp. x_1) direction. Then

$$\text{Tr}[e^{-\tau H_P} + e^{-\tau H_A} + e^{-\tau H_{AP}} + e^{-\tau H_{PA}} - 2e^{-\tau H_N} - 2e^{-\tau H_D}] = -1 + \tau V(0) + o(\tau) \text{ as } \tau \downarrow 0. \quad (4.9)$$

For a different kind of two-dimensional trace formula for $V(x)$ comparing the heat kernels for $H = -\Delta + V$ and $H_0 = -\Delta$ with Dirichlet boundary conditions on a rectangular box, see [34]. Trace formulas for heat kernels of multi-dimensional Schrödinger operators in the short-range case have also recently been derived in [4].

Finally, we illustrate a possible new abstract approach to the trace formulas (4.7) based on certain commutation (supersymmetric) techniques in the noninteracting case where $V(x) = 0$, $x \in \mathbb{R}^\nu$. We need a bit of notation. Let \mathcal{H} be a (complex separable) Hilbert space, F a closed densely defined linear operator in \mathcal{H} and define the self-adjoint operators

$$H_1 = F^* F, \quad H_2 = F F^* \quad (4.10)$$

in \mathcal{H} and

$$Q = \begin{pmatrix} 0 & F^* \\ F & 0 \end{pmatrix}, \quad P = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (4.11)$$

in $\mathcal{H} \oplus \mathcal{H}$. Moreover, we denote by $\text{tr}(\cdot)$ the trace in \mathcal{H} , by $\text{Tr}(\cdot)$ the trace in $\mathcal{H} \oplus \mathcal{H}$, and by $\mathcal{B}(\mathcal{H})$ (resp. $\mathcal{B}_1(\mathcal{H})$) the set of bounded (resp. trace class) operators in \mathcal{H} .

Lemma 4.6. One infers that

(i)

$$QP + PQ = 0. \quad (4.12)$$

(ii)

$$Q^2 = \begin{pmatrix} H_1 & 0 \\ 0 & H_2 \end{pmatrix}. \quad (4.13)$$

(iii)

$$F e^{-tH_1} \supseteq e^{-tH_2} F, \quad F^* e^{-tH_2} \supseteq e^{-tH_1} F^*. \quad (4.14)$$

Proof. While (i) and (ii) are obvious, (iii) follows from

$$Q e^{-tQ^2} \supseteq e^{-tQ^2} Q.$$

Lemma 4.7. Assume $B \in \mathcal{B}(\mathcal{H} \oplus \mathcal{H})$ is bounded and commutes with Q , i.e., $QB \supseteq BQ$. Suppose $e^{-tQ^2}, Q^2 e^{-tQ^2} \in \mathcal{B}_1(\mathcal{H} \oplus \mathcal{H})$, $t > 0$. Then

$$\frac{d}{dt} \text{Tr}[P e^{-tQ^2} B] = 0. \quad (4.15)$$

Proof.

$$\begin{aligned} \frac{d}{dt} \text{Tr}[P e^{-tQ^2} B] &= -\text{Tr}[P Q^2 e^{-tQ^2} B] \\ &= \text{Tr}[P Q e^{-tQ^2} Q B] = \dots = \text{Tr}[P Q^2 e^{-tQ^2} B] \end{aligned} \quad (4.16)$$

using commutativity of Q and B and anticommutativity of Q and P in (4.12) and cyclicity of the trace. The fact that Q is unbounded is offset by the trace class hypotheses in Lemma 4.7. In fact, rewriting

$$-\text{Tr}[P Q^2 e^{-tQ^2} B] = -\text{Tr}[P Q (1 + |Q|)^{-1} Q (1 + |Q|) e^{-tQ^2} B]$$

enables one to prove (4.16) in a trivial manner by reshuffling $Q(1 + |Q|)^{-1} \in \mathcal{B}(\mathcal{H} \oplus \mathcal{H})$ as opposed to Q in (4.16).

Next we introduce the closed densely defined linear operators F_n , $1 \leq n \leq \nu$ as in \mathcal{H} and define $H_{1,n} = F_n^* F_n$, $H_{2,n} = F_n F_n^*$, $1 \leq n \leq \nu$ as in (4.10). Moreover, assume

$$e^{-tH_{j,n}}, \quad H_{j,n} e^{-tH_{j,n}} \in \mathcal{B}_1(\mathcal{H}), \quad 1 \leq n \leq \nu$$

and

$$[F_m, F_n] \subseteq 0, \quad [F_m, F_n^*] \subseteq 0, \quad m \neq n$$

implying

$$[H_{j,m}, H_{\ell,n}] \subseteq 0, \quad j, \ell = 1, 2, \quad m \neq n.$$

We also denote

$$Q_n = \begin{pmatrix} 0 & F_n^* \\ F_n & 0 \end{pmatrix}, \quad 1 \leq n \leq \nu \quad (4.17)$$

in $\mathcal{H} \oplus \mathcal{H}$ as in (4.11) and define for any $A \in \mathcal{P}_\nu$ (the power set of $\{1, 2, \dots, \nu\}$) the self-adjoint operator

$$H_A^0 = \sum_{n \in A} H_{1,n} + \sum_{n \notin A} H_{2,n}. \quad (4.18)$$

Then an abstract version of (4.7) in the noninteracting case reads as follows.

Theorem 4.8.

$$\sum_{A \in \mathcal{P}_\nu} (-1)^{|A|} \text{tr}(e^{-tH_A^0}) = \sum_{A \in \mathcal{P}_\nu} (-1)^{|A|} \dim \text{Ran}[P_{H_A^0}(\{0\})], \quad (4.19)$$

where $P_{H_A^0}(\Omega)$, $\Omega \subseteq \mathbb{R}$, denote the spectral projections of H_A^0 .

Proof. One computes

$$\begin{aligned} \frac{d}{dt} \sum_{A \in \mathcal{P}_\nu} (-1)^{|A|} \text{tr}(e^{-tH_A^0}) &= - \sum_{A \in \mathcal{P}_\nu} (-1)^{|A|} \text{tr}(H_A^0 e^{-tH_A^0}) \\ &= - \sum_{n=1}^{\nu} \text{Tr}[PQ_n^2 e^{-tQ_n^2} B_{\nu,n}] = 0 \end{aligned} \quad (4.20)$$

by (4.15), where

$$\begin{aligned} B_{1,1} &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \\ B_{\nu,n} &= \begin{pmatrix} b_{\nu,n} & 0 \\ 0 & b_{\nu,n} \end{pmatrix}, \quad b_{\nu,n} = - \prod_{\substack{m=1 \\ m \neq n}}^{\nu} (e^{-tH_{2,m}} - e^{-tH_{1,m}}), \quad \nu \geq 2 \end{aligned} \quad (4.21)$$

are bounded and commute with Q_n . Thus the left-hand-side in (4.19) is independent of t and taking $t \uparrow \infty$ then determines the right-hand-side of (4.19).

Identifying $A_n = 1 \otimes \cdots \otimes 1 \otimes \frac{\partial}{\partial x_n} \Big|_D \otimes 1 \otimes \cdots \otimes 1$ in $L^2([0,1]^\nu)$ with

$$\frac{\partial}{\partial x_n} \Big|_D = \overline{\frac{d}{dx} \Big|_{C_0^\infty((0,1))}}, \quad 1 \leq n \leq \nu \quad (4.22)$$

in $L^2([0,1])$ then yields (4.7) in the case $V(x) = 0$ since only the zero-energy eigenvalue of the Neumann operator H_ϕ^0 contributes on the right-hand-side of (4.19). More generally, if A_n has the tensor product structure

$$A_n = 1 \otimes \cdots \otimes 1 \otimes a_n \otimes 1 \otimes \cdots \otimes 1$$

in $\mathcal{H} = \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_\nu$, then clearly $[A_m, A_n] \subseteq 0$ and one evaluates

$$\sum_{A \in \mathcal{P}_\nu} (-1)^{|A|} \text{tr}(e^{-tH_A^0}) = \prod_{n=1}^{\nu} \text{tr}(e^{-ta_n a_n^*} - e^{-ta_n^* a_n}). \quad (4.23)$$

In the special case (4.22), where $a_n = \frac{\partial}{\partial x_n} \Big|_D$, one confirms that

$$\text{tr}(e^{-ta_n a_n^*} - e^{-ta_n^* a_n}) = 1, \quad 1 \leq n \leq \nu.$$

5. Trace Formulas and Point Interactions in Dimensions One, Two, and Three.

In this section we describe a different kind of multi-dimensional trace formula based on point interactions [2] and hence rank-one perturbations of resolvents first derived in [17] in a slightly different form. Since point interactions (also called contact interactions or δ -interactions) are limited to $\nu = 1, 2, 3$ space dimensions, so will be our approach below.

Assuming V to be real-valued, continuous and bounded from below on \mathbb{R}^ν , $\nu = 1, 2, 3$, we introduce $H = -\Delta + V$ as in (4.3). The resolvent of the self-adjoint Hamiltonian $H_{\alpha,x}$, modeling H plus a point interaction centered at $x \in \mathbb{R}^\nu$ (whose strength is parameterized in terms of $\alpha \in \mathbb{R}$), is defined as follows (see, e.g., [2], [42])

$$(H_{\alpha,x} - z)^{-1} = (H - z)^{-1} + D_{\alpha,x}(z)^{-1} (\overline{G(z, x, \cdot)}, \cdot) G(z, \cdot, x), \quad z \in \mathbb{C} \setminus \{\sigma(H_{\alpha,x}) \cup \sigma(H)\}, \quad (5.1)$$

where

$$D_{\alpha,x}(z) = \begin{cases} -\alpha^{-1} - \Gamma_\nu(z, x), & \nu = 1, \alpha \in \mathbb{R} \cup \{\infty\}, \alpha \neq 0 \\ \alpha - \Gamma_\nu(z, x), & \nu = 2, 3, \alpha \in \mathbb{R}, \end{cases} \quad (5.2)$$

$$\Gamma_1(z, x) = G(z, x, x), \quad \Gamma_2(z, x) = \lim_{|\epsilon| \downarrow 0} [G(z, x, x + \epsilon) - (2\pi)^{-1} \ln(|\epsilon|)], \quad (5.3)$$

$$\Gamma_3(z, x) = \lim_{|\epsilon| \downarrow 0} [G(z, x, x + \epsilon) - (4\pi |\epsilon|)^{-1}],$$

and $G(z, x, x')$ denotes the Green's function of H . In analogy to (2.5) one then computes

$$\text{Tr}[(H_{\alpha,x} - z)^{-1} - (H - z)^{-1}] = -\frac{d}{dz} \ln[D_{\alpha,x}(z)]. \quad (5.4)$$

Krein's spectral shift function for the pair $(H_{\alpha,x}, H)$ is then introduced via

$$\text{Tr}[(H_{\alpha,x} - z)^{-1} - (H - z)^{-1}] = -\int_{E_{\alpha,x,0}}^{\infty} d\lambda \frac{\xi_{\alpha,x}(\lambda)}{(\lambda - z)^2}, \quad (5.5)$$

with $E_{\alpha,x,0} = \inf\{\sigma(H_{\alpha,x}) \cup \sigma(H)\}$ and the normalization

$$\xi_{\alpha,x}(\lambda) = 0, \quad \lambda < E_{\alpha,x,0}. \quad (5.6)$$

$\xi_{\alpha,x}(\lambda)$ is related to $D_{\alpha,x}(z)$ as $\xi(\lambda, x)$ is to $g(z, x, x)$ in (2.24). The high-energy expansion (see, e.g., [35], [41])

$$\lim_{|\epsilon| \downarrow 0} [G(z, x, x + \epsilon) - G^{(0)}(z, x, x + \epsilon)] = -V(x) \begin{cases} 1/4(-z)^{3/2} + o(z^{-3/2}), & \nu = 1 \\ -1/4\pi z + o(z^{-1}), & \nu = 2 \\ 1/8\pi(-z)^{1/2} + o(z^{-1/2}), & \nu = 3 \end{cases} \quad (5.7)$$

then yields

$$D_{\alpha,x}(z) = \begin{cases} -\alpha^{-1} - \frac{i}{2}z^{-1/2} - \frac{i}{4}V(x)z^{-3/2} + o(z^{-3/2}), & \nu = 1 \\ (2\pi)^{-1} \ln((-iz)^{1/2}) + \tilde{\alpha} - (4\pi)^{-1}V(x)z^{-1} + o(z^{-1}), & \nu = 2 \\ -i(4\pi)^{-1}z^{1/2} + \alpha + i(8\pi)^{-1}V(x)z^{-1/2} + o(z^{-1/2}), & \nu = 3 \end{cases}, \quad (5.8)$$

where

$$\tilde{\alpha} = \alpha + (2\pi)^{-1}\gamma - (2\pi)^{-1} \ln(2)$$

with $\gamma = .5772\dots$ being Euler's constant. A combination of (5.4), (5.5), and (5.8) then implies the following trace formula.

Theorem 5.1. [17]

$\nu = 1$:

$$V(x) = \begin{cases} \lim_{z \downarrow -\infty} \left\{ -z - 2 \int_{\inf[\sigma(H)]}^{\infty} d\lambda z^2 (\lambda - z)^{-2} \xi_{\infty,x}(\lambda) \right\}, & \alpha = \infty, \\ \frac{1}{6}\alpha^2 + \lim_{z \downarrow -\infty} \left\{ -\frac{2}{3}z + \frac{i}{3}\alpha z^{1/2} + \frac{8i}{3}\alpha^{-1} z^{5/2} \int_{E_{\alpha,x,0}}^{\infty} d\lambda (\lambda - z)^{-2} \xi_{\alpha,x}(\lambda) \right\}, & \alpha \in \mathbb{R} \setminus \{0\}. \end{cases} \quad (5.9)$$

$\nu = 2$:

$$V(x) = \lim_{z \downarrow -\infty} \left\{ -z + 4\pi[(2\pi)^{-1} \ln(-iz^{1/2}) + \tilde{\alpha}] \int_{E_{\alpha,x,0}}^{\infty} d\lambda z^2 (\lambda - z)^{-2} \xi_{\alpha,x}(\lambda) \right\}. \quad (5.10)$$

$\nu = 3$:

$$V(x) = 16\pi^2\alpha^2 + \lim_{z \downarrow -\infty} \left\{ -z + 4\pi i\alpha z^{1/2} + 2 \int_{E_{\alpha,x,0}}^{\infty} d\lambda z^2 (\lambda - z)^{-2} \xi_{\alpha,x}(\lambda) \right\}. \quad (5.11)$$

Using the systematic high-energy expansion of $\lim_{|\epsilon| \downarrow 0} [G(z, x, x + \epsilon) - G^{(0)}(z, x, x + \epsilon)]$ in terms of (multi-dimensional) KdV invariants (see, e.g., [35], [41]) one can extend Theorem 5.1 to higher-order trace relations in analogy to (2.29) and (2.54).

In the special case where $V^{(0)} \equiv 0$, one obtains explicitly,

$$D_\alpha^{(0)}(z) = \begin{cases} -\alpha^{-1} - (-4z)^{-1/2}, & \nu = 1 \\ \tilde{\alpha} + (2\pi)^{-1} \ln((-z)^{1/2}), & \nu = 2 \\ \tilde{\alpha} + (4\pi)^{-1} (-z)^{1/2}, & \nu = 3, \end{cases} \quad (5.12)$$

and

$$\text{Tr}[(H_{\alpha,x}^{(0)} - z)^{-1} - (H^{(0)} - z)^{-1}] = - \int_{E_{\alpha,0}^{(0)}}^{\infty} d\lambda \frac{\xi_\alpha^{(0)}(\lambda)}{(\lambda - z)^2}. \quad (5.13)$$

Here, for $\nu = 1$,

$$\xi_\alpha^{(0)}(\lambda) = \begin{cases} 0, & \lambda < -\alpha^2/4 \\ -1, & -\alpha^2/4 < \lambda < 0 \\ a_\alpha(\lambda), & \lambda > 0 \\ \alpha < 0 \end{cases} \quad \begin{cases} 0, & \lambda < 0 \\ \frac{1}{2}, & \lambda > 0 \\ \alpha = 0 \end{cases} \quad \begin{cases} 0, & \lambda < 0 \\ 1 + a_\alpha(\lambda), & \lambda > 0 \\ \alpha \in (0, \infty] \end{cases} \quad (5.14)$$

writing $a_\alpha(\lambda) = -\pi^{-1} \arctan(|\alpha|/2\lambda^{1/2})$, and, for $\nu = 2$,

$$\xi_\alpha^{(0)}(\lambda) = \begin{cases} 0, & \lambda < -e^{-4\pi\tilde{\alpha}} \\ -1, & -e^{-4\pi\tilde{\alpha}} < \lambda \leq 0 \\ -\pi^{-1} \arctan[\pi/(4\pi\tilde{\alpha} + \ln(\lambda))] - 1, & 0 \leq \lambda \leq e^{-4\pi\tilde{\alpha}} \\ -\pi^{-1} \arctan[\pi/(4\pi\tilde{\alpha} + \ln(\lambda))], & \lambda \geq e^{-4\pi\tilde{\alpha}} \end{cases} \quad (5.15)$$

and, finally, for $\nu = 3$,

$$\xi_\alpha^{(0)}(\lambda) = \begin{cases} 0, & \lambda < -(4\pi\alpha)^2 \\ -1, & -(4\pi\alpha)^2 < \lambda < 0 \\ A_\alpha(\lambda), & \lambda > 0 \\ \alpha < 0 \end{cases} \quad \begin{cases} 0, & \lambda < 0 \\ -\frac{1}{2}, & \lambda > 0 \\ \alpha = 0 \end{cases} \quad \begin{cases} 0, & \lambda < 0 \\ A_\alpha(\lambda), & \lambda > 0 \\ \alpha > 0 \end{cases}, \quad (5.16)$$

writing $A_\alpha(\lambda) = -\pi^{-1} \arctan(\lambda^{1/2}/4\pi|\alpha|)$, and

$$E_{\alpha,0}^{(0)} = \begin{cases} -\alpha^2/4, & \alpha < 0 \\ 0, & \alpha \in [0, \infty] \end{cases} \quad \begin{cases} -e^{-4\pi\tilde{\alpha}} & \\ & \end{cases} \quad \begin{cases} -(4\pi\alpha)^2, & \alpha < 0 \\ 0, & \alpha \geq 0 \end{cases} \quad \begin{matrix} \nu = 1 \\ \nu = 2 \\ \nu = 3 \end{matrix}. \quad (5.17)$$

6. A Uniqueness Result for Three-Dimensional Schrödinger Operators.

Finally, we briefly sketch a uniqueness result in the context of three-dimensional Schrödinger operators with spherically symmetric potentials originally derived in [19]. Consider the potential $V : \mathbb{R}^3 \rightarrow \mathbb{R}$,

$$V(x) = v(|x|), \quad v \in L^1([0, R]) \text{ for all } R > 0 \quad (6.1)$$

and define the self-adjoint Schrödinger operator H in $L^2(\mathbb{R}^3)$ associated with the differential expression $-\Delta + v(|x|)$ by decomposition with respect to angular momenta. This represents H as an infinite direct sum of half-line operators in $L^2((0, \infty); r^2 dr)$ associated with differential expressions of the type

$$\hat{\tau}_\ell = -\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} + \frac{\ell(\ell+1)}{r^2} + v(r), \quad r = |x| > 0, \quad \ell \in \mathbb{N}_0. \quad (6.2)$$

A simple unitary transformation (see, e.g., [36], Appendix to Sect. X.1) reduces (6.2) to

$$\tau_\ell = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + v(r) \quad (6.3)$$

and associated Hilbert space $L^2((0, \infty); dr)$. Next, let $G(z, x, x')$, $x \neq x'$ denote the Green's function of H and define $H_{\alpha,0}$ in $L^2(\mathbb{R}^3)$, $\alpha \in \mathbb{R}$ as in (5.1) (with $x = 0$) and the corresponding Krein spectral shift function $\xi_{\alpha,0}(\lambda)$ as in (5.5), i.e.,

$$\xi_{\alpha,0}(\lambda) = \lim_{\epsilon \downarrow 0} \pi^{-1} \operatorname{Im}\{\ln[D_{\alpha,0}(\lambda + i\epsilon)]\} \quad \text{a.e.} \quad (6.4)$$

Then the following uniqueness result holds.

Theorem 6.1. [19] Define $H_j, H_{j,\alpha_j,0}$, $\alpha_j \in \mathbb{R}$ associated with $-\Delta + v_j(|x|)$, $x \in \mathbb{R}^3$, $j = 1, 2$ as above and introduce Krein's spectral shift function $\xi_{j,\alpha_j,0}(\lambda)$ for the pair $(H_{j,\alpha_j,0}, H_j)$, $j = 1, 2$. Then the following are equivalent:

(i)

$$\xi_{1,\alpha_1,0}(\lambda) = \xi_{2,\alpha_2,0}(\lambda) \quad \text{for a.e. } \lambda \in \mathbb{R}. \quad (6.5)$$

(ii)

$$\alpha_1 = \alpha_2 \quad \text{and} \quad V_1(x) = V_2(x) \quad \text{for a.e. } x \in \mathbb{R}^3. \quad (6.6)$$

The proof of this result in [19] is based on detailed Weyl- m -function investigations associated with the angular momentum channel $\ell = 0$.

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