On Trace Formulas for Schrödinger–Type Operators

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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 $L^2(R)$ 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 $r^{-2}[-(p^2 f')' + q f]$ 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
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

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

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

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

$$h^D_y f = \frac{1}{y^2}[-(p^2f')' + qf],$$

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

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

$$g(z, x, x') = (h - z)^{-1}(x, x'), \quad g^D_y(z, x, x') = (h^D_y - z)^{-1}(x, x').$$

One verifies

$$g^D_y(z, x, x') = g(z, x, x') - \frac{g(z, x, y)g(z, y, x')}{g(z, y, y)},$$

and hence

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

To proceed further, we need a high-energy expansion, i.e., $z \to \infty$, 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

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

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

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

and introduce the unitary operator

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

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

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

$$Hf = -f'' + Vf,$$

$$f \in \mathcal{D}(H) = \{g \in L^2(\mathbb{R}; dt) | g, g' \in AC_{loc}(\mathbb{R}), Hg \in L^2(\mathbb{R}; dt)\},$$
where
\[
V(t) = \frac{Q(t)}{R(t)^2} + \frac{1}{(R(t)P(t))^2} \left[ \frac{1}{2} (R(t)P(t))(R(t)P(t))_t - \frac{1}{4} ((R(t)P(t))^2) ight]
\]
\[
= \frac{g(x)}{r(x)} + \frac{p(x)}{2r(x)^3} (r(x)p(x))_{xx} + \frac{(r(x)p(x))_x}{2r(x)^2} \left( \frac{p(x)}{r(x)} \right)_x - \frac{1}{4r(x)^4} (r(x)p(x))^2,
\]
:= \nu(x), \quad x = x(t). \tag{2.10}
\]
Furthermore,
\[
g(z, x, x') = \frac{G(z, t(x), t(x'))}{[r(x)p(x)r(x')p(x')]^{1/2}}, \quad x, x' \in \mathbb{R}, \quad z \in \mathbb{C}, \tag{2.11}
\]
where \(G\) is the Green's function of \(H\). Moreover,
\[
H^D_u = U H^D y U^{-1} = -\frac{d^2}{dt^2} + V \tag{2.12}
\]
with \(V\) given by (2.10), is the Schrödinger operator with a Dirichlet boundary condition imposed at the point \(u = \int_0^1 dx \left[ p(x)/r(x) \right] \). Let \(G^D_u\) denote the Green's function of \(H^D_u\). Then
\[
g^D_y(z, x, x') = \frac{G^D_y(z, t(x), t(x'))}{[p(x)r(x)p(x')r(x')]^{1/2}}. \tag{2.13}
\]
Hence we find, using known results for \(H\) [22, 24] that
\[
\text{Tr} \left[ e^{-\tau h^D_x} - e^{-\tau h} \right] \bigg|_{\tau=0} \sum_{\ell=0}^\infty s_\ell(x) r^{\ell}, \tag{2.14}
\]
\[
\text{Tr} \left[ (h^D_x - z)^{-1} - (h - z)^{-1} \right] |_{z=\perp} \sum_{x \in C \setminus \ell} r_j(x) z^{-j-1}, \tag{2.15}
\]
where \(C_\epsilon\) is a cone with apex at \(E_0 := \inf \{ \sigma(H) \} \) and opening angle \(\epsilon > 0\). Recursion relations for \(s_\ell\) and \(r_j\) are given by (cf. [22],[24])
\[
s_\ell(x) = (-1)^{\ell+1} \frac{r_\ell(x)}{\ell!}, \quad \ell \in \mathbb{N}_0, \tag{2.16}
\]
\[
r_0(x) = \frac{1}{2}, \quad r_1(x) = \frac{1}{2} \nu(x), \tag{2.17}
\]
\[
r_j(x) = j \gamma_j(x) - \sum_{\ell=1}^{j-1} \gamma_{j-\ell}(x) r_\ell(x), \quad j = 2, 3, \ldots,
\]
\[
\gamma_0 = 1, \quad \gamma_1 = \frac{1}{2} \nu,
\]
\[
\gamma_{j+1} = -\frac{1}{2} \sum_{\ell=1}^j \gamma_\ell \gamma_{j+1-\ell} + \frac{1}{2} \sum_{\ell=0}^j \left[ \nu \gamma_\ell \gamma_{j-\ell} + \frac{1}{4} \gamma_\ell \gamma_{j-\ell} - \frac{1}{2} \gamma_{\ell,x} \gamma_{j-\ell} - \frac{1}{2} \gamma_{j,x} \gamma_{j-\ell} \right], \quad j = 1, 2, \ldots.
\]
Explicitly, one computes
\[
s_0 = \frac{1}{2}, \quad s_1(x) = \frac{1}{2} \nu(x), \quad \text{etc.} \tag{2.19}
\]
The proof of (2.17) in [22] follows from the well-known differential equation for $\Gamma(z,t) = G(z,t,t)$, namely

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

and the asymptotic expansion

$$\Gamma(z,t)_{z=\infty} \sum_{j=0}^{\infty} \Gamma_j(t)z^{-j},$$

with $\Gamma_j(t)$ defined in (2.18) but $\nu(x)$ 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., $g(\cdot,x,x): \mathbb{C}_+ \to \mathbb{C}_+$ is analytic, $\mathbb{C}_+ = \{z \in \mathbb{C} \mid \text{Im } z > 0\}$. Hence $g$ allows a representation [3]

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

where $\xi(\lambda,x)$ is Krein’s spectral shift function for the pair $(h^D_x,h)$ [28], satisfying $0 \leq \xi(\lambda,x) \leq 1$, $\xi(\cdot,x) \in L^1_{loc}(\mathbb{R};d\lambda)$, 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 real parts 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

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

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

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

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

In particular,

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

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

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

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

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

$$s_0(x) = -\frac{1}{2}, \quad s_\ell(x) = \frac{(-1)^{\ell - 1}}{\ell!} \left\{ \frac{E_0^\ell}{2} + \ell \lim_{\tau \to 0} \int_{E_0}^{\infty} d\lambda e^{-\tau \lambda} \lambda^{\ell - 1} \left[ \frac{1}{2} - \xi(\lambda,x) \right] \right\}, \quad \ell \in \mathbb{N}. \quad (2.29)$$
From the high-energy behavior of the Green’s function we find that
\[ p(x) r(x) = i \lim_{z \to \pm i \infty} \sqrt{z} g(z, x, x) \]  
\[ (2.30) \]

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 \( \Xi \) and \( \xi \) 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 \( (H^D, H) \). By choosing any positive \( p \in C^\infty(R) \) we may define the Sturm-Liouville operator \( h \) using (2.10) (or (2.11) for the Green’s function). By construction, the pair \( (h^D_x, h) \) 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 \( \lambda \in R - \sigma(h) \). More precisely, suppose \( (\lambda_1, \lambda_2) \subset R - \sigma(h) \) and assume that \( \mu(x) \in (\lambda_1, \lambda_2) \) is an eigenvalue of \( h^D_x \). Then one has
\[ \xi(\lambda, x) = \begin{cases} 0, & \lambda_1 < \lambda < \mu(x) \\ 1, & \mu(x) < \lambda < \lambda_2. \end{cases} \]
\[ (2.31) \]

Next, assume that \( p, q, \) and \( r \) are periodic, i.e.,
\[ p(x + a) = p(x), \quad q(x + a) = q(x), \quad r(x + a) = r(x), \quad x \in R \]
\[ (2.32) \]
for some \( a > 0 \). Then Floquet theory implies that
\[ \sigma(h) = \bigcup_{n=1}^\infty [E_{2(n-1)}, E_{2n-1}], \quad E_0 < E_1 < E_2 < E_3 < \cdots \]
\[ (2.33) \]
and
\[ \sigma(h^D_x) = \sigma(h) \cup \{ \mu_n(x) \}_{n \in N}, \quad E_{2n-1} \leq \mu_n(x) \leq E_{2n}, \quad x \in R, \quad n \in N. \]
\[ (2.34) \]
In the periodic case \( g(\lambda + i0, x, x) \) is purely imaginary on the spectrum, and hence
\[ \xi(\lambda, x) = \begin{cases} 0, & \lambda < E_0, \mu_n(x) < \lambda < E_{2n}, \quad n \in N \\ 1, & E_{2n-1} < \lambda < \mu_n(x), \quad n \in N \\ \frac{1}{2}, & E_{2(n-1)} < \lambda < E_{2n-1}, \quad n \in N \end{cases} \]
\[ (2.35) \]
Combining (2.29) and (2.35) we obtain the following result.

**Theorem 2.3.** Let \( p, q, r \in C^\infty(R) \), \( p, r > 0 \) be periodic, \( p(x + a) = p(x), q(x + a) = q(x), r(x + a) = r(x) \) for some \( a > 0 \). Then
\[ 2(-1)^{\ell+1} \ell! s_\ell(x) \equiv E_0^\ell + \sum_{n=1}^\infty [E_{2n-1}^\ell + E_{2n}^\ell - 2\mu_n(x)^\ell], \quad \ell \in N, \quad x \in R. \]
\[ (2.36) \]
In particular,
\[ 2s_1(x) = v(x) = E_0 + \sum_{n=1}^\infty [E_{2n-1} + E_{2n} - 2\mu_n(x)], \]
\[ (2.37) \]
Finally, we turn to the case where the Dirichlet boundary condition is replaced by a family of (Robin-type) self-adjoint boundary conditions. Define

\[
h_{\beta,y} f = \frac{1}{r^2} [- (p^2 f')' + qf],
\]

\[
f \in \mathcal{D}(h_{\beta,y}) = \{ g \in L^2(\mathbb{R}; r^2 dx) \mid g, g' \in AC([y, \pm R]), \quad R > 0, \quad \lim_{\epsilon \to 0} [g'(y \pm \epsilon) + \beta g(y \pm \epsilon)] = 0, \quad h_{\beta,y} g \in L^2(\mathbb{R}; r^2 dx) \}.
\]

(\beta = 0 \text{ 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

\[
H_{\nu(\beta,u),u} = - \frac{d^2}{dt^2} + V,
\]

\[
\mathcal{D}(H_{\nu(\beta,u),u}) = \{ g \in L^2(\mathbb{R}; dt) \mid g, g' \in AC([u, \pm R]), \quad R > 0, \quad \lim_{\epsilon \to 0} [g'(u \pm \epsilon) + \nu(\beta, u) g(u \pm \epsilon)] = 0, \quad H_{\nu(\beta,u),u} g \in L^2(\mathbb{R}; dt) \},
\]

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

\[
u(\beta, u) = \frac{\int_{x_0}^y dx}{p(x)},
\]

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

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

The Green’s function of \(h_{\beta,y}\) is given by

\[
g_{\beta,y}(z, x, x') = (h_{\beta,y} - z)^{-1}(x, x')
\]

\[
= g(z, x, x') - \frac{(\beta + \partial_2) g(z, x, y)(\beta + \partial_1) g(z, y, x')}{(\beta + \partial_1)(\beta + \partial_2) g(z, y, y)},
\]

where we abbreviate

\[
\partial_1 g(z, y, x') = \partial_x g(z, x, x')|_{x=y}, \quad \partial_2 g(z, y, x) = \partial_x g(z, x, x')|_{x=y}, \text{ etc.}
\]

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

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

and it satisfies

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

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

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

\[
\text{Tr}[e^{-\tau h_{\beta,x}} - e^{-\tau h}] = \sum_{\ell=0}^{\infty} s_{\beta,\ell}(x) \tau^\ell,
\]
where
\[ s_{\beta, \ell}(x) = (-1)^{\ell+1} \frac{r_{\beta, \ell}(x)}{\ell!}, \quad \ell \in \mathbb{N}_0, \] (2.48)

with (cf. [22],[24]),
\[
\begin{align*}
    r_{\beta, 0}(x) &= -\frac{1}{2}, \\
    r_{\beta, 1}(x) &= \nu(\beta, u(x))^2 - \frac{1}{2} v(x), \\
    r_{\beta, j}(x) &= j \gamma_{\beta, j-1}(x) - \sum_{\ell=1}^{j-1} \gamma_{\beta, j-\ell-1}(x) r_{\beta, \ell}(x), \quad j = 2, 3, \ldots, \\
    \gamma_{\beta, -1} &= 1, \\
    \gamma_{\beta, 0} &= \nu^2 - \frac{1}{2} v, \\
    \gamma_{\beta, 1} &= \frac{1}{2} \nu^2 v + \frac{1}{2} \nu v_x - \frac{1}{8} v^2 + \frac{1}{8} v_{xx}, \\
    \gamma_{\beta, 2} &= \frac{1}{16} v^3 + \frac{3}{8} \nu^2 v^2 + \frac{3}{16} v_x (4 \nu v + v_x) + \frac{1}{8} v_{xx} (v - \nu^2) - \frac{1}{8} \nu v_{xxx} - \frac{1}{64} v_{xxxx}, \\
    \gamma_{\beta, j+1} &= \frac{1}{8} \sum_{\ell=1}^{j} \left[ 2 (v - \nu^2) \gamma_{\beta, \ell-1, x} \gamma_{\beta, j-\ell, x} - (v - \nu^2) \gamma_{\beta, \ell-1, x} \gamma_{\beta, j-\ell, x} - 4 \gamma_{\beta, \ell-1, x} \gamma_{\beta, j-\ell, x} - 2 v_x \gamma_{\beta, \ell-1, x} \gamma_{\beta, j-\ell, x} + \gamma_{\beta, \ell-1} \gamma_{\beta, j-\ell} \right] \\
    &\quad + \frac{1}{8} \sum_{\ell=0}^{j} \left[ \gamma_{\beta, \ell, x} \gamma_{\beta, j-\ell, x} - 2 \gamma_{\beta, \ell} \gamma_{\beta, j-\ell, x} - 4 (v^2 - 2v) \gamma_{\beta, \ell} \gamma_{\beta, j-\ell} \right], \quad j = 2, 3, \ldots 
\end{align*}
\] (2.49)

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

The proof of (2.49) in [22] is based on the differential equation for \( \Gamma_\nu(z, t) = (\nu + \partial_t) (\nu + \partial_z) G(z, t, t) \), namely
\[
\begin{align*}
    2 [V(t) - \nu - z] \Gamma_{\nu, \ell}(z, t) \Gamma_\nu(z, t) - [V(t) - \nu - z] \Gamma_{\nu, \ell}(z, t)^2 - 2 V(t) \Gamma_{\nu, \ell}(z, t) \Gamma_\nu(z, t) - 4 [V(t) - \nu - z] [V(t) - \nu - z - \nu V(t)] \Gamma_\nu(z, t)^2 &= - [V(t) - \nu - z]^3 
\end{align*}
\] (2.52)

and the asymptotic expansion
\[
\Gamma_\nu(z, t) \mid_{z \to \infty} = \frac{i}{2} \sum_{j=-1}^{\infty} \frac{1}{\ell} \Gamma_{\nu, \ell}(t) z^{-\ell-j}, 
\] (2.53)

with \( \Gamma_{\nu, \ell}(t) \) defined as in (2.50) with \( \beta \) replaced by \( \nu \) and \( v(x) \) by \( V(t) \).

The analog of Theorem 2.2 now reads
\[
\begin{align*}
    s_{\beta, \ell}(x) &= \frac{(-1)^{\ell}}{\ell!} \left\{ \frac{\zeta_{\beta, 0}(x)}{2} + \ell \lim_{\tau \to 0} \int_{\xi_{\beta, 0}(x)}^{\infty} d\lambda e^{-\tau \lambda} \lambda^{\ell-1} \left[ -\frac{1}{2} + \xi_{\beta}(\lambda, x) \right] \right\}, \quad \ell \in \mathbb{N}, 
\end{align*}
\] (2.54)

and, in particular,
\[
\begin{align*}
    s_{\beta, 1}(x) &= \nu(\beta, u(x))^2 - \frac{1}{2} v(x) \\
    &= -\frac{1}{2} \zeta_{\beta, 0}(x) - \lim_{\tau \to 0} \int_{\xi_{\beta, 0}(x)}^{\infty} d\lambda e^{-\tau \lambda} \left[ -\frac{1}{2} + \xi_{\beta}(\lambda, x) \right],
\end{align*}
\] (2.55)

Our last example in this section will be the periodic case, assuming (2.32) to hold.
In this case
\[
\sigma(h_{\beta,x}) = \sigma(h) \cup \{\zeta_{\beta,n}(x)\}_{n \in \mathbb{N}_0},
\]
\[
\zeta_{\beta,0}(x) \leq E_0, \ E_{2n-1} \leq \zeta_{\beta,n}(x) \leq E_{2n}, \ x \in \mathbb{R}, \ n \in \mathbb{N},
\]
with \(\sigma(h)\) given as in (2.33). The spectral shift function now reads
\[
\xi_{\beta}(\lambda, x) = \begin{cases} 
0, & \lambda < \zeta_{\beta,0}(x), \ E_{2n-1} < \lambda < \zeta_{\beta,n}(x), \ n \in \mathbb{N} \\
-1, & \zeta_{\beta,n}(x) < \lambda < E_{2n}, \ n \in \mathbb{N}_0 \\
-\frac{1}{2}, & E_{2(n-1)} < \lambda < E_{2n-1}, \ n \in \mathbb{N}
\end{cases}
\]
and the trace formula (2.54) in the periodic case now equals
\[
2(-1)^{\ell}! s_{\beta,\ell}(x) = 2\zeta_{\beta,0}(x)^{\ell} - E_0^{\ell} + \sum_{n=1}^{\infty} [2\zeta_{\beta,n}(x)^{\ell} - E_{2n-1}^{\ell} - E_{2n}^{\ell}], \ \ell \in \mathbb{N}, \ x \in \mathbb{R}. \quad (2.58)
\]
In the case \(\ell = 1\) we find
\[
-2s_{\beta,1}(x) = v(x) = \frac{q(x)}{r(x)} + \frac{p(x)}{2r(x)^2} (r(x)p(x))_{xx} + \frac{(r(x)p(x))_x}{2r(x)^2} \left( \frac{p(x)}{r(x)} \right)_x - \frac{(r(x)p(x))^2}{2r(x)^3}.
\]
Subtracting this equation from (2.37) yields
\[
-\left( \frac{p(x)}{r(x)} \right)_x - \frac{(p(x)r(x))^2}{2r(x)^2} \right)^2 = E_0 - \zeta_{\beta,0}(x) + \sum_{n=1}^{\infty} [E_{2n-1} + E_{2n} - \mu_n(x) - \zeta_{\beta,n}(x)].
\]


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
\[
Hf = -I_m f'' + Qf,
\]
\[
f \in \mathcal{D}(H) = \{g \in L^2(\mathbb{R})^m \mid g_j, g_j' \in AC_{loc}(\mathbb{R}), 1 \leq j \leq m; Hg \in L^2(\mathbb{R})^m \},
\]
where \(f = (f_1, \ldots, f_m)^T\), \(I_m\) denotes the identity in \(\mathbb{C}^m\), and \(Q = (Q_{j,k})_{1 \leq j, k \leq m}\) denotes a self-adjoint matrix satisfying
\[
Q_{j,k} \in C(\mathbb{R}) \text{ bounded from below, } 1 \leq j, k \leq m.
\]
Closely associated with the equation
\[
Hf = zf
\]
is the first-order \(2m \times 2m\) system
\[
L(z)(f, f')^T = 0,
\]
where \((f, f')^T = (f_1, \ldots, f_m, f_1', \ldots, f_m')^T\) and
\[
L(z) = I_{2m} \frac{d}{dx} - A(z), \quad A(z) = \begin{pmatrix} 0 & I_m \\ Q - z & 0 \end{pmatrix},
\]
\[
L(z) = I_{2m} \frac{d}{dx} - A(z), \quad A(z) = \begin{pmatrix} 0 & I_m \\ Q - z & 0 \end{pmatrix},
\]
\[
(3.5)
\]
with $I_{2m}$ the identity in $C^{2m}$. If $\Psi(z, x)$ denotes a fundamental matrix for $L(z)$, that is,
\begin{equation}
L(z)\Psi(z) = 0,
\end{equation}
or equivalently,
\begin{equation}
\Psi'(z, x) = A(z, x)\Psi(z, x),
\end{equation}
then $\tilde{\Psi}(z, x)$ defined by
\begin{equation}
\tilde{\Psi}(z, x) = \Psi(z, x)^{-1}
\end{equation}
satisfies the adjoint system
\begin{equation}
\tilde{\Psi}'(z, x) = -\tilde{\Psi}(z, x)A(z, x).
\end{equation}

Moreover, the fundamental matrices $\Psi(z, x)$ and $\tilde{\Psi}(z, x)$ are of the form
\begin{equation}
\Psi(z, x) = \begin{pmatrix}
\psi_1(z, x) & \psi_2(z, x) \\
\psi'_1(z, x) & \psi'_2(z, x)
\end{pmatrix}, 
\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},
\end{equation}
and one verifies that
\begin{equation}
-\psi'_j(z, x) + Q(x)\psi_j(z, x) = z\psi_j(z, x), 
-\tilde{\psi}'_j(z, x) + \tilde{\psi}_j(z, x)Q(x) = z\tilde{\psi}_j(z, x), 
\end{equation}
for $j = 1, 2$.

In particular, assuming $\psi_j(z, x)$, $\tilde{\psi}_j(z, x)$ to be unique solutions of (3.11) (up to right resp. left multiplication of matrices constant with respect to $x$) satisfying
\begin{equation}
\psi_1(z, \cdot) := \psi_{\pm}(z, \cdot) \in L^2([R, \pm \infty))^m, 
\tilde{\psi}_1(z, \cdot) := \tilde{\psi}_{\pm}(z, \cdot) \in L^2([R, \pm \infty))^m, \quad R \in \mathbb{R}, \quad z \in \mathbb{C} \setminus \sigma(H),
\end{equation}
the Green’s matrix $G(z, x, x')$ of $H$ becomes
\begin{equation}
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}
\end{equation}
and hence the resolvent of $H$ is given by
\begin{equation}
((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).
\end{equation}

Since
\begin{equation}
-\psi''_j(z, x) + \psi_j(z, x)Q(x) = z\psi_j(z, x), \quad j = 1, 2,
\end{equation}
$\tilde{\psi}_j(z, x)$ are of the type
\begin{equation}
\tilde{\psi}_j(z, x) = A_{j, 1}(z)\psi_1(z, x) + B_{j, 2}(z)\psi_2(z, x), \quad j = 1, 2
\end{equation}
for matrices $A_{j, k}(z), B_{j, k}(z), 1 \leq j, k \leq 2$ in $C^m$ constant with respect to $x$. Introducing the “Wronskian” $W(\phi, \psi)(x)$ of $m \times m$ matrices $\phi$ and $\psi$ by
\begin{equation}
W(\phi, \psi)(x) = \phi(x)\psi'(x) - \phi'(x)\psi(x),
\end{equation}
one verifies that
\begin{equation}
\frac{d}{dx}W(\phi(z), \psi(z))(x) = 0
\end{equation}
for solutions \( \psi(z, x) \) and \( \phi(\bar{z}, x)^* \) of

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

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

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

and hence

\[
G(z, x, x) = -\psi_+(z, x)W(\psi_-(\bar{z})^*, \psi_+(z))^{{-1}} \psi_-(\bar{z}, x)^* = \psi_-(z, x)W(\psi_+(\bar{z})^*, \psi_-(z))^{{-1}} \psi_+(\bar{z}, x)^*.
\] (3.21)

The corresponding matrix-valued Dirichlet Schrödinger operator \( H^D_y \) in \( L^2(R)^m \) then reads

\[
H^D_y f = -I_m f'' + Qf, \\
 f \in D(H^D_y) = \{ g \in L^2(R)^m \mid g_j \in AC_{loc}(R), g'_j \in AC_{loc}(R \setminus \{y\}), \\
\lim_{e \to 0} g_j(y \pm e) = 0, H^D_y g \in L^2(R)^m \}
\] (3.22)

and its Green’s matrix \( G^D_y(z, x, x') \), the analog of (2.4), is given by

\[
G^D_y(z, x, x') = G(z, x, x') - G(z, y, x')^{-1} G(y, y, x').
\] (3.23)

The analog of (2.5) then becomes

\[
Tr[(H^D_x - z)^{-1} - (H - z)^{-1}] = -Tr[G(z, \cdot, x)G(z, x, x)^{-1} G(z, \cdot, x)]
\]

\[
= -Tr[G(z, x, x)^{-1} G(z, \cdot, x)G(z, x, \cdot)] = -Tr_{C^m}\{G(z, x, x)^{-1} \left[ \frac{d}{dz} G(z, x, x) \right] \}
\]

\[
= -\frac{d}{dz} Tr_{C^m}\{\ln[G(z, x, x)]\} = -\frac{d}{dz}\ln[\det_{C^m}[G(z, x, x)]],
\] (3.24)

where we used cyclicity of the trace,

\[
(H - z)^{-2}(x, x')_{j,k} = \frac{d}{dz} G(z, x, x')_{j,k} = \sum_{l=1}^m \int_R dx'' G(z, x, x'')_{j,l} G(z, x'', x')_{l,k},
\] (3.25)

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

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

\[
\Gamma(z, x) = G(z, x, x),
\] (3.26)

the matrix analog of (2.20) reads

\[
-\Gamma(z, x) \Gamma_{xx}(z, x) - \Gamma_{xx}(z, x) \Gamma(z, x) + \Gamma(x, x)^2 + \Gamma(z, x)^2 Q(x) + Q(x) \Gamma(z, x)^2 + 2 \Gamma(z, x) Q(x) \Gamma(z, x) - 4 z \Gamma(z, x)^2 = I_m
\] (3.27)

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

\[
\Gamma(z, x) \big|_{x \in \C \setminus \Gamma_0} = \frac{i}{2} z^{-1/2} \sum_{j=0}^{\infty} \Gamma_j(x) z^{-j},
\] (3.28)

with

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

$$-\frac{d}{dz} \ln[G(z, x, x)]_{|z|=\infty} \sum_{j=0}^{\infty} R_j(x) z^{-j-1},$$

(3.30)

where

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

(3.31)

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

$$\Xi(\lambda, x) = \frac{1}{\pi} \lim_{\epsilon \to 0} \Im \{ \ln[G(\lambda + i\epsilon, x, x)] \} \text{ for a.e. } \lambda \in \mathbb{R},$$

$$\Xi(\lambda, x) = 0, \lambda < E_0 := \inf \{ \sigma(H) \},$$

(3.32)

where \(\Im(M), \Re(M)\), in obvious notation, abbreviate

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

(3.33)

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

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

(3.34)

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

$$C_{R,\epsilon} = \{ z = E_0 + e^{i\phi} \mid \frac{3\pi}{2} \geq \phi \geq \frac{\pi}{2} \} \cup \{ z = E_0 + \lambda + i\epsilon \mid 0 \leq \lambda \leq R \}$$

$$\cup \{ z = E_0 + \Re e^{i\phi} \mid \arctan(\epsilon/R) \leq \phi \leq 2\pi - \arctan(\epsilon/R) \}$$

$$\cup \{ z = E_0 + \lambda - i\epsilon \mid 0 \leq \lambda \leq R \}, \quad R > \epsilon > 0.$$  

(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

$$\{\ln[G(z', x, x)]\}_{j,k} = \frac{1}{2\pi i} \oint_{C_{R,\epsilon}} dz' \{\ln[G(z', x, x)]\}_{j,k}$$

$$= \frac{1}{2\pi i} \oint_{C_{R,\epsilon}} dz' \{\ln[G(z', x, x)]\}_{j,k} \frac{z'}{1 + z'^2}$$

$$+ \frac{1}{2\pi i} \oint_{C_{R,\epsilon}} dz' \{\ln[G(z', x, x)]\}_{j,k} \left[ \frac{1}{z' - z} - \frac{z'}{1 + z'^2} \right]$$

$$= \text{Re} \{\ln[G(i, x, x)]\}_{j,k} + \frac{1}{\pi} \int_{E_0}^{R} d\lambda \Im \{\ln[G(\lambda + i0, x, x)]\}_{j,k}$$

$$+ \frac{1}{\lambda - z} - \frac{\lambda}{1 + \lambda^2} \left( \frac{1}{1 + \lambda^2} \right)$$

$$\xrightarrow{R \to \infty, \epsilon \to 0} \text{Re} \{\ln[G(i, x, x)]\}_{j,k} + \int_{E_0}^{\infty} d\lambda \Xi(\lambda, x)_{j,k}$$

$$1 \leq j, k \leq m.$$  

(3.36)

Thus

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

(3.37)
and the matrix analog of (2.28) then reads
\[ Q(x) = E_0 I_m + \lim_{z \to \infty} \int_{E_0}^{\infty} d\lambda \frac{z^2}{(\lambda - z)^2} [I_m - 2\Xi(\lambda, x)], \] (3.38)
where we used a resolvent instead of a heat kernel regularization.

Defining
\[ \xi(\lambda, x) = Tr_{C^m}[\Xi(\lambda, x)], \] (3.39)
one infers from (3.24) that
\[ Tr[(H^D_x - z)^{-1} - (H - z)^{-1}] = -\int_{E_0}^{\infty} d\lambda \xi(\lambda, x)(\lambda - z)^{-2} \] (3.40)
and that
\[ \xi(\lambda, x) = \frac{1}{\pi} \lim_{\epsilon \to 0} \arg\{\det_{C^m}[G(\lambda + i\epsilon, x, x)]\}, \quad 0 \leq \xi(\lambda, x) \leq m \quad \text{for a.e. } \lambda \in \mathbb{R}. \] (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),
\[ 2Tr[\epsilon^{-\tau H} - \epsilon^{-\tau H^D_x}] = 1 - \tau V(x) + o(\tau) \quad \text{as } \tau \downarrow 0 \] (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
\[ Tr[\epsilon^{-\tau H^N_x} - \epsilon^{-\tau H^D_x}] = 1 - \tau V(x) + o(\tau) \quad \text{as } \tau \downarrow 0, \] (4.2)
where \( H^N_x = H^D_x \) 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 \( \mathbb{R}^\nu \) bounded from below and define the self-adjoint operator
\[ H = -\Delta u V \] (4.3)
as a form sum in \( L^2(\mathbb{R}^\nu) \). Next, let \( A \subseteq \{1, \ldots, \nu\} \) and denote by \( |A| \) the number of elements of \( A \). Moreover, let \( B_\alpha^{(x)}, \alpha \subseteq \{1, \ldots, \nu\} \) be the \( 2^\nu \) blocks obtained by removing the hyperplanes \( \mathcal{P}_\ell = \{y \in \mathbb{R}^\nu \mid y_\ell = x_\ell\} \) from \( \mathbb{R}^\nu \), 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 \( \mathcal{P}_\nu \) the power set of \( \{1, \ldots, \nu\} \). 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 \( \{B_j^{(x)}\}_{j \in A} \) and Neumann boundary conditions on \( \{B_j^{(x)}\}_{j \notin A} \).

**Theorem 4.1.** [25] Define \( C_\tau = \sum_{A \in \mathcal{B}_\nu} (-1)^{|A|} \epsilon^{-\tau H_{A,0}}, \tau > 0 \). Then the integral kernel of \( C_\tau \) is given by
\[ C_\tau(x, x') = \begin{cases} \epsilon^{-\tau H}(x, -x'), & x, x' \text{ in the same orthant} \\ 0, & \text{otherwise}. \end{cases} \] (4.4)
Moreover, \( C_\tau, \tau > 0 \) is a trace class operator in \( L^2(\mathbb{R}^\nu) \) and
\[ Tr(C_\tau) = 2^\nu \int_{\mathbb{R}^\nu} dx \epsilon^{-\tau H}(x, -x), \quad \tau > 0. \] (4.5)
The proof of (4.4) in [25] is based on the method of images while the trace class property of \( C_t \) and (4.5) follow from the direct sum decomposition of \( C_t \) in \( \bigoplus_{\alpha \in \mathbb{P}_d} L^2(B_{\alpha}(x)) \).

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

**Theorem 4.2.** [25]

\[
T \left( \sum_{A \in \mathbb{P}_v} (-1)^{|A|} e^{-\tau H_A} \right) = 1 - \tau V(x) + o(\tau) \quad \text{as } \tau \downarrow 0. \tag{4.6}
\]

While Theorem 4.2 represents a multidimensional trace formula for Schrödinger operators associated with unbounded regions in \( \mathbb{R}^\nu \), 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 \( A \subseteq \{1, \ldots, \nu\} \), 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 \( j \not\in A \). Let \( \langle V \rangle \) be the average of \( V \) at the \( 2^\nu \) corners of \([0,1]^\nu\). Then

\[
\sum_{A \in \mathbb{P}_v} (-1)^{|A|} T \left( e^{-\tau H_A} \right) = 1 - \tau \langle V \rangle + o(\tau) \quad \text{as } \tau \downarrow 0. \tag{4.7}
\]

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 \( A \subseteq \{1, \ldots, \nu\} \) 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 \( j \not\in A \) or \( x_k = 1 \) for all \( k \in \{1, \ldots, \nu\} \). Then

\[
\sum_{A \in \mathbb{P}_v} (-1)^{|A|} T \left( e^{-\tau \tilde{H}_A} \right) = 2^\nu \left[ 1 - \tau V(0) + o(\tau) \right] \quad \text{as } \tau \downarrow 0. \tag{4.8}
\]

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 \( H_P, H_A, H_{PA}, H_{PA}, H_N, \) 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

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

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

\[
H_1 = F^* F, \quad H_2 = F F^* \tag{4.10}
\]
in $\mathcal{H}$ and
\[ Q = \begin{pmatrix} 0 & F^* \\ F & 0 \end{pmatrix}, \quad P = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4.11} \]
in $\mathcal{H} \oplus \mathcal{H}$. Moreover, we denote by $tr(.)$ the trace in $\mathcal{H}$, by $Tr(.)$ 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) \[ QP + PQ = 0. \tag{4.12} \]

(ii) \[ Q^2 = \begin{pmatrix} H_1 & 0 \\ 0 & H_2 \end{pmatrix}. \tag{4.13} \]

(iii) \[ Fe^{-tH_1} \supset e^{-tH_2} F, \quad F^* e^{-tH_2} \supset e^{-tH_1} F^*. \tag{4.14} \]

*Proof.* While (i) and (ii) are obvious, (iii) follows from
\[ e^{-tQ} \supset e^{-tQ^2} Q. \]

**Lemma 4.7.** Assume $B \in \mathcal{B}(\mathcal{H} \oplus \mathcal{H})$ is bounded and commutes with $Q$, i.e., $QB \supset BQ$. Suppose $e^{-tQ^2}, Q^2 e^{-tQ^2} \in \mathcal{B}_1(\mathcal{H} \oplus \mathcal{H}), t > 0$. Then
\[ \frac{d}{dt} Tr[P e^{-tQ^2} B] = 0. \tag{4.15} \]

*Proof.*
\[ \frac{d}{dt} Tr[P e^{-tQ^2} B] = -Tr[PQ^2 e^{-tQ^2} B] = Tr[PQe^{-tQ^2} QB] = \cdots = Tr[PQ^2 e^{-tQ^2} B] \tag{4.16} \]
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, in rewriting
\[ -Tr[PQ^2 e^{-tQ^2} B] = -Tr[PQ(1 + |Q|)^{-1} Q(1 + |Q|)e^{-tQ^2} B] \]
ensures 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
\[ e^{-tH_{1,n}}, \quad H_{j,n} e^{-tH_{1,n}} \in \mathcal{B}_1(\mathcal{H}), \quad 1 \leq n \leq \nu \]
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

\[ Q_n = \begin{pmatrix} 0 & F_n^* \\ F_n & 0 \end{pmatrix}, \quad 1 \leq n \leq \nu \]  

(4.17)

in \( \mathcal{H} \oplus \mathcal{H} \) as in (4.11) and define for any \( A \in \mathcal{P}_2 \) (the power set of \( \{1, 2, \ldots, \nu\} \)) the self-adjoint operator

\[ H^0_A = \sum_{n \in A} H_{1,n} + \sum_{n \notin A} H_{2,n}. \]  

(4.18)

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

**Theorem 4.8.**

\[ \sum_{A \in \mathcal{P}_2} (-1)^{|A|} \text{tr} (e^{-i H^0_A}) = \sum_{A \in \mathcal{P}_2} (-1)^{|A|} \dim \text{Ran}[P_{H^0_A}(\{0\})], \]  

(4.19)

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

**Proof.** One computes

\[
\begin{align*}
\frac{d}{dt} \sum_{A \in \mathcal{P}_2} (-1)^{|A|} \text{tr}(e^{-i H^0_A}) &= -\sum_{A \in \mathcal{P}_2} (-1)^{|A|} \text{tr}(H^0_A e^{-i H^0_A}) \\
&= -\sum_{n=1}^{\nu} \text{tr} [P Q_n^2 e^{-i Q_n^2 B_{\nu,n}}] = 0
\end{align*}
\]

by (4.15), where

\[ B_{1,1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \]  

(4.21a)

\[ B_{\nu,n} = \begin{pmatrix} b_{\nu,n} & 0 \\ 0 & b_{\nu,n} \end{pmatrix}, \quad b_{\nu,n} = -\prod_{m=1}^{\nu} \left( e^{-i H_{2,n,m}} - e^{-i H_{1,m}} \right), \quad \nu \geq 2 \]  

(4.21b)

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

\[
\frac{\partial}{\partial x_n} |_D = \frac{d}{dx} |_{C^\infty((0,1))}, \quad 1 \leq n \leq \nu
\]  

(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 \( H^0_\nu \) 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

\[ \sum_{A \in \mathcal{P}_2} (-1)^{|A|} \text{tr}(e^{-i H^0_A}) = \prod_{n=1}^{\nu} \text{tr}(e^{-i a_n a_n^*} - e^{-i a_n^* a_n}). \]  

(4.23)

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

\[ \text{tr} \left( e^{-i a_n a_n^*} - e^{-i a_n^* a_n} \right) = 1, \quad 1 \leq n \leq \nu. \]
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 ν = 1, 2, 3 space dimensions, so will be our approach below.

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

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

where

$$D_{α,x}(z) = \begin{cases} -α^{-1} - \Gamma_ν(z, x), & ν = 1, \quad α \in \mathbb{R} \cup \{∞\}, \quad α \neq 0 \\ α - \Gamma_ν(z, x), & ν = 2, 3, \quad α \in \mathbb{R}, \end{cases} \quad (5.2)$$

$$\Gamma_1(z, x) = G(z, x, x), \quad Γ_2(z, x) = \lim_{|d| \to 0} [G(z, x, x + ε) - (2π)^{-1} \ln(|ε|)], \quad (5.3)$$

$$Γ_3(z, x) = \lim_{|d| \to 0} [G(z, x, x + ε) - (4π |ε|)^{-1}],$$

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

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

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

$$Tr[(H_{α,x} - z)^{-1} - (H - z)^{-1}] = -\int_{E_{α,x,0}}^∞ dλ \frac{ξ_{α,x}(λ)}{(λ - z)^2}, \quad (5.5)$$

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

$$ξ_{α,x}(λ) = 0, \quad λ < E_{α,x,0}. \quad (5.6)$$

$ξ_{α,x}(λ)$ is related to $D_{α,x}(z)$ as $ξ(λ, x)$ is to $g(z, x, x)$ in (2.24). The high-energy expansion (see, e.g., [35], [41])

$$\lim_{|d| \to 0} [G(z, x, x + ε) - G^{(0)}(z, x, x + ε)] = -V(x) \begin{cases} 1/4(-z)^{3/2} + o(z^{-3/2}), & ν = 1 \\ -1/4πz + o(z^{-1}), & ν = 2 \\ 1/8π(-z)^{1/2} + o(z^{-1/2}), & ν = 3 \end{cases}, \quad (5.7)$$

then yields

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

where

$$\tilde{α} = α + (2π)^{-1} γ - (2π)^{-1} \ln(2)$$

with $γ = 0.5772\ldots$ being Euler’s constant. A combination of (5.4), (5.5), and (5.8) then implies the following trace formula.
Theorem 5.1. [17]
\[ \nu = 1: \]
\[ V(x) = \left\{ \begin{array}{ll}
\lim_{z \to -\infty} \{-z - 2 \int_{[\inf \mathcal{H}, \infty)} d\lambda z^2 (\lambda - z)^{-2} \xi_{\alpha, x}(\lambda)\}, & \alpha = \infty, \\
\frac{1}{6} \alpha^2 + \lim_{z \to -\infty} \left\{ \frac{2}{3} z + \frac{1}{3} \alpha z^{1/2} + \frac{8i}{3} \alpha^{-1} z^{5/2} \int_{E_{\alpha, x, 0}} d\lambda (\lambda - z)^{-2} \xi_{\alpha, x}(\lambda) \right\}, & \alpha \in \mathbb{R} \setminus \{0\}. 
\end{array} \right. \]
\[ (5.9) \]
\[ \nu = 2: \]
\[ V(x) = \lim_{z \to -\infty} \{-z + 4\pi [(2\pi)^{-1} \ln(-iz^{1/2}) + \tilde{\alpha}] \int_{E_{\alpha, x, 0}} d\lambda z^2 (\lambda - z)^{-2} \xi_{\alpha, x}(\lambda)\}. \]
\[ (5.10) \]
\[ \nu = 3: \]
\[ V(x) = 16\pi^2 \alpha^2 + \lim_{z \to -\infty} \left\{ -z + 4\pi i \alpha z^{1/2} + 2 \int_{E_{\alpha, x, 0}} d\lambda z^2 (\lambda - z)^{-2} \xi_{\alpha, x}(\lambda) \right\}. \]
\[ (5.11) \]

Using the systematic high-energy expansion of \( \lim_{|\epsilon| \to 0} [G(z, x, x + \epsilon) - G^{(0)}(z, x, x + \epsilon)] \) in terms of (multi-dimensional) KdV invariants (see, e.g., [34, 35]) 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,
\[ D^{(0)}_{\alpha}(z) = \left\{ \begin{array}{ll}
-\alpha^{-1} - (-4\alpha)^{-1/2}, & \nu = 1 \\
\tilde{\alpha} + (2\pi)^{-1} \ln((-z)^{1/2}), & \nu = 2 \\
\tilde{\alpha} + (4\pi)^{-1} (-z)^{1/2}, & \nu = 3,
\end{array} \right. \]
\[ (5.12) \]
and
\[ Tr[(H^{(0)}_{\alpha, x} - z)^{-1} - (H^{(0)} - z)^{-1}] = -\int_{E_{\alpha, x, 0}}^\infty d\lambda \xi_{\alpha, x}(\lambda) (\lambda - z)^{-2}. \]
\[ (5.13) \]
Here, for \( \nu = 1 \),
\[ \xi^{(0)}_{\alpha, x}(\lambda) = \left\{ \begin{array}{llllll}
0, & \lambda < -\alpha^2/4 \\
-1, & -\alpha^2/4 < \lambda < 0 \\
a_{\alpha}(\lambda), & \lambda > 0
\end{array} \right. \]
\[ (5.14) \]
writing \( a_{\alpha}(\lambda) = \pi^{-1} \arctan(|\alpha|/2\lambda^{1/2}) \), and, for \( \nu = 2 \),
\[ \xi^{(0)}_{\alpha}(\lambda) = \left\{ \begin{array}{llll}
0, & \lambda < -e^{-4\alpha} \\
-1, & -e^{-4\alpha} < \lambda < 0 \\
-\pi^{-1} \arctan[\pi/(4\pi\alpha + \ln(\lambda))] - 1, & 0 < \lambda \leq e^{-4\alpha} \\
-\pi^{-1} \arctan[\pi/(4\pi\tilde{\alpha} + \ln(\lambda))], & \lambda \geq e^{-4\alpha}
\end{array} \right. \]
\[ (5.15) \]
and, finally, for \( \nu = 3 \),
\[ \xi^{(0)}_{\alpha}(\lambda) = \left\{ \begin{array}{llll}
0, & \lambda < -(4\pi \alpha)^2 \\
-1, & -(4\pi \alpha)^2 < \lambda < 0 \\
A_{\alpha}(\lambda), & \lambda > 0 \\
A_{\alpha}, & \lambda > 0
\end{array} \right. \]
\[ (5.16) \]
writing \( A_{\alpha}(\lambda) = \pi^{-1} \arctan(\lambda^{1/2}/4\pi |\alpha|) \), and
\[ E^{(0)}_{\alpha, 0} = \left\{ \begin{array}{llllll}
-\alpha^2/4, & \alpha < 0 \\
0, & \alpha \in [0, \infty]
\end{array} \right. \]
\[ (5.17) \]
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 \( V : \mathbb{R}^3 \to \mathbb{R} \),

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

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 \( L^2((0, \infty); r^2dr) \) associated with differential expressions of the type

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

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

\[
\tau_\ell = -\frac{d^2}{dr^2} + \frac{\ell(\ell + 1)}{r^2} + v(r)
\]  

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.,

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

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 \( \xi_{i,j,0}(\lambda) \) for the pair \((H_{j,\alpha,j,0}, H_j)\), \( j = 1, 2 \). Then the following are equivalent:

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

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

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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