Spectral shift function and trace formula

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Abstract. The complete proofs of Krein's theorem on the spectral shift function and the trace formula are given for a pair of self-adjoint operators such that either (i) their difference is trace-class or (ii) the difference of their resolvents is trace-class. The proofs, essentially due to Krein, is based on Herglotz's theorem on the boundary value of the analytic functions whose imaginary part is non-negative on the upper half plane, and an almost optimal class of functions are obtained for which the trace formula is valid. Also an alternative method based on Weyl-von Neumann's theorem for self-adjoint operators, avoiding the complex function theory and inspired by Voiculescu's work, is given for the first case. Furthermore, some applications of the spectral shift function have been discussed.

Keywords. Spectral shift function; trace formula; Krein's theorem.

1. Introduction

Krein's spectral shift function and associated trace formulas [9, 18, 19, 20, 30] have been of considerable interest as an abstract mathematical statement as well as for various applications. The original proof of Krein (see for example [20]) uses analytic function theory and we use the same in §2 and §4. Voiculescu [28] gave a proof of the trace formula without using function theory for the case of bounded self-adjoint operators. We extend this method in §3 to a pair of arbitrary self-adjoint operators with their difference trace-class. In the appendix we collect some of the necessary results from analytic function theory without proof as well as the definition and some properties of the perturbation determinant. Section 5 deals with some applications.

In this article, $\mathscr{H}$ will denote the Hilbert space we work in; $\mathscr{B}(\mathscr{H})$, $\mathscr{B}_1(\mathscr{H})$ and $\mathscr{B}_2(\mathscr{H})$ standing for the set of bounded, trace-class and Hilbert-Schmidt operators respectively. We shall often have H and H_0 as a pair of self-adjoint operators in $\mathscr{H}$ with $\sigma(H)$, $\sigma(H_0)$ their spectra; $\rho(H)$, $\rho(H_0)$ their resolvent sets with R_z and R_z^0 their resolvents and E_λ, E_λ^0 the associated spectral families. The symbols $\|\cdot\|$, $\|\cdot\|_1$ and $\|\cdot\|_2$ will denote operator norm, trace norm and Hilbert-Schmidt norm respectively, while $\operatorname{Tr} B$ will stand for the trace of a trace-class operator B.

In a finite dimensional Hilbert space the problem is easy to state and prove.

Theorem 1.1. *Let H and H_0 be two self-adjoint operators in a finite dimensional Hilbert space $\mathscr{H}$. Then there exists a unique real-valued bounded function ξ such that*

(i) $\xi(\lambda) = \operatorname{Tr}(E_\lambda^0 - E_\lambda), \quad \lambda \in \mathbb{R}$,
(ii) $\int \xi(\lambda) \mathrm{d}\lambda = \operatorname{Tr}(H - H_0)$,

(iii) for $\varphi \in C^1$ ($\mathbb{R}$),

$$\mathrm{Tr}[\varphi(H) - \varphi(H_0)] = \int \varphi'(\lambda)\xi(\lambda)\mathrm{d}\lambda. \tag{1.1}$$

Furthermore, ξ is a constant in every real open interval in $\rho(H) \cap \rho(H_0)$ and has support in $[a, b]$, where $a = \min\{\inf \sigma(H), \inf \sigma(H_0)\}$, $b = \max\{\sup \sigma(H), \sup \sigma(H_0)\}$.

(iv) *If $H - H_0 = \tau |g\rangle\langle g|$ with $\tau > 0$, $\|g\| = 1$ (we have used Dirac notation for rank one operators), then ξ is a $\{0, 1\}$-valued function. More precisely, $\xi(\lambda) = \Sigma_{j=1}^{r} \chi_{\Delta_j}(\lambda)$ for r disjoint intervals $\Delta_j \subseteq \mathbb{R}$, $1 \leqslant r \leqslant n$.*

Proof. In fact, we define ξ by (i). Then ξ is a bounded real-valued function with the stated support property. We only prove (iii). Given the support of ξ, the integral on the right hand side of (1.1) is over a finite interval only. By functional calculus, $\mathrm{Tr}[\varphi(H) - \varphi(H_0)] = -\int \varphi(\lambda)\mathrm{d}\xi(\lambda) = -\xi(\lambda)\varphi(\lambda)|_{-\infty}^{\infty} + \int \varphi'(\lambda)\xi(\lambda)\mathrm{d}\lambda$, and the result follows. That ξ is constant in every open real interval in $\rho(H) \cap \rho(H_0)$ is a consequence of the definition of the spectral families.

Let $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n$ and $\mu_1 \leqslant \mu_2 \leqslant \cdots \leqslant \mu_n$ be the eigenvalues of H_0 and H respectively. Then since $H - H_0$ is positive rank one, it is a consequence of the minimax principle for eigenvalues [14] that $\lambda_j \leqslant \mu_j \leqslant \lambda_{j+1} (1 \leqslant j \leqslant n-1)$ and $\lambda_n \leqslant \mu_n$. From this it is clear that if $\lambda_j = \lambda_{j+1} = \lambda_{j+2} = \cdots = \lambda_{j+s}$ for some j and s, then $\mu_j = \mu_{j+1} = \cdots = \mu_{j+s-1} = \lambda_j$. This and the expression (i) for ξ leads to:

$$\xi(\lambda) = \Sigma_{j=1}^{n} \chi_{[\lambda_j, \mu_j]}(\lambda),$$

where we set $\chi_{[\lambda_j, \mu_j]}(\lambda) = 0$ for those j for which $\lambda_j = \mu_j$. ∎

The next corollary follows easily from the theorem.

COROLLARY 1.2

For $t \in \mathbb{R}$, $\mathrm{Tr}(e^{itH} - e^{itH_0}) = it \int e^{it\lambda}\xi(\lambda)\mathrm{d}\lambda$.

In an infinite dimensional Hilbert space, the relation $\xi(\lambda) = \mathrm{Tr}(E_\lambda^0 - E_\lambda)$ will not make sense in general because $E_\lambda^0 - E_\lambda$ may not be trace-class. Next we give a counter example due to Krein [18] where $H - H_0$ is rank one and yet $E_\lambda - E_\lambda^0$ is not trace-class.

Counter example. Let $\mathscr{H} = L^2[0, \infty)$ and $L = -\dfrac{\mathrm{d}^2}{\mathrm{d}x^2}$ be the differential operator with $D(L) = C_0^\infty(0, \infty)$. It is known that L has several self-adjoint extensions depending upon the boundary conditions on the corresponding differential equation. Of them choose two, namely h_0 and h as

$$D(h_0) = \left\{ \begin{array}{l} f \in \mathscr{H} : f \text{ and } f' \text{ are absolutely continuous,} \\ f'' \in \mathscr{H} \text{ and } f(0) = 0 \end{array} \right\}$$

and

$$D(h) = \left\{ \begin{array}{l} f \in \mathscr{H} : f \text{ and } f' \text{ are absolutely continuous,} \\ f'' \in \mathscr{H} \text{ and } f'(0) = 0. \end{array} \right\}$$

Note that both h_0 and h are positive operators. One can compute the spectral families F_λ^0 and F_λ of h_0 and h respectively by solving the associated ordinary differential equations and get for $\lambda \geqslant 0$

$$F_\lambda^0(x, y) = \frac{2}{\pi} \int_0^{(\lambda)^{1/2}} \sin tx \ \sin ty \, dt \tag{1.2}$$

and

$$F_\lambda(x, y) = \frac{2}{\pi} \int_0^{(\lambda)^{1/2}} \cos tx \ \cos ty \, dt.$$

Let $H_0 = (h_0 + I)^{-1}$ and $H = (h + I)^{-1}$. The Green's functions associated with $(h_0 + I)^{-1}$ and $(h + I)^{-1}$ are

$$\begin{aligned} G_0(x, y) = {} & e^{-y} \sinh x, \quad x \leqslant y \\ & e^{-x} \sinh y, \quad x \geqslant y \end{aligned} \tag{1.3}$$

and

$$\begin{aligned} G(x, y) = {} & e^{-y} \cosh x, \quad x \leqslant y \\ & e^{-x} \cosh y, \quad x \geqslant y \end{aligned}$$

respectively. Then $H - H_0 = \frac{1}{2}|\psi\rangle\langle\psi|$, where $\psi(x) = \sqrt{2}e^{-x}$ so that $\|\psi\| = 1$. Let $\mu = \dfrac{1}{1+\lambda}$. Then $E_\mu^0 = I - F_\lambda^0$ and $E_\mu = I - F_\lambda$ are the spectral families of H_0 and H respectively and

$$E_\mu(x, y) - E_\mu^0(x, y) = F_\lambda^0(x, y) - F_\lambda(x, y) = (-2/\pi) \frac{\sin \sqrt{\lambda}(x+y)}{(x+y)}. \tag{1.4}$$

Note that $E_\mu - E_\mu^0$ is not trace-class since the Hilbert-Schmidt norm

$$\begin{aligned} \iint |E_\mu(x, y) - E_\mu^0(x, y)|^2 \, dx \, dy &= (2/\pi)^2 \int_0^\infty \int_0^\infty \frac{\sin^2 \sqrt{\lambda}(x+y)}{(x+y)^2} \, dx \, dy \\ &= \begin{cases} \infty & \text{if } \lambda \neq 0, \text{ equivalently if } 0 < \mu < 1, \\ 0 & \text{if } \lambda = 0, \text{ equivalently if } \mu = 1. \end{cases} \end{aligned}$$

If $E_\mu - E_\mu^0$ were trace class, then since its integral kernel (1.4) is continuous, we could evaluate the trace (see p. 523 of [16]) as:

$$\begin{aligned} \mathrm{Tr}(E_\mu^0 - E_\mu) &= \int_0^\infty (E_\mu^0 - E_\mu)(x, x) \, dx \\ &= \frac{2}{\pi} \int_0^\infty \frac{\sin 2\sqrt{\lambda}x}{2x} \, dx \\ &= \frac{1}{2} \quad \text{if} \quad 0 < \mu < 1 \text{ and} \\ &= 0 \quad \text{if} \quad \mu = 1. \end{aligned} \tag{1.5}$$

In §2 we shall define Krein's spectral shift function ξ when the difference of H and H_0 is trace class, and in remark 2.7 (iv) it will be shown that ξ in the above example is precisely the expression (1.5) though $E^0_\mu - E_\mu$ is not trace class.

Here we mention some other authors who have also dealt with this subject, in particular Clancy [10] and Kuroda [17]. There is also the interesting approach of Birman and Solomyak [8] using the theory of double spectral integrals, also developed by them. They obtain a trace formula of the type (1.1) for a function class somewhat larger than what we have described in §2–4.

2. Spectral shift function and trace formula: the case of trace-class perturbation

In this section we shall establish the existence of the spectral shift function and prove the trace formula (1.1) for a large class of functions under the assumption $V \in \mathscr{B}_1$. The following theorem concerns the first assertion, (see also [20], [25], [10]).

Theorem 2.1 *Let H and H_0 be two self-adjoint operators in $\mathscr{H}$ such that $V = H - H_0 \in \mathscr{B}_1$. Let $\Delta(z) = \det(I + VR^0_z)$, for $\operatorname{Im} z \neq 0$, be the perturbation determinant (see appendix for definition and its properties). Then there exists a unique real valued $L^1(\mathbb{R})$ – function ξ satisfying*

$$\text{(i)} \qquad \xi(\lambda) = \frac{1}{\pi} \lim_{\varepsilon \to 0+} \operatorname{Im} \ln \Delta(\lambda + i\varepsilon) \tag{2.1}$$

$$\text{(ii)} \qquad \int_{-\infty}^{\infty} |\xi(\lambda)| d\lambda \leqslant \|V\|_1, \quad \int_{-\infty}^{\infty} \xi(\lambda) d\lambda = \operatorname{Tr} V$$

$$\text{(iii)} \qquad \ln \Delta(z) = \int_{-\infty}^{\infty} \frac{\xi(\lambda)}{\lambda - z} d\lambda \quad \text{for} \quad \operatorname{Im} z \neq 0,$$

$$\text{(iv)} \qquad \operatorname{Tr}(R_z - R^0_z) = -\int_{-\infty}^{\infty} \frac{\xi(\lambda)}{(\lambda - z)^2} d\lambda \quad \text{for} \quad \operatorname{Im} z \neq 0,$$

Proof. Let V be self-adjoint, rank one, i.e. $V = \tau|g\rangle\langle g|$, $\tau \neq 0$ and $\|g\| = 1$. Then for $\operatorname{Im} z \neq 0$,

$$\Delta(z) = 1 + \tau(g, R^0_z g) = 1 + \tau \int \frac{d\|E^0_\lambda g\|^2}{\lambda - z}. \tag{2.2}$$

In the following by ln we mean the principal branch of the logarithm function. If $\operatorname{Im} z > 0$, then by (2.2), $\tau^{-1} \operatorname{Im} \Delta(z) = (\operatorname{Im} z) \int \frac{d\|E^0_\lambda g\|^2}{|\lambda - z|^2} > 0$ or equivalently $0 \leqslant (\operatorname{sgn} \tau) \operatorname{Im} \ln \Delta(z) < \pi$, where $\operatorname{sgn} \tau = \pm 1$ according as $\tau >$ or < 0. Since $\Delta(z)$ is analytic and has no zeros there, $G(z) \equiv (\operatorname{sgn} \tau) \ln \Delta(z)$ is analytic in the upper half-plane $\{z \in \mathbb{C} : \operatorname{Im} z > 0\}$ and, by (2.2), $|G(z)| = O\left(\frac{1}{\operatorname{Im} z}\right)$ as $\operatorname{Im} z \to \infty$. So by theorem A.1 there exists a non-negative function $\zeta \in L^1$, given by $\zeta(\lambda) = \frac{1}{\pi} \lim_{\varepsilon \to 0+} \operatorname{Im} G(\lambda + i\varepsilon)$ for almost all λ such that

$$(\operatorname{sgn} \tau) \ln \Delta(z) = G(z) = \int_{-\infty}^{\infty} \frac{\zeta(\lambda)}{\lambda - z} d\lambda.$$

Set $\xi(\lambda) = (\operatorname{sgn}\tau)\zeta(\lambda)$. Then by theorem A.5 (i) and the above relation one obtains

$$\operatorname{Tr}(R_z - R_z^0) = -\frac{d}{dz}\ln\Delta(z) = -\int_{-\infty}^{\infty}\frac{\xi(\lambda)}{(\lambda - z)^2}d\lambda, \tag{2.3}$$

since the integral in the right hand side converges uniformly in z for $\operatorname{Im} z \geqslant \delta > 0$.

Using the resolvent identity $R_z - R_z^0 = -R_z V R_z^0$ and the fact $s-\lim_{y\to\infty} iyR_{iy} = s-\lim_{y\to\infty} iyR_{iy}^0 = -I$, one gets $y^2(R_{iy} - R_{iy}^0) \to V$ in $\mathscr{B}_1$-norm as $y \to \infty$ (see lemma 8.23 of [1]). Since $\xi \in L^1$, an application of dominated convergence theorem then yields

$$\tau = \operatorname{Tr} V = \lim_{y\to\infty} y^2 \operatorname{Tr}(R_{iy} - R_{iy}^0)$$

$$= -\lim_{y\to\infty}\int_{-\infty}^{\infty}\frac{\xi(\lambda)y^2}{(\lambda - iy)^2} = \int_{-\infty}^{\infty}\xi(\lambda)d\lambda. \tag{2.4}$$

So by (2.4)

$$\int_{-\infty}^{\infty}|\xi(\lambda)|d\lambda = \int_{-\infty}^{\infty}\zeta(\lambda)d\lambda = (\operatorname{sgn}\tau)\int_{-\infty}^{\infty}\xi(\lambda)d\lambda = (\operatorname{sgn}\tau)\tau = |\tau| = \|V\|_1.$$

Next, let $V \in \mathscr{B}_1$ and write $V = \Sigma_{j=1}^{\infty}\tau_j|g_j\rangle\langle g_j|$ with $\Sigma_{j=1}^{\infty}|\tau_j| < \infty$, $\|g_j\| = 1$ for each j. Set for $k = 1, 2, \ldots, H_k = H_0 + V_k \equiv H_0 + \Sigma_{j=1}^{k}\tau_j|g_j\rangle\langle g_j|$, $R_z^{(k)} = (H_k - z)^{-1}$ and $\Delta_k(z) = \det(I + (H_k - H_{k-1})R_z^{(k-1)})$. Then, as before, for each $k \geqslant 1$, there exists a real valued function $\xi_k \in L^1$ such that $\int\xi_k(\lambda)d\lambda = \tau_k$ and $\int|\xi_k(\lambda)|d\lambda = |\tau_k|$. Define $\xi(\lambda) = \Sigma_{k=1}^{\infty}\xi_k(\lambda)$; the right hand side converges in L^1-norm since $\Sigma_{k=1}^{\infty}|\tau_k| < \infty$. This also shows that $\xi \in L^1(\mathbb{R})$. Note that ξ is unique since each ξ_k is. Moreover

$$\int_{-\infty}^{\infty}|\xi(\lambda)|d\lambda \leqslant \sum_{k=1}^{\infty}\int_{-\infty}^{\infty}|\xi_k(\lambda)|d\lambda = \sum_{k=1}^{\infty}|\tau_k| = \|V\|_1,$$

and

$$\int_{-\infty}^{\infty}\xi(\lambda)d\lambda = \sum_{k=1}^{\infty}\int_{-\infty}^{\infty}\xi_k(\lambda)d\lambda = \sum_{k=1}^{\infty}\tau_k = \operatorname{Tr} V$$

This proves (ii).

By theorem A.5 (i)

$$\ln\det(I + V_k R_z^0) = \sum_{j=1}^{k}\ln\Delta_j(z)$$

$$= \int d\lambda\left\{\sum_{j=1}^{k}\xi_j(\lambda)\right\}\ (\lambda - z)^{-1}.$$

As $k \to \infty$, the right hand side converges to $\int\frac{\xi(\lambda)}{\lambda - z}d\lambda$ for $\operatorname{Im} z \neq 0$, whereas by the continuity property of determinant (see theorem A.3 (ii)) the left hand side converges to $\ln\Delta(z)$ since $V_k \to V$ in $\mathscr{B}_1$-norm and $\det(I + V_k R_z^0) \neq 0$ for $\operatorname{Im} z \neq 0$ and all k. Thus we get

$$\ln\Delta(z) = \int_{-\infty}^{\infty}\frac{\xi(\lambda)}{\lambda - z}d\lambda. \tag{2.5}$$

which proves (iii). The property (i) follows from theorem 13 in [27].

By theorem A.5 (i) and (2.5) we have $\mathrm{Tr}(R_z - R_z^0) = -\int_{-\infty}^{\infty} \frac{\xi(\lambda)}{(\lambda - z)^2} \mathrm{d}\lambda$ by differentiating inside the integral of (2.5), which is allowed since second integral converges uniformly in z for $\mathrm{Im}\, z \geqslant \delta > 0$. ■

Next we study the class of functions φ for which $\varphi(H) - \varphi(H_0) \in \mathscr{B}_1$ and the trace formula (1.1) holds. For example, let $\varphi(\lambda) = e^{it\lambda}$ for fixed $t \in \mathbb{R}$. Note that for $t \neq 0$

$$\frac{e^{itH} - e^{itH_0}}{it} = \frac{1}{t} e^{itH_0} \int_0^t \mathrm{d}s\, e^{-isH_0} V e^{isH} \tag{2.6}$$

on $D(H_0)$. Since $s \to e^{-isH_0}, e^{isH}$ are strongly continuous and since $V \in \mathscr{B}_1$, it follows by lemma 8.23 of [1] that $s \to e^{-isH_0} V e^{isH}$ is $\mathscr{B}_1$-continuous. This means that the Riemann integral exists in $\mathscr{B}_1$-norm, the left hand side of (2.6) converges to V as $t \to 0$ in $\mathscr{B}_1$-norm and we have the estimate:

$$\left\| \frac{e^{itH} - e^{itH_0}}{it} \right\|_1 \leqslant \| V \|_1. \tag{2.7}$$

Therefore $\varphi(H) - \varphi(H_0) \in \mathscr{B}_1$. It is also clear that $t \to \frac{e^{itH} - e^{itH_0}}{it}$ is a $\mathscr{B}_1$-continuous map.

We will prove an abstract theorem from which the trace formula for $\varphi(\lambda) = e^{it\lambda}$ will follow. Using that the trace formula for a large class of functions will be established. We start with the following lemma.

Lemma 2.2. *Let A be a self-adjoint operator in $\mathscr{H}$, so that $\Psi_z \equiv (A - i)(A - z)^{-1} \in \mathscr{B}(\mathscr{H})$ for $\mathrm{Im}\, z \neq 0$. Then for any $\varepsilon \neq 0$ and $g \in \mathscr{H}$*

(i) $$\int_{-\infty}^{\infty} \mathrm{d}\lambda \| (A - \lambda - i\varepsilon)^{-1} g \|^2 = \pi |\varepsilon|^{-1} \| g \|^2$$

(ii) $$\int_{-\infty}^{\infty} \frac{\mathrm{d}\lambda}{1 + \lambda^2} \| \Psi_{\lambda + i\varepsilon} g \|^2 \leqslant 2\pi (1 + |\varepsilon|^{-1}) \| g \|^2$$

Proof. Let $\{F_\lambda\}$ be the spectral family of A. Then by functional calculus and Fubini's theorem,

$$\int_{-\infty}^{\infty} \mathrm{d}\lambda \| (A - \lambda - i\varepsilon)^{-1} g \|^2 = \int_{-\infty}^{\infty} \mathrm{d}\lambda \int_{-\infty}^{\infty} \frac{\mathrm{d} \| F_\mu g \|^2}{(\mu - \lambda)^2 + \varepsilon^2}$$
$$= \int_{-\infty}^{\infty} \mathrm{d} \| F_\mu g \|^2 \int_{-\infty}^{\infty} \frac{\mathrm{d}\lambda}{(\mu - \lambda)^2 + \varepsilon^2}$$
$$= \pi |\varepsilon|^{-1} \| g \|^2.$$

Similarly,

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}\lambda}{1 + \lambda^2} \| \Psi_{\lambda + i\varepsilon} g \|^2 = \int_{-\infty}^{\infty} \frac{\mathrm{d}\lambda}{1 + \lambda^2} \int_{-\infty}^{\infty} \mathrm{d} \| F_\mu g \|^2 \frac{(\mu^2 + 1)}{(\mu - \lambda)^2 + \varepsilon^2}$$
$$= \int_{-\infty}^{\infty} \mathrm{d} \| F_\mu g \|^2 \int_{-\infty}^{\infty} \frac{(\mu^2 + 1)\mathrm{d}\lambda}{\{(\mu - \lambda)^2 + \varepsilon^2\}(1 + \lambda^2)},$$

from which part (ii) follows since the integrand is dominated by

$$\frac{2(\mu-\lambda)^2+2(\lambda^2+1)}{\{(\mu-\lambda)^2+\varepsilon^2\}(1+\lambda^2)} \leqslant \frac{2}{1+\lambda^2}+\frac{2}{(\mu-\lambda)^2+\varepsilon^2}. \tag{2.8}$$

■

Let $\varphi \in C(\mathbb{R})$ be bounded. For $\varepsilon > 0$, define

$$\varphi_\varepsilon(\lambda) = \frac{\varepsilon}{\pi}\int_{-\infty}^{\infty} \frac{\varphi(\mu)}{(\mu-\lambda)^2+\varepsilon^2}\,\mathrm{d}\mu. \tag{2.9}$$

Remark 2.3. If φ and φ_ε are as above, then it is easy to see that for any self-adjoint operator A, $\varphi(A)$ and $\varphi_\varepsilon(A)$, defined by functional calculus, are bounded operators and $\varphi_\varepsilon(A)$ converges strongly to $\varphi(A)$ as $\varepsilon \to 0$.

Theorem 2.4. *Let H and H_0 be two self-adjoint operators in $\mathscr{H}$ such that $V = H - H_0 \in \mathscr{B}_1$. Let $\varphi \in C(\mathbb{R})$ be bounded and φ_ε be given by* (2.9). *Then*

(i) $\varphi_\varepsilon(H) - \varphi_\varepsilon(H_0) \in \mathscr{B}_1$.
(ii) *If furthermore $\varphi \in C^1(\mathbb{R})$ and φ' is bounded, then*

$$\lim_{\varepsilon\to\infty} \mathrm{Tr}\{\varphi_\varepsilon(H) - \varphi_\varepsilon(H_0)\} = \int \varphi'(\lambda)\xi(\lambda)\,\mathrm{d}\lambda,$$

where ξ is the function given by theorem 2.1.
(iii) *If also $\varphi_\varepsilon(H) - \varphi_\varepsilon(H_0)$ converges in $\mathscr{B}_1$-norm as $\varepsilon \to 0$, then the trace formfula* (1.1) *holds.*

Proof. Let $\varepsilon > 0$ be fixed. Then by (2.9)

$$\varphi_\varepsilon(H) - \varphi_\varepsilon(H_0) = \frac{1}{\pi}\int \mathrm{d}\lambda\, \varphi(\lambda)\,\mathrm{Im}(R_{\lambda+i\varepsilon} - R^0_{\lambda+i\varepsilon}). \tag{2.10}$$

Since φ is bounded, for part (i) it suffices to show that $T_\pm(\lambda) \equiv \|R_{\lambda\pm i\varepsilon} - R^0_{\lambda\pm i\varepsilon}\|_1 \in L^1(\mathbb{R}; \mathrm{d}\lambda)$. We give the proof of positive sign only, the other case being similar.

Let $V = \Sigma_{k=1}^\infty \tau_k |g_k\rangle\langle g_k|$ with $\Sigma_{k=1}^\infty |\tau_k| < \infty$ and $\{g_k\}$ an orthonormal set. Then the resolvent identity $R_z - R_z^0 = -R_z V R_z^0$ leads to the estimate:

$$\begin{aligned} \|R_z - R_z^0\|_1 &\leqslant \sum_{k=1}^\infty |\tau_k| \, \| |R_z g_k\rangle\langle R_{\bar z}^0 g_k| \|_1 \\ &= \sum_{k=1}^\infty |\tau_k| \, \|R_z g_k\| \, \|R_{\bar z}^0 g_k\|. \end{aligned}$$

Setting $z = \lambda + i\varepsilon$ and integrating both the sides of the above inequality with respect to λ and using Schwarz's inequality and lemma 2.2 (i) we obtain

$$\begin{aligned} &\int_{-\infty}^{\infty} \mathrm{d}\lambda \, \|R_{\lambda+i\varepsilon} - R^0_{\lambda+i\varepsilon}\|_1 \\ &\leqslant \sum_{k=1}^\infty |\tau_k| \int_{-\infty}^{\infty} \mathrm{d}\lambda \, \|R^0_{\lambda-i\varepsilon} g_k\| \, \|R_{\lambda+i\varepsilon} g_k\| \end{aligned}$$

$$\leqslant \sum_{k=1}^{\infty} |\tau_k| \left\{ \int_{-\infty}^{\infty} d\lambda \| R^0_{\lambda-i\varepsilon} g_k \|^2 \right\}^{1/2} \left\{ \int_{-\infty}^{\infty} d\lambda \| R_{\lambda+i\varepsilon} g_k \|^2 \right\}^{1/2}$$
$$= (\pi/\varepsilon) \| V \|_1.$$

Assume φ' to be bounded and continuous. Then by (2.10), theorem 2.1 (iii) and integration by parts we get

$$\begin{aligned}
\operatorname{Tr}\{\varphi_\varepsilon(H) - \varphi_\varepsilon(H_0)\} &= \frac{1}{\pi} \int_{-\infty}^{\infty} d\lambda \varphi(\lambda) \operatorname{Tr}\{\operatorname{Im}(R_{\lambda+i\varepsilon} - R^0_{\lambda+i\varepsilon})\} \\
&= -\frac{1}{\pi} \int_{-\infty}^{\infty} d\lambda \varphi(\lambda) \left\{ \operatorname{Im} \int_{-\infty}^{\infty} \frac{\xi(\mu) d\mu}{(\mu - \lambda - i\varepsilon)^2} \right\} \\
&= -\frac{1}{\pi} \int_{-\infty}^{\infty} d\lambda \varphi(\lambda) \frac{d}{d\lambda} \left\{ \varepsilon \int_{-\infty}^{\infty} \frac{\xi(\mu)}{(\mu - \lambda)^2 + \varepsilon^2} d\mu \right\} \\
&= -\frac{\varepsilon}{\pi} \left[\varphi(\lambda) \int_{-\infty}^{\infty} \frac{\xi(\mu)}{(\mu - \lambda)^2 + \varepsilon^2} d\mu \right]_{\lambda=-\infty}^{\lambda=+\infty} \\
&\quad + \frac{\varepsilon}{\pi} \int_{-\infty}^{\infty} d\lambda \varphi'(\lambda) \int_{-\infty}^{\infty} \frac{\xi(\mu)}{(\mu - \lambda)^2 + \varepsilon^2} d\mu.
\end{aligned}$$

Note that $\varphi(\lambda) \int_{-\infty}^{\infty} \frac{\xi(\mu)}{(\mu - \lambda)^2 + \varepsilon^2} d\mu \to 0$ as $|\lambda| \to \infty$ by dominated convergence theorem. Hence the boundary terms in the above vanishes, and thus

$$\begin{aligned}
\operatorname{Tr}\{\varphi_\varepsilon(H) - \varphi_\varepsilon(H_0)\} &= \frac{\varepsilon}{\pi} \int_{-\infty}^{\infty} d\lambda \varphi'(\lambda) \int_{-\infty}^{\infty} \frac{\xi(\mu)}{(\mu - \lambda)^2 + \varepsilon^2} d\mu \\
&= \int_{-\infty}^{\infty} d\mu \xi(\mu) \left\{ \frac{\varepsilon}{\pi} \int_{-\infty}^{\infty} \frac{\varphi'(\lambda)}{(\mu - \lambda)^2 + \varepsilon^2} d\lambda \right\} \\
&\equiv \int_{-\infty}^{\infty} d\mu \xi(\mu) \Phi_\varepsilon(\mu),
\end{aligned}$$

which converges to $\int_{-\infty}^{\infty} \varphi'(\mu)\xi(\mu) d\mu$ by dominated convergence theorem since $\Phi_\varepsilon(\mu) \to \varphi'(\mu)$ for every μ (see theorem 13 of [27]) as $\varepsilon \to 0$ and is bounded by $\left(\sup_{\lambda \in \mathbb{R}} |\varphi'(\lambda)| \right) \frac{\varepsilon}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{(\mu - \lambda)^2 + \varepsilon^2} = \sup_{\lambda \in \mathbb{R}} |\varphi'(\lambda)|$. This proves (ii).

If $\varphi_\varepsilon(H) - \varphi_\varepsilon(H_0)$ converges in $\mathscr{B}_1$ as $\varepsilon \to 0$, then it converges to $\varphi(H) - \varphi(H_0)$ since $\varphi_\varepsilon(H)$ and $\varphi_\varepsilon(H_0)$ converge strongly to $\varphi(H)$ and $\varphi(H_0)$ respectively. Hence the trace formula follows from part (ii). ∎

As a corollary of this theorem we obtain

COROLLARY 2.5

Let H, H_0 and ξ be as in theorem 2.1. Then for each $t \in \mathbb{R}$, $e^{itH} - e^{itH_0} \in \mathscr{B}_1$ and

$$\operatorname{Tr}(e^{itH} - e^{itH_0}) = it \int_{-\infty}^{\infty} e^{it\lambda} \xi(\lambda) d\lambda. \qquad (2.11)$$

Proof. Let $t \in \mathbb{R}$ be fixed. Then the first part follows from (2.7). Set $\varphi(\lambda) = e^{it\lambda}$. Then $\varphi_\varepsilon(\lambda)$, given in (2.9), can be easily computed: $\varphi_\varepsilon(\lambda) = e^{-\varepsilon|t|}e^{it\lambda}$. Clearly φ satisfies the hypotheses of theorem 2.4, and $\varphi_\varepsilon(H) - \varphi_\varepsilon(H_0) = e^{-\varepsilon|t|}(e^{itH} - e^{itH_0})$ converges in $\mathscr{B}_1$ to $e^{itH} - e^{itH_0}$ as $\varepsilon \to 0$. Thus the result follows from theorem 2.4 (iii). ■

A function φ on $\mathbb{R}$ is said to be in Krein class $\mathscr{K}$ if φ is given by

$$\varphi(\lambda) = \int_{-\infty}^{\infty} \frac{e^{it\lambda} - 1}{it} \nu(\mathrm{d}t) + C \tag{2.12}$$

for some constant C and complex measure ν on $\mathbb{R}$. Note that such a function is necessarily continuously differentiable and the derivative is the Fourier transform of the measure ν i.e.,

$$\varphi'(\lambda) = \int e^{it\lambda} \nu(\mathrm{d}t).$$

It is also worth observing that $\varphi(H)$ and $\varphi(H_0)$ are not necessarily bounded operators (see remark 2.7 (ii)) though defined on $D(H) = D(H_0)$.

Theorem 2.6. *Let H, H_0 and ξ be as in theorem 2.1, and $\varphi \in \mathscr{K}$. Then $\varphi(H) - \varphi(H_0) \in \mathscr{B}_1$ and* $\mathrm{Tr}\{\varphi(H) - \varphi(H_0)\} = \int_{-\infty}^{\infty} \varphi'(\lambda)\xi(\lambda)\mathrm{d}\lambda.$

Proof. By functional calculus

$$\varphi(H) - \varphi(H_0) = \int_{-\infty}^{\infty} \frac{e^{itH} - e^{itH_0}}{it} \nu(\mathrm{d}t), \tag{2.13}$$

where we have observed that by the discussion following the proof of theorem 2.1. and estimate (2.7), the integral in (2.13) exists as a $\mathscr{B}_1$-valued Bochner integral (page 30 of [5]). It also follows that

$$\|\varphi(H) - \varphi(H_0)\|_1 \leqslant \|V\|_1 \int_{-\infty}^{\infty} |\nu|(\mathrm{d}t) < \infty,$$

and we have by (2.11)

$$\begin{aligned}
\mathrm{Tr}\{\varphi(H) - \varphi(H_0)\} &= \int_{-\infty}^{\infty} \frac{\nu(\mathrm{d}t)}{it} \mathrm{Tr}(e^{itH} - e^{itH_0}) \\
&= \int_{-\infty}^{\infty} \frac{\nu(\mathrm{d}t)}{it} it \int_{-\infty}^{\infty} e^{it\lambda}\xi(\lambda)\mathrm{d}\lambda \\
&= \int_{-\infty}^{\infty} \mathrm{d}\lambda\, \xi(\lambda) \int_{-\infty}^{\infty} e^{it\lambda}\nu(\mathrm{d}t) \\
&= \int_{-\infty}^{\infty} \varphi'(\lambda)\xi(\lambda)\mathrm{d}\lambda.
\end{aligned}$$

In the above the change in the order of integration is justified since

$$\int_{-\infty}^{\infty} \mathrm{d}\lambda |\xi(\lambda)| \int_{-\infty}^{\infty} |\nu|(\mathrm{d}t) < \infty.$$

∎

Remark 2.7. (i) If supp ν does not contain 0, then $\varphi \in \mathscr{K}$ is a bounded function. On the other hand if we set $\nu(\mathrm{d}t) = \delta(t)\mathrm{d}t$ or $= \frac{it}{2\pi}\hat{\zeta}(t)\mathrm{d}t$ (with $C = 0$ or $= \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{\zeta}(t)\mathrm{d}t$ respectively), where $\zeta \in \mathscr{S}(\mathbb{R})$, the Schwartz class of smooth functions of rapid decrease, and $\hat{\zeta}$ its Fourier transform, then $\varphi(\lambda) = \lambda$ or $= \zeta(\lambda)$ respectively.

(ii) Since $\left\| \frac{1}{it}(e^{itH} - I)f \right\| \leq \|Hf\|$, $\varphi(H)$ is well defined on $D(H) = D(H_0)$ for $\varphi \in \mathscr{K}$, and by (2.7), $\varphi(H) - \varphi(H_0)$ can be extended to whole of $\mathscr{H}$ as a trace-class operator.

(iii) Let J be a real open interval in $\rho(H) \cap \rho(H_0)$, and let $\varphi \in C_0^\infty(J)$, the class of smooth functions with compact support in J. Then by functional calculus $\varphi(H) = \varphi(H_0) = 0$, and hence by the trace formula in theorem 2.6,

$$\int \varphi'(\lambda)\xi(\lambda)\mathrm{d}\lambda = 0 \tag{2.14}$$

for all $\varphi \in C_0^\infty(J) \subseteq \mathscr{K}$. Since $\xi \in L^1$, it follows that $\xi \in L^1_{\mathrm{loc}}(\mathbb{R})$, and hence ξ can be thought of as a distribution on J. Then the equation (2.14) can be viewed as $\langle \xi', \varphi \rangle = 0$ for all $\varphi \in C_0^\infty(J)$ where ξ' is the distributional derivative. By a standard theorem in the theory of distributions (see p. 105 of [12]) ξ is constant in J. Furthermore if J contains a neighbourhood of either $+\infty$ or $-\infty$, then $\xi = 0$ a.e. on J since by theorem 2.1, (ii) $\int_{-\infty}^{\infty} |\xi(\lambda)|\mathrm{d}\lambda \leq \|V\|_1 < \infty$. Thus, supp ξ lies in the interval $[a, b]$, where $a = \min\{\inf \sigma(H_0), \inf \sigma(H)\}$ and $b = \max\{\sup \sigma(H_0), \sup \sigma(H)\}$.

(iv) We would like to go back once again to the counterexample in § 1 and observe the curious fact that the "formal expression" for $\mathrm{Tr}(E^0_\mu - E_\mu)$ coincides exactly with the boundary value of the argument of the perturbation determinant in this case. Using the notation of section 1, we see that $(E^0_\mu \psi, \psi) = 2\int_0^{(\lambda)^{1/2}} \alpha^2(1+\alpha^2)^{-1}\mathrm{d}\alpha$ with $\mu = (1+\lambda)^{-1}$. Thus for $\mathrm{Im}\, z \neq 0$,

$$\begin{aligned}\Delta(z) &= 1 + \frac{1}{2}\int_0^1 \frac{\mathrm{d}(E^0_\mu \psi, \psi)}{\mu - z} \\ &= 1 + \frac{1}{\pi}\int_0^1 \left(\frac{1-\mu}{\mu}\right)^{1/2} (\mu - z)^{-1}\mathrm{d}\mu.\end{aligned}$$

The last integral can be evaluated using the calculus of residues (see for example [26]) and this yields

$$\Delta(z) = i\left(\frac{1-z}{z}\right)^{1/2}, \tag{2.15}$$

and

$$\xi(\mu)=\lim_{\varepsilon\to 0+}\frac{1}{\pi}\arg\Delta(\mu+i\varepsilon)$$
$$=\frac{1}{2}\quad\text{if}\quad 0<\mu<1$$
$$=0\quad\text{if}\quad \mu\notin[0,1].$$

(v) In some applications [13], $H-H_0$ may not be trace-class but $e^{-tH}-e^{-tH_0}$ is trace-class for some $t>0$ (with H and $H_0\geqslant 0$). Such a case can be treated by the results of this section. Let $A=e^{-H}$, $B=e^{-H_0}$ so that $0\leqslant A$, $B\leqslant I$ and assume that $A-B\in\mathscr{B}_1$. Then by theorem 2.1 and remark 2.7 (iii) one has $\eta\in L^1[0,1]$ such that $\int_0^1|\eta(\mu)|\mathrm{d}\mu\leqslant\|e^{-H}-e^{-H_0}\|_1$ and

$$\int_0^1\eta(\mu)\mathrm{d}\mu=\mathrm{Tr}(e^{-H}-e^{-H_0}).\tag{2.16}$$

By setting $\mu=e^{-\lambda}(0\leqslant\lambda<\infty)$ and $\xi(\lambda)=-\eta(e^{-\lambda})$ in (2.16) we have

$$\int_0^\infty|\xi(\lambda)|e^{-\lambda}\mathrm{d}\lambda\leqslant\|e^{-H}-e^{-H_0}\|_1$$

and

$$-\int_0^\infty\xi(\lambda)e^{-\lambda}\mathrm{d}\lambda=\mathrm{Tr}(e^{-H}-e^{-H_0}).$$

Consider the function $g(\mu)=\mu^t$ for $\mu\in[0,1]$ and $t>2$. Since g is $C^2[0,1]$ function with $g'''\in L^1[0,1]$, we can find a function $G\in\mathscr{K}$ such that $G(\mu)=g(\mu)$ for all $\mu\in[0,1]$. Thus

$$\mathrm{Tr}(e^{-tH}-e^{-tH_0})=\mathrm{Tr}[(e^{-H})^t-(e^{-H_0})^t]$$
$$=\int_0^1\frac{\mathrm{d}}{\mathrm{d}\mu}(\mu^t)\eta(\mu)\mathrm{d}\mu=-t\int_0^\infty e^{-t\lambda}\xi(\lambda)\mathrm{d}\lambda.\tag{2.17}$$

(vi) More generally one can use the formula (5.7) and the invariance principle of scattering theory to derive the trace formula. As in [23] a real valued function ψ on J, an open subset of $\mathbb{R}$, is said to be *admissible* if $J=\cup_1^N J_n$ where $J_n=(\alpha_n,\beta_n)$ are disjoint, N finite or infinite, and (i) $\psi''\in L^1_{loc}(J)$, (ii) $\psi'>0$ or <0 on each interval (α_n,β_n). Then one has

Theorem 2.8. [23] (invarience principle). *Let ψ be an admissible function on J, H and H_0 be selfadjoint operators such that $\sigma(H)$, $\sigma(H_0)\subset\bar{J}$ and that at each boundary point of J either ψ has a finite limit or both H and H_0 do not have point spectrum at that point. Suppose furthermore $H-H_0\in\mathscr{B}_1$. Then $\Omega_\pm(\psi(H),\psi(H_0))$ exist, are complete and*

$$\Omega_\pm(\psi(H),\psi(H_0))=\Omega_\pm(H,H_0)E_{J_1}(H_0)+\Omega_\mp(H,H_0)E_{J_2}(H_0),$$

where J_1 (respectively J_2) is the union of those intervals on which $\psi' > 0$ (respectively $\psi' < 0$).

Then using (5·4)–(5·7) one gets in the spectral representation of H_0:

$$\xi(\lambda; H, H_0) = \operatorname{sgn}(\psi'(\lambda))\cdot\xi(\psi(\lambda); \psi(H), \psi(H_0)). \tag{2.18}$$

The relation (2.18) can be turned around to give a definition of $\xi(\lambda; H, H_0)$ when $H - H_0$ is not trace-class but rather $\psi(H) - \psi(H_0)$ is trace-class. It is also clear then that $\psi(\lambda) = e^{-t\lambda}(\lambda \geqslant 0)$ is an admissible function for every $t > 0$, and this gives the example in (v).

Now, if ψ is an admissible function such that $\psi(H) - \psi(H_0) \in \mathscr{B}_1$ and $\varphi: \mathbb{R} \to \mathbb{R}$ be such that $\varphi \circ \psi^{-1}$ (note that ψ^{-1} exists) is again an admissible function, then writing $\varphi(H) - \varphi(H_0) = \varphi \circ \psi^{-1}(\psi(H)) - \varphi \circ \psi^{-1}(\psi(H_0))$, one has formally (by using (2.18) and a change of variable $\mu = \psi(\lambda)$)

$$\begin{aligned}\operatorname{Tr}[\varphi(H) - \varphi(H_0)] &= \int \xi(\mu; \psi(H), \psi(H_0))(\varphi \circ \psi^{-1})'(\mu)\mathrm{d}\mu \\ &= \int \xi(\lambda; H, H_0)(\varphi \circ \psi^{-1})'(\psi(\lambda))\operatorname{sgn}\psi'(\lambda)|\psi'(\lambda)|\mathrm{d}\lambda \\ &= \int \xi(\lambda; H, H_0)\varphi'(\lambda)\mathrm{d}\lambda.\end{aligned}$$

3. An alternative proof of the trace formula

Here we give a functional analytic proof (following Voiculescu [28]) of the results in §1. The strategy is to reduce the computation of $\operatorname{Tr}(e^{itH} - e^{itH_0})$ to that of $\operatorname{Tr}(e^{itH_m} - e^{itH_{0,m}})$ for suitable finite dimensional approximations H_m and $H_{0,m}$ of H and H_0 respectively and then apply theorem 1.1. We begin with a few lemmas which are extensions of Weyl-von Neumann result (see lemma 2.2 of p. 523 of [16]).

Lemma 3.1. *Let A be a self-adjoint operator in $\mathscr{H}$, $f \in \mathscr{H}$ and $\varepsilon > 0$, K a compact set in $\mathbb{R}$. Then there exist a projection P of finite rank in $\mathscr{H}$ such that*

(i) $\|(I - P)e^{itA}P\|_2 < \varepsilon$ *uniformly for $t \in K$*
(ii) $\|(I - P)f\| < \varepsilon$.

Proof. Let $F(\,)$ be the spectral measure associated with the self-adjoint operator A. Choose $a > 0$ such that $\|(I - F(-a, a])f\| < \varepsilon$. For each positive integer n and $1 \leqslant k \leqslant n$, set $F_k = F\left(\frac{2k - 2 - n}{n}a, \frac{2k - n}{n}a\right]$ and note that $F_k F_j = \delta_{kj} F_j$, $\sum_{k=1}^{n} F_k = F(-a, a]$. We also set $g_k = \begin{cases} F_k f/\|F_k f\| & \text{if } F_k f \neq 0 \\ 0 & \text{otherwise.}\end{cases}$ Then $g_k \in D(A)$ and $Ag_k \in F_k\mathscr{H}$. Let P be the projection on to the sub-space generated by $\{g_1, \ldots, g_n\}$ so that $\dim P\mathscr{H} \leqslant n$. With $\lambda_k = \frac{2k - n - 1}{n}a$, it is easy to verify that

$$\|(A-\lambda_k)g_k\|^2=\int_{[(2k-n-2)/n]a}^{[(2k-n)/n]a}(\lambda-\lambda_k)^2 d\|F(\lambda)g_k\|^2\leqslant(a/n)^2,$$

and

$$\|(I-P)APu\|^2=\left\|\sum_{k=1}^{n}(u,g_k)(I-P)Ag_k\right\|^2\leqslant(a/n)^2\|u\|^2$$

for $u\in\mathscr{H}$ and hence

$$\|(I-P)AP\|_2\leqslant a/\sqrt{n}.$$

Thus

$$\begin{aligned}\alpha(t)&\equiv\|(I-P)e^{itA}P\|_2=\|(I-P)(e^{itA}-I)P\|_2\\&=\|(I-P)\int_0^t e^{isA}iA\,\mathrm{d}s\,P\|_2\\&\leqslant\int_0^t\{\|(I-P)e^{isA}P\|_2\|AP\|+\|(I-P)e^{isA}(I-P)\|\,\|(I-P)AP\|_2\}\,\mathrm{d}s\\&\leqslant 2a\int_0^t\alpha(s)\mathrm{d}s+Ta/\sqrt{n}\end{aligned}\tag{3.1}$$

for $|t|<T$. We can solve this Gronwall-type inequality (3.1) to conclude that

$$\alpha(t)\leqslant(Tae^{2at})/\sqrt{n}\leqslant(Tae^{2aT})/\sqrt{n}.$$

On the other hand, $(I-P)F(-a,a]f=\Sigma_{k=1}^{n}\|F_kf\|(I-P)g_k=0$ so that $\|(I-P)f\|=\|(I-P)(I-F(-a,a])f\|<\varepsilon$. ∎

Lemma 3.2 Let H and H_0 be two selfadjoint operators such that $V\equiv H-H_0$ is positive and of rank one. Set $V=\tau|g\rangle\langle g|$ with $\tau>0$ and $\|g\|=1$. Then given any $\varepsilon>0$, there exists a projection P of finite rank such that for all t with $|t|<T$.

(i) $\|(I-P)g\|<\varepsilon,\quad \|(I-P)e^{itH_0}P\|_2<\varepsilon,\quad \|(I-P)e^{itH_0}g\|<2\varepsilon,$
(ii) $\|(I-P)HP\|_2<\varepsilon(1+\tau),\quad \|(e^{itH}-e^{itH_0})(I-P)\|_1<2T\tau\varepsilon,$
(iii) $\|P(e^{itH_0}-e^{itPH_0P})P\|_1<\varepsilon^2T,\quad \|P(e^{itH}-e^{itPHP})P\|_1\leqslant\varepsilon^2T(1+\tau),$
(iv) $|\mathrm{Tr}(e^{itH}-e^{itH_0})-\mathrm{Tr}\{P(e^{itPHP}-e^{itPH_0P})P\}|\leqslant T\varepsilon[\tau(4+\varepsilon)+2\varepsilon].$

Proof. Given $\varepsilon>0$, g and H_0, we construct P as in lemma 3.1 so that the first two conclusions of (i) are satisfied. The third one follows from the first two trivially. Since $(I-P)HP=(I-P)H_0P+\tau|(I-P)g\rangle\langle Pg|$, the first part of (ii) follows from the estimate of lemma 3.1 and (i). Now

$$\begin{aligned}\|(e^{itH_0}-e^{itH})(I-P)\|_1&=\|i\tau\int_0^t|e^{i(t-s)H}g\rangle\langle(I-P)e^{isH_0}g|\mathrm{d}s\|_1\\&\leqslant\tau\int_0^{|t|}\|(I-P)e^{isH_0}g\|\,\mathrm{d}s\leqslant 2T\tau\varepsilon.\end{aligned}$$

This easily leads to the fact that

$$\|(1-P)(e^{itH}-e^{itH_0})P\|_1 < 2T\tau\varepsilon.$$

For (iii) we observe that

$$\|P(e^{itH_0}-e^{itPH_0P})P\|_1 \leqslant \int_0^{|t|} \|Pe^{i(t-s)H_0}(I-P)H_0 e^{isPH_0P}P\|_1 \mathrm{d}s$$

$$\leqslant \int_0^{|t|} \|Pe^{i(t-s)H_0}(I-P)\|_2 \|(I-P)H_0 P\|_2 \mathrm{d}s$$

and an application of (i) and the estimate in lemma 3.1 gives the result. A similar computation and the estimates in (ii) give the second result in (iii).

Finally since $\|e^{itH}-e^{itH_0}\|_1 \leqslant \tau \int_0^{|t|} \||e^{i(t-s)H}g\rangle\langle e^{isH_0}g|\|_1 \mathrm{d}s \leqslant \tau T$, it follows that $e^{itH}-e^{itH_0}\in\mathscr{B}_1$ and we have by (ii) and (iii)

$$\begin{aligned}&|\mathrm{Tr}(e^{itH}-e^{itH_0})-\mathrm{Tr}\{P(e^{itPHP}-e^{itPH_0P})P\}|\\&\leqslant \|P(e^{itH}-e^{itPHP})P\|_1+\|P(e^{itH_0}-e^{itPH_0P})P\|_1\\&\quad+\|(e^{itH}-e^{itH_0})(I-P)\|_1+\|(I-P)(e^{itH}-e^{itH_0})P\|_1\\&\leqslant T\varepsilon[\tau(4+\varepsilon)+2\varepsilon].\end{aligned}$$

■

Now we are ready to prove the main theorem of this section.

Theorem 3.3. *Let H_0 be a selfadjoint operator and $H=H_0+V$ with V self-adjoint trace-class. Then there exists a unique real-valued function ξ in $L^1(\mathbb{R})$ such that*

(i) $\mathrm{Tr}(e^{itH}-e^{itH_0}) = it\int e^{it\lambda}\xi(\lambda)\mathrm{d}\lambda$,

(ii) $\int\xi(\lambda)\mathrm{d}\lambda = \mathrm{Tr}\, V$, $\int|\xi(\lambda)|\mathrm{d}\lambda \leqslant \|V\|_1$,

(iii) *for every function $\varphi\in\mathscr{K}$ (defined in (2.12)), $\varphi(H)-\varphi(H_0)\in\mathscr{B}_1$ and*

$$\mathrm{Tr}(\varphi(H)-\varphi(H_0)) = \int_{-\infty}^{\infty} \varphi'(\lambda)\xi(\lambda)\mathrm{d}\lambda,$$

(iv) *the function $\lambda\to(\lambda-z)^{-1}$ (with $\mathrm{Im}\, z\neq 0$) belongs to the class $\mathscr{K}$ and hence*

$$\mathrm{Tr}(R_z-R_z^0) = -\int(\lambda-z)^{-2}\xi(\lambda)\mathrm{d}\lambda.$$

Proof. At first we let $V\equiv\tau|g\rangle\langle g|$, $\tau>0$, $\|g\|=1$. Then we rephrase the conclusion (iv) of lemma 3.2 as: there exists a sequence P_m of finite rank projections such that $P_m g\to g$ strongly and

$$\mathrm{Tr}(e^{itH}-e^{itH_0}) = \lim_{m\to\infty}\mathrm{Tr}[P_m(e^{itH_m}-e^{itH_{0,m}})P_m], \tag{3.2}$$

where $H_{0,m}=P_m H_0 P_m$ and $H_m=P_m H P_m$, and the convergence is uniform in t for

$|t| < T$. Note that by construction $P_m\mathscr{H} \subseteq D(H_0) = D(H)$ and hence both $H_{0,m}$ and H_m are self-adjoint operators in the finite-dimensional space $P_m\mathscr{H}$. Next we use theorem 1.1 (iv) and corollary 1.2 in the right hand side of (3.2) to get a $\{0, 1\}$-valued L^1-function ξ_m such that

$$\operatorname{Tr}[P_m(e^{itH_m} - e^{itH_{0,m}})P_m] = it \int_{-\infty}^{\infty} e^{it\lambda}\xi_m(\lambda)\mathrm{d}\lambda. \tag{3.3}$$

Hence

$$\operatorname{Tr}(e^{itH} - e^{itH_0}) = it \lim_{m\to\infty} \int_{-\infty}^{\infty} e^{it\lambda}\xi_m(\lambda)\mathrm{d}\lambda, \tag{3.4}$$

the convergence being uniform in t. It is easy to see from (3.3) that

$$\begin{aligned}\int \xi_m(\lambda)\mathrm{d}\lambda &= \lim_{t\to 0}\frac{1}{it}\operatorname{Tr}[P_m(e^{itH_m} - e^{itH_{0,m}})P_m] \\ &= \lim_{t\to 0}\frac{1}{t}\int_0^t \operatorname{Tr}[P_m e^{i(t-s)H_m}P_m V P_m e^{isH_{0,m}}P_m]\mathrm{d}s \\ &= \operatorname{Tr} P_m V P_m,\end{aligned} \tag{3.5}$$

since $t \to e^{itH_m}$, $e^{itH_{0,m}}$ are norm continuous in $P_m\mathscr{H}$ and $P_m V P_m$ is rank one. Thus $\int \xi_m(\lambda)\mathrm{d}\lambda = \tau\|P_m g\|^2 > \tau(1-\varepsilon)^2$ by lemma 3.2 (i) and setting $\mu_m(\Delta) = (\tau\|P_m g\|^2)^{-1} \int_\Delta \xi_m(\lambda)\mathrm{d}\lambda$ for every Borel set $\Delta \subseteq \mathbb{R}$, we have a family $\{\mu_m\}$ of probability measures by (3.5). Also note that by (3.4) the family $\{\hat{\mu}_m(t)\}$ of their Fourier transforms converges to $\hat{\mu}(t) = \dfrac{1}{it\tau}\operatorname{Tr}(e^{itH} - e^{itH_0})$ uniformly in t in compact sets in $\mathbb{R}\backslash\{0\}$. On the other hand $\hat{\mu}_m(0) = (\tau/\|P_m g\|^2)^{-1}\int \xi_m(\lambda)\mathrm{d}\lambda = 1$ for all m and a calculation identical to that in (3.5) shows that $\lim_{t\to 0}\hat{\mu}(t) = \tau^{-1}\operatorname{Tr} V = 1 \equiv \hat{\mu}(0)$, by definition. Thus by Levy-Cramer continuity theorem [22], there exists a probability measure μ on $\mathbb{R}$ such that $\mu_m \to \mu$ weakly i.e. $\int \varphi(\lambda)\mathrm{d}\mu_m(\lambda) \to \int \varphi(\lambda)\mathrm{d}\mu(\lambda)$ as $m \to \infty$ for every bounded continuous function φ.

Let $\Delta = (a, b] \subseteq \mathbb{R}$ and let $\{\varphi_n\}$ be a sequence of smooth functions of support in $\left(a - \frac{1}{n}, b + \frac{1}{n}\right]$ such that $0 \leqslant \varphi_n \leqslant 1$ and $\|\chi_\Delta - \varphi_n\|_1 \to 0$ as $n \to \infty$ where χ_Δ is the indicator function of Δ. Choosing a subsequence if necessary and using the bounded convergence theorem, we have

$$\lim_{n\to\infty}\lim_{m\to\infty}\int \varphi_n(\lambda)\mathrm{d}\mu_m(\lambda) = \lim_{n\to\infty}\int \varphi_n(\lambda)\mathrm{d}\mu(\lambda) = \mu(\Delta).$$

Thus

$$\begin{aligned}\mu(\Delta) &= \lim_{n\to\infty}\lim_{m\to\infty}\frac{1}{\tau\|P_m g\|^2}\int \varphi_n(\lambda)\xi_m(\lambda)\mathrm{d}\lambda \\ &= \frac{1}{\tau}\lim_{n\to\infty}\lim_{m\to\infty}\int \varphi_n(\lambda)\xi_m(\lambda)\mathrm{d}\lambda \\ &\leqslant \tau^{-1}\lim_{n\to\infty}(b - a + 2/n) = \tau^{-1}(b - a),\end{aligned}$$

since $0 \leqslant \xi_m(\lambda) \leqslant 1$ for all m and all λ. This shows that μ is absolutely continuous and we set $\xi(\lambda) = \tau \cdot \frac{d\mu(\lambda)}{d\lambda}$. Then ξ is a non-negative L^1 function and we have that $\hat{\mu}(t) = \int e^{it\lambda} d\mu(\lambda) = \tau^{-1} \int e^{it\lambda} \xi(\lambda) d\lambda$ and hence

$$\mathrm{Tr}(e^{itH} - e^{itH_0}) = it \int e^{it\lambda} \xi(\lambda) d\lambda. \tag{3.6}$$

Also dividing both sides of (3.6) by it and taking limit $t \to 0$ as in (3.5) we conclude that

$$\int \xi(\lambda) d\lambda = \mathrm{Tr}\, V = \tau \geqslant 0.$$

If V is rank one and negative, then we interchange the role of H and H_0 and write $H_0 = H - V$ with $-V$ rank one and positive and obtain as above a non-negative L^1-function η such that

$$\mathrm{Tr}(e^{itH_0} - e^{itH}) = it \int e^{it\lambda} \eta(\lambda) d\lambda$$

and

$$\int \eta(\lambda) d\lambda = \mathrm{Tr}(-V) = -\mathrm{Tr}\, V \geqslant 0.$$

Defining $\xi(\lambda) = -\eta(\lambda)$, we get that relation (3.6) is valid for all V rank one with some real-valued L^1-function ξ.

Now let $V \in \mathscr{B}_1$ and let $V = \Sigma_{k=1}^{\infty} \tau_k |g_k\rangle\langle g_k|$ be its canonical decomposition with $\|V\|_1 \equiv \Sigma_{k=1}^{\infty} |\tau_k| < \infty$ and $\|g_k\| = 1$. We write for $k = 1, 2, \ldots, H_k = H_0 + \Sigma_{j=1}^{k} \tau_j |g_j\rangle\langle g_j| = H_{k-1} + \tau_k |g_k\rangle\langle g_k|$. Then we have a real valued L^1-function ξ_k such that

$$\mathrm{Tr}(e^{itH_k} - e^{itH_{k-1}}) = it \int e^{it\lambda} \xi_k(\lambda) d\lambda,$$

$$\int \xi_k(\lambda) d\lambda = \tau_k \quad \text{and} \quad \int |\xi_k(\lambda)| d\lambda = |\tau_k|.$$

Set $\xi(\lambda) = \sum_{k=1}^{\infty} \xi_k(\lambda)$, then by the above relations $\int |\xi(\lambda)| d\lambda \leqslant \Sigma_{k=1}^{\infty} \int |\xi_k(\lambda)| d\lambda = \Sigma_{k=1}^{\infty} |\tau_k| = \|V\|_1$ and thus ξ is a real-valued L^1 function and $\Sigma_{k=1}^{\infty} \xi_k$ converges in L^1-norm. Therefore

$$\begin{aligned}
it \int e^{it\lambda} \xi(\lambda) d\lambda &= it \sum_{k=1}^{\infty} \int e^{it\lambda} \xi_k(\lambda) d\lambda \\
&= \sum_{k=1}^{\infty} \mathrm{Tr}(e^{itH_k} - e^{itH_{k-1}}) \\
&= \lim_{k \to \infty} \mathrm{Tr}(e^{itH_k} - e^{itH_0}) \\
&= \mathrm{Tr}(e^{itH} - e^{itH_0}),
\end{aligned}$$

since

$$\|e^{itH} - e^{itH_k}\|_1 = \|i \sum_{j=k+1}^{\infty} \tau_j \int_0^t |e^{i(t-s)H} g_j\rangle\langle e^{-isH_k} g_j| \mathrm{d}s\|_1$$

$$\leqslant |t| \sum_{j=k+1}^{\infty} |\tau_j| \to 0 \quad \text{as} \quad k \to \infty.$$

Also

$$\int \xi(\lambda)\mathrm{d}\lambda = \sum_{k=1}^{\infty} \int \xi_k(\lambda)\mathrm{d}\lambda = \sum_{k=1}^{\infty} \tau_k = \operatorname{Tr} V.$$

This completes the proof of (i) and (ii). The proof of part (iii) follows as in theorem 2.6. For (iv) we just note that $(\lambda - z)^{-1} + z^{-1} = \int \frac{e^{it\lambda} - 1}{it} \nu(\mathrm{d}t)$ with $\nu(\mathrm{d}t) = -t\chi_{\mp}(t)e^{-izt}\mathrm{d}t$, according as $\operatorname{Im} z \gtrless 0$, where $\chi_{\pm}$ are the indicator functions of the intervals $[0, \infty)$ and $(-\infty, 0]$ respectively. ■

4. The trace formula: the case when the difference of resolvents is trace-class

In this section we shall follow essentially the methods of § 2, but for the case when the perturbation V is not necessarily of trace class but is such that the difference of resolvents $R_z - R_z^0$ is trace-class for some $z \in \rho(H) \cap \rho(H_0)$. It is not difficult to see that if $R_z - R_z^0 \in \mathscr{B}_1$ for some such z, then it is so for all such z and hence we shall, in this section, take $z = i$ as the reference point and assume that $R_i - R_i^0 \in \mathscr{B}_1$. Also it is worth noting that in $L^2(\mathbb{R}^3)$, if $H_0 = -\Delta$ and V is the multiplication operator by a function $V \in L^2(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$, then $R_i - R_i^0 \in \mathscr{B}_1$ (see p. 546 of [16]).

We set $U_0 = \dfrac{H_0 + i}{H_0 - i} = I + 2iR_i^0$ and $U = \dfrac{H + i}{H - i} = I + 2iR_i$ so that $U - U_0 = 2i(R_i - R_i^0) \in \mathscr{B}_1$. If we also set $U - U_0 = U_0 T$ then it is clear that T is a normal trace-class operator and $I + T$ is unitary. Let $T = \sum_{j=1}^{\infty} \tau_j |g_j\rangle\langle g_j|$ be the canonical decomposition for T with $\|g_j\| = 1$ and $1 + \tau_j = \exp(i\theta_j)$, $-\pi < \theta_j \leqslant \pi$. Then it follows that

$$\sum_{j=1}^{\infty} |\theta_j| = \sum_{j=1}^{\infty} \left| e^{-i\theta_j/2} \left[\frac{\theta_j/2}{\sin(\theta_j/2)} \right] \tau_j \right| \leqslant \frac{\pi}{2} \sum_{j=1}^{\infty} |\tau_j|$$

$$= \frac{\pi}{2} \|T\|_1 < \infty \tag{4.1}$$

since $\left|\dfrac{\sin\theta}{\theta}\right| \geqslant 2/\pi$ for $0 \leqslant \theta \leqslant \pi/2$. Thus the determinant

$$\Delta(\omega) \equiv \det[(U - \omega)(U_0 - \omega)^{-1}] = \det[I + U_0 T(U_0 - \omega)^{-1}]$$

is analytic for $|\omega| < 1$ and has no zeroes there (see theorem A.5 (ii)). Next we obtain the Krein's spectral shift function in this case essentially following the same route as in § 2.

Theorem 4.1. *Let $R_t - R_t^0 \in \mathscr{B}_1$ and U and U_0 be defined as above. Then there exists a real-valued function ξ on $\mathbb{R}$ such that*

(i) $\xi(\lambda)(1+\lambda^2)^{-1} \in L^1(\mathbb{R})$,

(ii) $\int_{-\infty}^{\infty} |\xi(\lambda)|(1+\lambda^2)^{-1}\mathrm{d}\lambda \leqslant (\pi/4)\|T\|_1$ and $\int_{-\infty}^{\infty} \xi(\lambda)(1+\lambda^2)^{-1}\mathrm{d}\lambda = \frac{-i}{2}\ln\det(I+T)$,

(iii) $\xi(\lambda) \equiv \eta(\alpha) = \frac{1}{\pi}\lim_{\rho\uparrow 1}\operatorname{Im}\ln\left[\exp\left(-\frac{i}{2}\sum_{j=1}^{\infty}\theta_j\right)\Delta(\rho e^{i\alpha})\right]$, with $e^{i\alpha} = (\lambda+i)(\lambda-i)^{-1}$,

(iv) $\operatorname{Tr}(R_z - R_z^0) = -\int_{-\infty}^{\infty}(\lambda - z)^{-2}\xi(\lambda)\mathrm{d}\lambda$ *for* $\operatorname{Im} z \neq 0$.

Furthermore, ξ is unique up to an additive constant function.

Proof. At first let T be rank one i.e. $T = \tau|g\rangle\langle g|$ with $1+\tau = e^{i\theta}\,(-\pi < \theta \leqslant \pi)$, $\|g\| = 1$. Then

$$\begin{aligned}\Delta(\omega) &= \det[I + \tau|U_0 g\rangle\langle (U_0^* - \bar{\omega})^{-1} g|] = 1 + \tau(g, U_0(U_0 - \omega)^{-1} g)\\ &= e^{i\theta/2}\left[\cos(\theta/2) + i\sin(\theta/2)\int_{-\pi}^{\pi}\frac{e^{i\alpha}+\omega}{e^{i\alpha}-\omega}\, d\|F_0(\alpha)g\|^2\right],\end{aligned} \tag{4.2}$$

where F_0 is the spectral family of the unitary operator U_0. Thus

$$\operatorname{Im}[e^{-i\theta/2}\Delta(\omega)] = \sin(\theta/2)\int_{-\pi}^{\pi}\frac{1-\rho^2}{1+\rho^2 - 2\rho\cos(\alpha-\beta)}\,\mathrm{d}\|F_0(\alpha)g\|^2, \tag{4.3}$$

where we have set $\omega = \rho\exp(i\beta)$, $0 \leqslant \rho < 1$; and hence $(\operatorname{sgn}\theta)\cdot\operatorname{Im}[e^{-i\theta/2}\Delta(\omega)] \geqslant 0$ or equivalently $0 \leqslant (\operatorname{sgn}\theta)\cdot\operatorname{Im}\ln[e^{-i\theta/2}\Delta(\omega)] \leqslant \pi$. Since $\Delta(\omega)$ is analytic in the interior or the exterior of the unit circle and has no zeroes there, $\ln\Delta(\omega)$ is also analytic there. Therefore by theorem A.2 there exists a real-valued $L^1[-\pi,\pi]$ function $\eta(\alpha)$ such that

$$\ln[e^{-i\theta/2}\Delta(\omega)] = \operatorname{Re}\ln[e^{-i\theta/2}\Delta(0)] + \frac{i}{2}\int_{-\pi}^{\pi}\frac{e^{i\alpha}+\omega}{e^{i\alpha}-\omega}\eta(\alpha)\mathrm{d}\alpha.$$

Now $\Delta(0) = \det(UU_0^{-1}) = \det[U_0(I+T)U_0^{-1}] = \det(I+T) = e^{i\theta}$ by theorem A.3 (v), so that $\operatorname{Re}\ln[e^{-i\theta/2}\Delta(0)] = 0$ and we have

$$\ln\Delta(\omega) = i\theta/2 + \frac{i}{2}\int_{-\pi}^{\pi}\frac{e^{i\alpha}+\omega}{e^{i\alpha}-\omega}\eta(\alpha)\mathrm{d}\alpha. \tag{4.4}$$

We also know from the theorem A.2 that $\eta(\alpha) = \frac{1}{\pi}\lim_{\rho\uparrow 1}\operatorname{Im}\ln[e^{-i\theta/2}\Delta(\rho e^{i\alpha})]$ and

$$\int_{-\pi}^{\pi}\eta(\alpha)\mathrm{d}\alpha = 2\operatorname{Im}\ln[e^{-i\theta/2}\Delta(0)] = \theta. \tag{4.5}$$

Equation (4.3) implies that $0 \leqslant (\operatorname{sgn}\theta)\eta(\alpha) \leqslant 1$ and therefore

$$\int_{-\pi}^{\pi}|\eta(\alpha)|\mathrm{d}\alpha = (\operatorname{sgn}\theta)\int_{-\pi}^{\pi}\eta(\alpha)\mathrm{d}\alpha = |\theta| \tag{4.6}$$

In the general case, $T=\sum_{j=1}^{\infty}(e^{i\theta_j}-1)|g_j\rangle\langle g_j|$ as before, and write $U_j=U_{j-1}(I+\tau_j|g_j\rangle\langle g_j|)$, $(j=1,2,\ldots)$. Since $\tau_j=e^{i\theta_j}-1$ and since $(g_j,g_k)=\delta_{jk}$, it is easy to see that each U_j is unitary and that,

$$U_j=U_0(I+\tau_1|g_1\rangle\langle g_1|)(I+\tau_2|g_2\rangle\langle g_2|)\cdots(I+\tau_j|g_j\rangle\langle g_j|)$$
$$=U_0\left(I+\sum_{k=1}^{j}\tau_k|g_k\rangle\langle g_k|\right)$$

and therefore $U_j-U_0\to U-U_0$ in $\mathscr{B}_1$-norm as $j\to\infty$. As in the last paragraph, let $\eta_j(t)$ be the real $L^1[-\pi,\pi]$-function for the pair $\{U_j,U_{j-1}\}$ with $U_j-U_{j-1}=\tau_jU_{j-1}|g_j\rangle\langle g_j|$, an operator of rank one. Then we have from (4.4)–(4.6):

$$\operatorname{Im}\Delta_j(\omega)=e^{i\theta_j/2}+\frac{i}{2}\int_{-\pi}^{\pi}\frac{e^{i\alpha}+\omega}{e^{i\alpha}-\omega}\eta_j(\alpha)\mathrm{d}\alpha$$

$$0\leqslant(\operatorname{sgn}\theta_j)\eta_j(\alpha)\leqslant 1,\quad\int_{-\pi}^{\pi}\eta_j(\alpha)\mathrm{d}\alpha=\theta_j, \tag{4.7}$$

$$\int_{-\pi}^{\pi}|\eta_j(\alpha)|\mathrm{d}\alpha=|\theta_j|,$$

where $\Delta_j(\omega)=\det[(U_j-\omega)(U_{j-1}-\omega)^{-1}]$.

Set $\eta(\alpha)=\sum_{j=1}^{\infty}\eta_j(\alpha)$. It follows easily from (4.7) that the series converges in $L^1[-\pi,\pi]$-norm and defines an L^1-function η and we have

$$\int_{-\pi}^{\pi}|\eta(\alpha)|\mathrm{d}\alpha\leqslant\sum_{j=1}^{\infty}\int_{-\pi}^{\pi}|\eta_j(\alpha)|\mathrm{d}\alpha=\sum_{j=1}^{\infty}|\theta_j|\leqslant\frac{\pi}{2}\|T\|_1,$$
$$=\frac{\pi}{2}\|U-U_0\|_1=\pi\|R_i-R_i^0\|_1,$$

and

$$\int_{-\pi}^{\pi}\eta(\alpha)\mathrm{d}\alpha=\sum_{j=1}^{\infty}\theta_j=-i\ln\det(I+T). \tag{4.8}$$

By theorem A.5 (ii) we have that

$$\ln\det[(U_n-\omega)(U_0-\omega)^{-1}]=\ln\det[I+(U_n-U_0)(U_0-\omega)^{-1}]$$
$$=\sum_{j=1}^{n}\ln\Delta_j(\omega)$$
$$=\frac{i}{2}\sum_{j=1}^{n}\theta_j+\frac{i}{2}\int_{-\pi}^{\pi}\frac{e^{i\alpha}+\omega}{e^{i\alpha}-\omega}\left(\sum_{j=1}^{n}\eta_j(\alpha)\right)\mathrm{d}\alpha. \tag{4.9}$$

The fact the $U_n-U_0\to U-U_0$ in $\mathscr{B}_1$ and the continuity of the determinant with respect to its argument in $\mathscr{B}_1$-norm (theorem A.3 (ii)) lead to

$$\ln\Delta(\omega)=\frac{i}{2}\sum_{j=1}^{\infty}\theta_j+\frac{i}{2}\int_{-\pi}^{\pi}\frac{e^{i\alpha}+\omega}{e^{i\alpha}-\omega}\eta(\alpha)\mathrm{d}\alpha \tag{4.10}$$

and hence

$$\eta(\alpha) = \frac{1}{\pi} \lim_{\rho \uparrow 1} \operatorname{Im} \ln \left[\exp\left(-\frac{i}{2} \sum_{j=1}^{\infty} \theta_j \right) \Delta(\rho e^{i\alpha}) \right]. \tag{4.11}$$

The transformation $e^{i\alpha} = \frac{\lambda + i}{\lambda - i}$ or conversely $\alpha = 2\cot^{-1}\lambda$ implies that as λ increases from $-\infty$ to 0 and then to $+\infty$, α moves from 0 to $-\pi$ and then from π to 0. If we now define $\xi: \mathbb{R} \to \mathbb{R}$ by setting $\xi(\lambda) = \eta(\alpha) \equiv \eta(2\cot^{-1}\lambda)$, then since $\frac{\mathrm{d}\alpha}{\mathrm{d}\lambda} = -\frac{2}{1+\lambda^2}$ one has by (4.8)

$$\int_{-\infty}^{\infty} |\xi(\lambda)|(1+\lambda^2)^{-1}\mathrm{d}\lambda = \frac{1}{2}\int_{-\pi}^{\pi} |\eta(\alpha)|\mathrm{d}\alpha \leqslant \frac{\pi}{4}\|T\|_1$$

and

$$\int_{-\infty}^{\infty} \xi(\lambda)(1+\lambda^2)^{-1}\mathrm{d}\lambda = \frac{1}{2}\int_{-\pi}^{\pi} \eta(\alpha)\mathrm{d}\alpha = -\frac{i}{2}\ln\det(I+T)$$

which proves (i) and (ii). The part (iii) is the statement (4.11) which also shows that ξ is real.

The map $z \to \omega = \frac{z+i}{z-i}$ maps the open lower half plane onto the open unit disc and we have $(U-\omega)^{-1} = \frac{i}{2}(z-i)[1+(z-i)R_z]$, $(U_0-\omega)^{-1} = \frac{i}{2}(z-i)[1+(z-i)R_z^0]$ for $\operatorname{Im} z < 0$. Thus by theorem A.5 (ii) and (4.10)

$$\begin{aligned}
\operatorname{Tr}[(U-\omega)^{-1} - (U_0-\omega)^{-1}] &= \frac{i}{2}(z-i)^2 \operatorname{Tr}(R_z - R_z^0) \\
&= -\frac{\mathrm{d}}{\mathrm{d}\omega}\ln\Delta(\omega) = -\frac{i}{2}\frac{\mathrm{d}}{\mathrm{d}\omega}\int_{-\pi}^{\pi}\frac{e^{i\alpha}+\omega}{e^{i\alpha}-\omega}\eta(\alpha)\mathrm{d}\alpha \\
&= -i\int_{-\pi}^{\pi}\frac{e^{i\alpha}}{(e^{i\alpha}-\omega)^2}\eta(\alpha)\mathrm{d}\alpha,
\end{aligned}$$

where the interchange of differentiation and integration can easily be justified by noting that the last integral is uniformly convergent for all ω such that $0 \leqslant |\omega| \leqslant \delta < 1$. Therefore for $\operatorname{Im} z < 0$, $\frac{i}{2}(z-i)^2\operatorname{Tr}(R_z - R_z^0) = -i\left\{-\int_{-\infty}^{\infty}\xi(\lambda)\frac{\mathrm{d}\alpha}{\mathrm{d}\lambda}\cdot \mathrm{d}\lambda \left(\frac{\lambda+i}{\lambda-i}\right)\left[2i\left(\frac{\lambda-z}{(\lambda-i)(z-i)}\right)\right]^{-2}\right\} = \frac{-i(z-i)^2}{2}\int_{-\infty}^{\infty}\frac{\xi(\lambda)}{(\lambda-z)^2}\mathrm{d}\lambda$ which leads to (iii) for $\operatorname{Im} z < 0$. Since ξ is real-valued, an identical formula for $\operatorname{Im} z > 0$ is obtained by complex conjugation of the one for $\operatorname{Im} z < 0$.

Finally, if ξ and ξ' are two shift functions satisfying (i) and (ii), then setting $\zeta(\lambda) = \xi(\lambda) - \xi'(\lambda)$ we have that for $z = \mu + i\varepsilon(\varepsilon > 0)$,

$$\int\frac{\zeta(\lambda)\mathrm{d}\lambda}{(\lambda-z)^2} = \int\frac{\zeta(\lambda)\mathrm{d}\lambda}{(\lambda-\mu)^2 - \varepsilon^2 - 2i\varepsilon(\lambda-\mu)} = 0.$$

Thus

$$0 = \operatorname{Im}\int \frac{\zeta(\lambda)\mathrm{d}\lambda}{(\lambda-\mu)^2-\varepsilon^2-2i\varepsilon(\lambda-\mu)} = \int \frac{\zeta(\lambda)2\varepsilon(\lambda-\mu)}{((\lambda-\mu)^2+\varepsilon^2)^2}\mathrm{d}\lambda = \frac{\mathrm{d}}{\mathrm{d}\mu}\int \frac{\zeta(\lambda)\varepsilon}{(\lambda-\mu)^2+\varepsilon^2}\mathrm{d}\lambda$$

or $\int\zeta(\lambda)\varepsilon((\lambda-\mu)^2+\varepsilon^2)^{-1}\mathrm{d}\lambda$ = constant for all $\mu\in\mathbb{R}$, $\varepsilon>0$. By taking limit $\varepsilon\to 0+$ of the above expression by theorem 13 of [27], $\zeta(\mu)$ = constant almost everywhere which implies uniqueness of ξ up to an additive constant. ■

Next we consider functions ψ of H and H_0 and obtain the trace formula for $\psi(H)-\psi(H_0)$.

Theorem 4.2. *Let $R_i - R_i^0 \in \mathscr{B}_1$, and let ψ be a bounded C^1-function on $\mathbb{R}$ such that $\sup_{\lambda\in\mathbb{R}}|\psi(\lambda)(1+\lambda^2)|<\infty$ and $\sup_{\lambda\in\mathbb{R}}|\psi'(\lambda)(1+\lambda^2)|<\infty$. Define ψ_ε as in (2.9). Then*

(i) $\psi_\varepsilon(H)-\psi_\varepsilon(H_0)\in\mathscr{B}_1$ for each $\varepsilon>0$.
(ii) If $\psi_\varepsilon(H)-\psi_\varepsilon(H_0)$ converges to $\psi(H)-\psi(H_0)$ in $\mathscr{B}_1$-norm, then

$$\operatorname{Tr}[\psi(H)-\psi(H_0)] = \int\psi'(\lambda)\xi(\lambda)\mathrm{d}\lambda,$$

where ξ is the spectral shift function obtained in theorem 4.1.

Proof. Let $z=\mu+i\varepsilon$ $(0<\varepsilon<1)$ and write $\Psi_z=(H-i)(H-z)^{-1}$, $\Psi_z^0=(H_0-i)(H_0-z)^{-1}$. Both Ψ_z and Ψ_z^0 are bounded and

$$\begin{aligned} R_z - R_z^0 &= R_z[1+(z-i)R_z^0]-[1+(z-i)R_z]R_z^0 \\ &= R_z(H_0-i)R_z^0 - R_z(H-i)R_z^0 \\ &= \Psi_z(R_i-R_i^0)\Psi_z^0, \end{aligned} \tag{4.12}$$

Now let $R_i-R_i^0=\sum_{j=1}^{\infty}\gamma_j|f_j\rangle\langle g_j|$ with $\sum_{j=1}^{\infty}|\gamma_j|=\|R_i-R_i^0\|_1<\infty$, $\|f_j\|=\|g_j\|=1$. Then by (4.12), Schwarz inequality and lemma 2.2 (ii) we have that

$$\begin{aligned} &\int\mathrm{d}\mu(1+\mu^2)^{-1}\|R_{\mu+i\varepsilon}-R^0_{\mu+i\varepsilon}\|_1 \\ &\leqslant \sum_{j=1}^{\infty}|\gamma_j|\int\mathrm{d}\mu(1+\mu^2)^{-1}\|\Psi_{\mu+i\varepsilon}f_j\|\,\|\Psi^0_{\mu-i\varepsilon}g_j\| \\ &\leqslant \|R_i-R_i^0\|_1 2\pi(1+\varepsilon^{-1}). \end{aligned}$$

Next by the definition of ψ_ε and functional calculus,

$$\|\psi_\varepsilon(H)-\psi_\varepsilon(H_0)\|_1 \leqslant \frac{1}{\pi}\int\mathrm{d}\mu|\psi(\mu)|\,\|\operatorname{Im}(R_{\mu+i\varepsilon}-R^0_{\mu+i\varepsilon})\|_1$$

$$\leq \frac{1}{\pi}\left(\sup_{\lambda\in\mathbb{R}}|(\psi(\lambda)(1+\lambda^2)|\right)\int d\mu(1+\mu^2)^{-1}\|R_{\mu+i\varepsilon}-R^0_{\mu+i\varepsilon}\|_1$$

$$\leq 2(1+\varepsilon^{-1})\left(\sup_{\lambda\in\mathbb{R}}|(\psi(\lambda)(1+\lambda^2)|\right)\|R_i-R^0_i\|_1$$

and this proves (i).

$$\begin{aligned}\mathrm{Tr}[\psi_\varepsilon(H)-\psi_\varepsilon(H_0)] &= \frac{1}{\pi}\int\psi(\lambda)\mathrm{Im}\,\mathrm{Tr}(R_{\lambda+i\varepsilon}-R^0_{\lambda+i\varepsilon})d\lambda\\ &= -\frac{\varepsilon}{\pi}\int d\lambda\psi(\lambda)\mathrm{Im}\int\frac{\xi(\mu)d\mu}{(\mu-\lambda-i\varepsilon)^2}\\ &= -\frac{\varepsilon}{\pi}\int\psi(\lambda)\frac{d}{d\lambda}\left(\int\frac{\xi(\mu)d\mu}{(\mu-\lambda)^2+\varepsilon^2}\right)d\lambda\\ &= -\frac{\varepsilon}{\pi}\psi(\lambda)\left(\int\frac{\xi(\mu)d\mu}{(\mu-\lambda)^2+\varepsilon^2}\right)\Bigg|_{-\infty}^{\infty}\\ &\quad+\frac{\varepsilon}{\pi}\int\psi'(\lambda)\left(\int\frac{\xi(\mu)}{(\mu-\lambda)^2+\varepsilon^2}d\mu\right)d\lambda. \end{aligned}\tag{4.13}$$

Since

$$\psi(\lambda)(1+\lambda^2)\leq C,\quad (1+\mu^2)=1+(\mu-\lambda+\lambda)^2\leq 2[(1+\lambda^2)+(\mu-\lambda)^2]$$

it follows that the boundary term in (4.13) can be estimated by $2C\varepsilon/\pi\int\frac{\xi(\mu)}{1+\mu^2}\frac{(1+\lambda^2)+(\mu-\lambda)^2}{(1+\lambda^2)[(\mu-\lambda)^2+\varepsilon^2]}d\mu$. Furthermore the integrand in the last expression converges to 0 as $\lambda\to\pm\infty$ and is bounded by $(1+\varepsilon^{-2})|\xi(\mu)|(1+\mu^2)^{-1}$ which is integrable, and hence the boudary term in (4.13) vanishes by an application of dominated convergence theorem. The same estimate allows us to interchange the order of integration in the second term in (4.13) to get

$$\begin{aligned}\mathrm{Tr}[\psi_\varepsilon(H)-\psi_\varepsilon(H_0)] &= \int\frac{\xi(\mu)}{1+\mu^2}\left[\frac{\varepsilon}{\pi}\int\frac{\psi'(\lambda)(1+\mu^2)}{(\mu-\lambda)^2+\varepsilon^2}d\lambda\right]d\mu\\ &\equiv\int\frac{\xi(\mu)}{1+\mu^2}\Psi_\varepsilon(\mu)d\mu.\end{aligned}\tag{4.14}$$

By theorem 13 of [27] we know that since ψ' is integrable by hypothesis $\Psi_\varepsilon(\mu)$ converges to $(1+\mu^2)\psi'(\mu)$ as $\varepsilon\to 0+$. On the other hand since $|\psi'(\lambda)(1+\lambda^2)|\leq C'$, as before we get the estimate

$$\begin{aligned}|\Psi_\varepsilon(\mu)| &\leq C'\left\{\frac{\varepsilon}{\pi}\int\frac{d\lambda}{(\lambda-\mu)^2+\varepsilon^2}+\frac{\varepsilon}{\pi}\int\frac{d\lambda}{1+\lambda^2}\right\}\\ &= C'(1+\varepsilon)\leq 2C',\end{aligned}$$

and we have the result by dominated convergence theorem. ■

Finally we have the main theorem of this section. For this we define the modified Krein Class of complex-valued functions on $\mathbb{R}$

$$\tilde{\mathscr{K}} = \{\psi : \mathbb{R} \to \mathbb{C} : \varphi(\lambda) \equiv (1+\lambda^2)\psi(\lambda) \in \mathscr{K}\} \tag{4.15}$$

where $\mathscr{K}$ is the Krein class defined in (2.12).

Theorem 4.3. *Let $R_i - R_i^0 \in \mathscr{B}_1$ and $D(H) = D(H_0)$. Then for $\psi \in \tilde{\mathscr{K}}$, $\psi(H) - \psi(H_0) \in \mathscr{B}_1$ and*

$$\operatorname{Tr}[\psi(H) - \psi(H_0)] = \int \psi'(\lambda)\xi(\lambda)\mathrm{d}\lambda.$$

We need a lemma.

Lemma 4.4. Assume the hypotheses of theorem 4.3 and set $\psi^{(t)}(\lambda) = (\lambda^2+1)^{-1}(e^{it\lambda}-1)$ for $\lambda \in \mathbb{R}$ and $t \neq 0$. Then (i) $\psi^{(t)}$ is a C^1-function for $t \neq 0$ and $\psi^{(t)}(\lambda)(1+\lambda^2)$ and $\psi^{(t)\prime}(\lambda)(1+\lambda^2)$ are both bounded in λ. Furthermore, $|\psi^{(t)\prime}(\lambda)(1+\lambda^2)|/|t|^{-1} \leqslant 3$.

(ii) $\psi_\varepsilon^{(t)}(\lambda) = \mp\chi_\pm(t)\left[\dfrac{1-e^{i\lambda t}e^{-\varepsilon|t|}}{1+(\lambda \pm i\varepsilon)^2} \mp \varepsilon\dfrac{1-e^{-|t|}}{(\lambda - i)^2+\varepsilon^2}\right]$ *for $t > 0$ and $t < 0$ respectively and $\varepsilon > 0$, where $\chi_\pm$ are the indicator functions defined at the end of § 3.*

(iii) $\psi^{(t)}(H) - \psi^{(t)}(H_0) \in \mathscr{B}_1$ *and*

$$\|\psi^{(t)}(H) - \psi^{(t)}(H_0)\|_1 \leqslant (2\|R_i - R_i^0\|_1 + \|R_{-i} - R_{-i}^0\|_1)|t|.$$

(iv) $\psi_{\varepsilon}^{(t)}(H) - \psi_\varepsilon^{(t)}(H_0) \in \mathscr{B}_1$ *for every $\varepsilon > 0$, $t \neq 0$ and $\psi_\varepsilon^{(t)}(H) - \psi_\varepsilon^{(t)}(H_0)$ converges to $\psi^{(t)}(H) - \psi^{(t)}(H_0)$ in $\mathscr{B}_1$-norm as $\varepsilon \to 0+$.*

(v) $\operatorname{Tr}[\psi^{(t)}(H) - \psi^{(t)}(H_0)] = \int \psi^{(t)\prime}(\lambda)\xi(\lambda)\mathrm{d}\lambda$.

Proof. The part (i) follows by direct verification. For example, $\dfrac{\mathrm{d}\psi^{(t)}}{\mathrm{d}\lambda}(\lambda) = \dfrac{ite^{it\lambda}}{1+\lambda^2} - \dfrac{(e^{it\lambda}-1)2\lambda}{(\lambda^2+1)^2}$ so that

$$|\psi^{(t)\prime}(\lambda)(1+\lambda^2)| = \left|ite^{it\lambda} - \frac{2\lambda}{1+\lambda^2}(e^{it\lambda}-1)\right| \leqslant 3|t|.$$

To evaluate $\psi_\varepsilon^{(t)}(\lambda) \equiv \dfrac{\varepsilon}{\pi}\displaystyle\int \frac{\psi^{(t)}(\mu)}{(\mu-\lambda)^2+\varepsilon^2}\mathrm{d}\mu = \frac{\varepsilon}{\pi}\int \frac{e^{it\mu}-1}{(1+\mu^2)((\mu-\lambda)^2+\varepsilon^2)}\mathrm{d}\mu$, we employ the method of complex integration by taking a semi-circular contour of radius R about origin in the upper half complex plane (for $t > 0$). It is easy to see that the contribution to the integral from the semi-circular arc converges to 0 as $R \to \infty$ and what remains are the residues at the two enclosed simple poles viz, at $z = i$ and $= \lambda + i\varepsilon$. This leads to

$$\psi_\varepsilon^{(t)}(\lambda) = \frac{e^{i\lambda t - \varepsilon t}-1}{(\lambda+i\varepsilon)^2+1} + \varepsilon\frac{e^{-t}-1}{(\lambda-i)^2+\varepsilon^2} \quad \text{for} \quad t > 0.$$

For $t<0$, one has to take a semi-circular contour in the lower half plane and these two together lead to (ii).

By functional calculus, one writes

$$\begin{aligned}\psi^{(t)}(H)-\psi^{(t)}(H_0) &= R_i(e^{itH}-I)R_{-i}-R_i^0(e^{itH_0}-I)R_{-i}^0\\ &=(R_i-R_i^0)(e^{itH}-I)R_{-i}+R_i^0(e^{itH_0}-I)(R_{-i}-R_{-i}^0)\\ &\quad+R_i^0(e^{itH}-e^{itH_0})R_i\{(H-i)R_{-i}\}. \end{aligned}\qquad (4.16)$$

The first term in (4.16) can be written as $(R_i-R_i^0)\int_0^t e^{isH}(iHR_{-i})\mathrm{d}s$ and hence is in $\mathscr{B}_1$ and admits a trace-norm estimate $|t|\,\|R_i-R_i^0\|_1$. An identical consideration leads to a trace-norm estimate for the second term in (4.16) by $|t|\,\|R_{-i}-R_{-i}^0\|_1$. Since $D(H)=D(H_0)$, the third term in (4.16) can be written as in (2.6)

$$i\int_0^t e^{i(t-s)H_0}R_i^0VR_ie^{isH}\{(H-i)R_{-i}\}\,\mathrm{d}s.$$

Since $R_i^0VR_i=R_i^0-R_i\in\mathscr{B}_1$ and since $\|(H-i)R_{-i}\|=1$, by a reasoning similar to the discussion following the proof of theorem 2.1, we conclude that the above integral exists in $\mathscr{B}_1$-norm and its trace-norm can be estimated by $\|R_i-R_i^0\|_1|t|$. This proves (iii).

We prove (iv) for $t>0$, the case for $t<0$ being similar. That $\psi_\varepsilon^{(t)}(H)-\psi_\varepsilon^{(t)}(H_0)\in\mathscr{B}_1$ follows from (i) and theorem 4.2. By (ii) and functional calculus,

$$\begin{aligned}&[\psi_\varepsilon^{(t)}(H)-\psi_\varepsilon^{(t)}(H_0)]-[\psi^{(t)}(H)-\psi^{(t)}(H_0)]\\ &=\varepsilon(1-e^{-t})[R_{i+i\varepsilon}R_{i-i\varepsilon}-R_{i+i\varepsilon}^0R_{i-i\varepsilon}^0]\\ &\quad-[\{R_{i-i\varepsilon}R_{-i-i\varepsilon}-R_{i-i\varepsilon}^0R_{-i-i\varepsilon}^0\}-\{R_iR_{-i}-R_i^0R_{-i}^0\}]\\ &\quad+[e^{-\varepsilon t}\{R_{i-i\varepsilon}e^{itH}R_{-i-i\varepsilon}-R_{i-i\varepsilon}^0e^{itH_0}R_{-i-i\varepsilon}^0\}\\ &\qquad-\{R_ie^{itH}R_{-i}-R_i^0e^{itH_0}R_{-i}^0\}].\end{aligned}\qquad (4.17)$$

Now by the first and second resolvent identity (since $D(H)=D(H_0)$), we have

$$\begin{aligned}&\varepsilon[R_{i+i\varepsilon}R_{i-i\varepsilon}-R_{i+i\varepsilon}^0R_{i-i\varepsilon}^0]\\ &=\frac{1}{2i}\{(R_{i+i\varepsilon}-R_{i+i\varepsilon}^0)-(R_{i-i\varepsilon}-R_{i-i\varepsilon}^0)\}\\ &=\frac{1}{2i}[\{R_{i+i\varepsilon}(H-i)\}(R_i-R_i^0)\{(H_0-i)R_{i+i\varepsilon}^0\}\\ &\qquad-\{R_{i-i\varepsilon}(H-i)\}(R_i-R_i^0)\{(H_0-i)R_{i+i\varepsilon}^0\}]\end{aligned}$$

$\to 0$ in $\mathscr{B}_1$-norm as $\varepsilon\to 0$ since $(H+i)R_{-i\pm i\varepsilon}$ and $(H_0-i)R_{i\pm i\varepsilon}^0\to I$ in operator norm. This shows that the first term in (4.17) converges to 0 in $\mathscr{B}_1$ and the second term in (4.17) can similarly be shown to converge to 0 in $\mathscr{B}_1$. For the third term in (4.17) we again use the two resolvent identities to see that the result (iv) follows if

$$\|(R_{i\pm i\varepsilon}e^{itH}-R_{i\pm i\varepsilon}^0e^{itH_0})-(R_ie^{itH}-R_i^0e^{itH_0})\|_1\to 0$$

as $\varepsilon\to 0+$. But the above expression

$$\begin{aligned}&=\|\pm i\varepsilon[R_{i\pm i\varepsilon}e^{itH}R_i-R^0_{i\pm i\varepsilon}e^{itH_0}R^0_i]\|_1\\&=\varepsilon\|R_{i\pm i\varepsilon}e^{itH}(R_i-R^0_i)+\{R_{i\pm i\varepsilon}(H-i)\}R_i(e^{itH}-e^{itH_0})R^0_i\\&\quad+[\{R_{i\pm i\varepsilon}(H-i)\}(R_i-R^0_i)e^{itH_0}R^0_{i\pm i\varepsilon}]\|_1.\end{aligned}\tag{4.18}$$

Since $\|R_{i\pm i\varepsilon}\|$ and $\|(H-i)R_{i\pm i\varepsilon}\|$ are bounded in ε for ε sufficiently small, the contributions from the first and third terms are zero in the limit $\varepsilon\to 0$. For the second term in (4.18) we need only to observe from (2.6) that

$$R_i(e^{itH}-e^{itH_0})R^0_i=i\int_0^t e^{i(t-s)H}R_iVR^0_ie^{isH_0}\,\mathrm{d}s=\\-i\int_0^t e^{i(t-s)H}(R_i-R^0_i)e^{isH_0}\,\mathrm{d}s.$$

■

The part (v) follows from (iii), (iv) and theorem 4.2 (ii).

Proof of theorem 4.3. By (2.12) and (4.15),

$$\begin{aligned}\psi(\lambda)&=(\lambda^2+1)^{-1}\left[\int\frac{e^{it\lambda}-1}{it}\nu(\mathrm{d}t)+C\right]\\&=\int\frac{\psi^{(t)}(\lambda)}{it}\nu(\mathrm{d}t)+C(\lambda^2+1)^{-1}.\end{aligned}$$

It is clear that $(H^2+I)^{-1}-(H_0^2+I)^{-1}\in\mathscr{B}_1$. Also by lemma 4.4 (iii)

$$\left\|\int\frac{\psi^{(t)}(H)-\psi^{(t)}(H_0)}{it}\nu(\mathrm{d}t)\right\|_1\\\leqslant|\nu|(\mathbb{R})(2\|R_i-R^0_i\|_1+\|R_{-i}-R^0_{-i}\|_1),$$

and hence $\psi(H)-\psi(H_0)\in\mathscr{B}_1$. By theorem 4.1 (iv),

$$\begin{aligned}\mathrm{Tr}[(H^2+I)^{-1}-(H_0^2+I)^{-1}]&=\mathrm{Im\,Tr}[(H-i)^{-1}-(H_0-i)^{-1}]\\&=-\mathrm{Im}\int\frac{\xi(\lambda)}{(\lambda-i)^2}\mathrm{d}\lambda\\&=-\int\frac{2\lambda}{(\lambda^2+1)^2}\xi(\lambda)\mathrm{d}\lambda=\int(\mathrm{d}/\mathrm{d}\lambda)\{(\lambda^2+1)^{-1}\}\xi(\lambda)\mathrm{d}\lambda.\end{aligned}$$

On the other hand by lemma 4.4 (v),

$$\begin{aligned}\mathscr{I}&\equiv\mathrm{Tr}\int\frac{\psi^{(t)}(H)-\psi^{(t)}(H_0)}{it}\nu(\mathrm{d}t)\\&=\int\frac{\nu(\mathrm{d}t)}{it}\mathrm{Tr}[\psi^{(t)}(H)-\psi^{(t)}(H_0)]\\&=\int\frac{\nu(\mathrm{d}t)}{it}\int\psi^{(t)\prime}(\lambda)\xi(\lambda)\mathrm{d}\lambda.\end{aligned}$$

Since by theorem 4.1 (i), $\xi(\lambda)(1+\lambda^2)^{-1}\in L^1$ and by lemma 4.4 (i), $|\psi^{(t)'}(\lambda)(1+\lambda^2|\leqslant C|t|$, and since ν is a finite measure, we can interchange the order of integration in the above and get

$$\begin{aligned}\mathscr{I} &= \int \xi(\lambda)\mathrm{d}\lambda \int \frac{1}{it}\left\{\frac{ite^{it\lambda}}{\lambda^2+1} - \frac{2\lambda(e^{it\lambda}-1)}{(\lambda^2+1)^2}\right\}\nu(\mathrm{d}t)\\ &= \int \xi(\lambda)\mathrm{d}\lambda \frac{\mathrm{d}}{\mathrm{d}\lambda}\left[\int \frac{e^{it\lambda}-1}{it(\lambda^2+1)}\nu(\mathrm{d}t)\right].\end{aligned}$$

The interchange of differentiation and integration in the last step is justified since

$$\left|\frac{1}{it}\left\{\frac{ite^{it\lambda}}{\lambda^2+1} - \frac{2\lambda(e^{it\lambda}-1)}{(\lambda^2+1)^2}\right\}\right| \leqslant 3(\lambda^2+1)^{-1}$$

for all $t\neq 0$ and hence the concerned integral converges uniformly. This completes the proof. ∎

Remark 4.5(i). If $\psi\in\mathscr{S}(\mathbb{R})$, the Schwartz class of smooth function of rapid decrease at ∞, then so is $\varphi(\lambda)=\psi(\lambda)(1+\lambda^2)$ and thus by remark 2.7 (i) $\mathscr{S}(\mathbb{R})\subseteq\tilde{\mathscr{K}}$. Also all functions of the type $(\lambda-z)^{-m}$ (for integer $m\geqslant 1$) are in $\tilde{\mathscr{K}}$. Krein in his original work considered functions ψ admitting integral representation

$$\psi(\lambda)=\int(\lambda-z)^{-1}\mathrm{d}\mu(z), \tag{4.19}$$

where μ is complex measure on the set of non-real points in $\mathbb{C}$ satisfying for $z=x+iy$, $\int|y|^{-j}|\mathrm{d}\mu(z)|<\infty\,(j=1,2)$. A simple calculation as in the proof of theorem 3.3 (v) shows that since $\int\exp(-|ty|)|\mathrm{d}\mu(z)|<\infty$ for every $t\neq 0$, this class of functions are contained in $\tilde{\mathscr{K}}$.

(ii) Let J be a real open interval in $\rho(H)\cap\rho(H_0)$, and let $\psi\in C_0^\infty(J)$, the class of smooth functions with compact support in J. Then by functional calculus $\psi(H)=\psi(H_0)=0$ and hence by the trace formula in theorem 4.3,

$$\int\xi(\lambda)\psi'(\lambda)\mathrm{d}\lambda=0 \quad \forall \quad \psi\in C_0^\infty(J). \tag{4.20}$$

Since $\xi(\lambda)(1+\lambda^2)^{-1}\in L^1$, it follows that $\xi\in L^1_{\mathrm{loc}}(\mathbb{R})$ and hence as in remark 2.7 (iii), the equation (4.20) can be viewed as $\langle\xi',\psi\rangle=0$ for $\psi\in C_0^\infty(J)$ where ξ' is the distributional derivative and we conclude that ξ is a constant in J.

Thus if H and H_0 are bounded below, which happens for many Schrödinger operators ([1], [23]), the shift function is constant in the neighbourhood of $-\infty$ and can be chosen to be zero there.

5. Applications

First of all we want to mention the relation between the spectral shift function and scattering theory. One of the earliest results in this direction is due to Birman and Krein [7]. More details can be found in ([20], [5]).

Let H and H_0 be self-adjoint and let $R_z - R_z^0 \in \mathscr{B}_1$ for some $z \in \rho(H) \cap \rho(H_0)$. Define wave operators $\Omega_\pm$ (if they exist) as:

$$\Omega_\pm(H, H_0) \equiv \Omega_\pm = s - \lim_{t \to \pm\infty} e^{iHt} e^{-iH_0 t} E_{ac}^0, \tag{5.1}$$

where E_{ac}^0 is the projection onto the absolutely continuous subspace of H_0. If $\Omega_\pm$ exist, then they are partial isometries with initial set $E_{ac}^0 \mathscr{H}$ and final set closed subspaces of $E_{ac}\mathscr{H}$, and satisfy the intertwining property:

$$\Omega_\pm H_{0,ac} = H_{ac} \Omega_\pm, \tag{5.2}$$

where H_{ac} and $H_{0,ac}$ are the absolutely continuous parts of H and H_0 respectively, and E_{ac} is the projection onto the absolutely continuous subspace of $\mathscr{H}$. The wave operators are said to be *complete* if their final sets are both $E_{ac}\mathscr{H}$ i.e. if

$$\text{Range}\,\Omega_+ = \text{Range}\,\Omega_- = E_{ac}\mathscr{H}. \tag{5.3}$$

If $\Omega_\pm$ exist and are complete, then one defines the *scattering operator* S:

$$S = \Omega_+^* \Omega_-, \tag{5.4}$$

and observes that S commutes with H_0 and $SS^* = S^*S = E_{ac}^0$. In such a case, $E_{ac}^0\mathscr{H}$ admits a direct integral representation (upto unitary isomorphism) [11]:

$$E_{ac}^0 \mathscr{H} = \int^\oplus \mathscr{H}_\lambda \mathrm{d}\lambda,$$

so that

$$H_{0,ac} = \int^\oplus \lambda \mathrm{d}\lambda \text{ and} \tag{5.5}$$

$$S = \int^\oplus S(\lambda) \mathrm{d}\lambda.$$

For almost all λ, $S(\lambda)$ is a unitary operator in $\mathscr{H}_\lambda$ and is called the *scattering matrix* or on-shell scattering operator. One can also define a self-adjoint operator-valued function $\Pi(\lambda)$ (called the *phase shift*) such that

$$S(\lambda) = \exp(-2\pi i \Pi(\lambda)). \tag{5.6}$$

We now state a theorem (without proof) which is typical of scattering theory and also relates the shift function ξ with the phase shift operator $\Pi(\lambda)$ in (5.6).

Theorem 5.1. *Let $R_z - R_z^0 \in \mathscr{B}_1$ for some z in $\rho(H) \cap \rho(H_0)$. Then the wave operators $\Omega_\pm$ in (5.1) exist and are complete. Furthermore, $\Pi(\lambda) \in \mathscr{B}_1(\mathscr{H}_\lambda)$ for almost all λ, $\xi(\lambda) = Tr(\Pi(\lambda))$ so that*

$$\det S(\lambda) = \exp(-2\pi i \xi(\lambda)), \tag{5.7}$$

where $\xi(\lambda)$ is the spectral shift function obtained in theorem 4.1.

For an introduction to scattering theory and a proof of the above theorem, the reader is referred to [1] and [5].

The expression (5.7) and the trace formula in theorem 4.3 has found applications in many areas. As an example, one may mention the derivation of the Eisenbud-Wigner relation between the average time-delay in a scattering process and the (distributional) derivative of the associated shift function $\xi(\lambda)$ [15].

In a series of papers the authors of [6] and [13] used the trace formula, in particular (2.17) appearing in remark 2.7 (v), to compute the Witten index in super-symmetric quantum mechanics. A typical theorem which we state without proof, is the following.

Theorem 5.2. *Let A be a closed operator in $\mathscr{H}$ such that $\exp(-A^*A)-\exp(-AA^*)$ is trace-class. If we assume that the associated shift function $\xi(\lambda)$ is right continuous at 0 and if we define the Witten index $W(A)\equiv\lim_{t\to\infty}\mathrm{Tr}(e^{-tA^*A}-e^{-tAA^*})$, then $W(A)=-\xi(0+)$.*

From the remark 2.7 (v), it is clear that $[\exp(-tA^*A)-\exp(-tAA^*)]\in\mathscr{B}_1$ for all $t>2$ and

$$\mathrm{Tr}[(\exp(-tA^*A)-\exp(-tAA^*))]=-t\int_0^\infty -e^{-t\lambda}\xi(\lambda)\mathrm{d}\lambda.$$

Then the result of theorem 5.2 follows from this expression and the hypothesis of right continuity. Under further assumptions, the authors in [13] prove an invariance property of the index for a class of perturbations.

Another interesting application is in relation to a pair of projections P, Q in a Hilbert space $\mathscr{H}$. An ordered pair of projections (P,Q) is said to be a *Fredholm pair* if $G\equiv QP$: Range $P\to$ Range Q is Fredholm i.e. if $\mathscr{R}(G)\equiv$ Range G is closed and if $\mathscr{N}(G)(\equiv$ the null space of $G)$ and $\mathscr{R}(G)$ have finite dimension and co-dimension respectively. In such a case, we define the index of the pair

$$\mathrm{Ind}(P,Q)\equiv\dim\mathscr{N}(G)-\dim\mathscr{R}(G)^{\perp}.$$

Then the following theorem ([2], [3]) can be proven.

Theorem 5.3. *Set $\mathscr{H}_{mn}(m,n=0,1)\equiv\{f\in\mathscr{H}\,|\,Pf=mf, Qf=nf\}$.*

(i) *If (P,Q) is a Fredholm pair, then $m_1=\dim\mathscr{H}_{10}$ and $m_{-1}=\dim\mathscr{H}_{01}$ are finite and*

$$\mathrm{Ind}(P,Q)=\dim\mathscr{H}_{10}-\dim\mathscr{H}_{01}\equiv m_1-m_{-1}.$$

(ii) *If $A\equiv P-Q\in\mathscr{B}_1$, then (P,Q) is a Fredholm pair and $A^{2n+1}\in\mathscr{B}_1$ for all positive integer n and $\mathrm{Tr}\,A^{2n+1}=\mathrm{Tr}\,A=\mathrm{Ind}(P,Q)=m_1-m_{-1}$, an integer.*

(iii) *If $A\in\mathscr{B}_1$, then the perturbation determinant $\Delta(z)$ (for $\mathrm{Im}\,z\neq 0$) is given as*

$$\Delta(z)=\left(\frac{z-1}{z}\right)^{m_1-m_{-1}}.$$

The shift function ξ in this case is given by

$$\xi(\lambda)=\begin{cases}0 & \text{if } \lambda\notin[0,1]\\ m_1-m_{-1} & \text{if } \lambda\in[0,1].\end{cases}$$

These results find application in the study of charge transport phenomenon in integer Hall effect [4] and a proof of the above theorem and its generalizations can be found in [2]. A recent survey of some further applications of the trace formula can be found in the lecture notes of Simon [24].

Appendix

In the first part we state some of the standard results on boundary values of functions analytic in half-plane and unit disc. These have been used in §2 and §4. Next we define the perturbation determinant and study some of its properties.

Theorem A.1. *Let $F(z)$ be analytic in the open upper half plane $\{z:\operatorname{Im} z>0\}$ with $0\leqslant \operatorname{Im} F(z)\leqslant C$ for some constant C, and $|F(z)|=O\left(\frac{1}{\operatorname{Im} z}\right)$ as $\operatorname{Im} z\to\infty$. Then there exists a unique real valued L^1 function ζ on $\mathbb{R}$ given by $\zeta(\lambda)=(1/\pi)\lim_{\varepsilon\to 0+}\operatorname{Im} F(\lambda+i\varepsilon)$ for almost all λ(Lebesgue) such that*

$$F(z)=\int_{-\infty}^{\infty}\frac{\zeta(\lambda)}{\lambda-z}\mathrm{d}\lambda.$$

Such a function F, analytic in the open upper half plane such that $\operatorname{Im} F(z)\geqslant 0$, is called a Herglotz function. A Herglotz function F satisfying $|F(z)|=O\left(\frac{1}{\operatorname{Im} z}\right)$ as $\operatorname{Im} z\to\infty$ admits the following representation (see theorem B3 of [29]): $F(z)=\int_{-\infty}^{\infty}\frac{\mathrm{d}\sigma(\lambda)}{\lambda-z}$, where σ is a right continuous non-decreasing bounded function on $\mathbb{R}$. The further restriction $\operatorname{Im} F(z)\leqslant C$ leads to the absolute continuity of σ such that $\zeta(\lambda)$ ($\equiv\sigma'(\lambda)$ a.e.) is integrable.

Theorem A.2. *Let $G(\omega)$ be analytic in open unit disc $|\omega|<1$ and let $0\leqslant \operatorname{Im} G(\omega)\leqslant C$ for some constant C. Then there exists a real valued function η in $L^1[-\pi,\pi]$ such that*

$$G(\omega)=\operatorname{Re} G(0)+\frac{i}{2}\int_{-\pi}^{\pi}\frac{e^{i\alpha}+\omega}{e^{i\alpha}-\omega}\eta(\alpha)\mathrm{d}\alpha,$$

and

$$\eta(\alpha)=(1/\pi)\lim_{\rho\uparrow 1}\operatorname{Im} G(\rho e^{i\alpha}) \text{ for almost all } \alpha.$$

For a proof of this, see for example pages 189–198 of [21].

In analogy with the case of operators in finite dimensional Hilbert space or of finite rank operators in infinite dimensional Hilbert space, the determinant of $(I+A)$ for $A\in\mathscr{B}_1$, is defined as:

$$\det(I+A)\equiv\prod_{j=1}^{\infty}(1+\lambda_j(A)), \tag{A.1}$$

where $\lambda_j(A)$'s are the eigenvalues of A counted as many times as their multiplicities.

The above definition makes sense since $\Sigma_{j=1}^{\infty}|\lambda_j(A)| \leqslant \|A\|_1$ for $A\in\mathscr{B}_1$. The following properties of determinant can be proven (see [14] for further details).

Theorem A.3. *Let $A\in\mathscr{B}_1$, and let $\{\lambda_j(A)\}$ be the eigenvalues of A. Then*

(i) $\det(I+A)=\exp[\int_\Gamma dz \operatorname{Tr}\{A(I+zA)^{-1}\}]$, *where Γ is a rectifiable path in $\mathbb{C}$ joining 0 and 1 such that none of the points $\{-\lambda_j(A)^{-1}\}$ lies on Γ,*

(ii) *given $\varepsilon>0$ there exists $\delta>0$ such that for every $B\in\mathscr{B}_1$ with $\|A-B\|_1<\delta$, $|\det(I+A)-\det(I+B)|<\varepsilon$, i.e. $A\to\det(I+A)$ is continuous in $\mathscr{B}_1$-norm.*

(iii) *If $B\in\mathscr{B}_1$, then*

$$\det[(I+A)(I+B)]=\det(I+A)\cdot\det(I+B).$$

(iv) $|\det(I+A)|\leqslant e^{\|A\|_1}$.

(v) *For every unitary operator S,* $\det(I+A)=\det(I+SAS^{-1})$.

Proof. Since A is compact, the intersection of the set $\{-\lambda_j(A)^{-1}\}$ with any bounded subset of $\mathbb{C}$ is finite (could be empty). For $z\in\mathbb{C}$, define

$$D(z)\equiv\det(I+zA)=\begin{cases}\prod_{j=1}^{\infty}(1+z\lambda_j(A)) & \text{if } z\neq-\lambda_j(A)^{-1} \text{ for any } j,\\ 0 & \text{if } z=-\lambda_j(A)^{-1} \text{ for some } j.\end{cases}$$

Then $D(z)$ is analytic in the complex plane with zeros accumulating at infinity. Taking the logarithmic derivative, at points away from these zeros,

$$\frac{D'(z)}{D(z)}=\sum_{j=1}^{\infty}\frac{\lambda_j(A)}{1+z\lambda_j(A)}=\operatorname{Tr}A(I+zA)^{-1}. \tag{A.2}$$

Let Γ be a rectifiable curve in $\mathbb{C}$ joining 0 and 1 such that none of $-\lambda_j(A)^{-1}$'s lie on Γ Integrating both the sides over Γ and then taking the exponential we get the required result. Apriori it seems, the integral depends on the path. But if we extend Γ to a closed contour by taking another rectifiable curve Γ' (say) from 1 to 0 such that none of the $-\lambda_j(A)^{-1}$'s lie on Γ', then $\operatorname{Int}(\Gamma\cup\Gamma')$ contains at most finitely many $-\lambda_j(A)^{-1}$, say $-\lambda_1(A)^{-1}, -\lambda_2(A)^{-1},\ldots,-\lambda_k(A)^{-1}$. Then the integration over $\Gamma\cup\Gamma'$ has the contribution $\Sigma_{j=1}^{k}2\pi i m_j$, where m_j is the multiplicity of $\lambda_j(A)$, which equals identity on exponentiation. This proves (i).

By the resolvent identity

$$(I+zA)^{-1}-(I+zB)^{-1}=z(I+zA)^{-1}(B-A)(I+zB)^{-1}$$

or

$$(I+zB)^{-1}=[I+z(I+zA)^{-1}(B-A)]^{-1}(I+zA)^{-1}.$$

If $B\in\mathscr{B}_1$ be such that

$$\|B-A\|_1\leqslant\min_{z\in\Gamma}\{|z|\|(I+zA)^{-1}\|\}^{-1}, \tag{A.3}$$

then $[I+z(I+zA)^{-1}(B-A)]^{-1}$ exists as a Neumann series, and

$$\sup_{z\in\Gamma}\|(I+zB)^{-1}\|\leqslant C\sup_{z\in\Gamma}\|(I+zA)^{-1}\|, \tag{A.4}$$

where the constant C depends only on Γ and A. Let $L(\Gamma)$ be the length of the arc Γ. Since

$$\|A(I+zA)^{-1}-B(I+zB)^{-1}\|_1=\|(I+zB)^{-1}(A-B)(I+zA)^{-1}\|_1 \leqslant \|(I+zB)^{-1}\|\,\|A-B\|_1\,\|(I+zA)^{-1}\|,$$

it follows from (A.4) that for any $\kappa>0$, there exists a $\delta>0$ such that

$$\begin{aligned}\left|\int_\Gamma \operatorname{Tr} A(I+zA)^{-1}-B(I+zB)^{-1}\}\mathrm{d}z\right| &\leqslant \int_\Gamma \|A(I+zA)^{-1}-B(I+zB)^{-1}\|_1\mathrm{d}z\\ &\leqslant L(\Gamma)C\left\{\sup_{z\in\Gamma}\|(I+zA)^{-1}\|\right\}^2\|A-B\|_1\\ &<\kappa\end{aligned}$$

whenever $\|A-B\|_1<\delta$. Using the inequality $|e^z-1|\leqslant\sqrt{2}e^{|z|}|z|$, and choosing κ sufficiently small we get

$$\begin{aligned}&|\det(I+B)-\det(I+A)|\\ &=\left|\exp\left[\int_\Gamma \mathrm{d}z\operatorname{Tr}\{B(I+zB)^{-1}\}\right]-\exp\left[\int_\Gamma \mathrm{d}z\operatorname{Tr}\{A(I+zA)^{-1}\}\right]\right|\\ &\leqslant\left|\exp\left[\int_\Gamma \mathrm{d}z\operatorname{Tr}\{A(I+zA)^{-1}\}\right]\right|\\ &\qquad\left|\exp\left[\int_\Gamma \mathrm{d}z\operatorname{Tr}\{B(I+zB)^{-1}-A(I+zA)^{-1}\}\right]-1\right|\\ &\leqslant\sqrt{2}e\kappa|\det(I+A)|\end{aligned}$$

which can be made arbitrarily small by choosing δ appropriately.

Let $\{P_n\}$ be a sequence of finite rank projections such that $P_n\uparrow I$. Then P_nAP_n and P_nBP_n converges to A and B respectively in $\mathscr{B}_1$-norm as $n\to\infty$. Hence

$$\begin{aligned}&(I+P_nAP_n)(I+P_nBP_n)-(I+A)(I+B)\\ &\qquad=(P_nAP_n-A)+(P_nBP_n-B)+P_nAP_nBP_n-AB\to 0\end{aligned}$$

in $\mathscr{B}_1$-norm as $n\to\infty$. Note that

$$\det(I+P_nAP_n)=\det(P_n+P_nAP_n),$$

where the determinant on the right hand side is taken on the finite dimensional Hilbert space $P_n\mathscr{H}$. By (ii),

$$\begin{aligned}&\det[(I+A)(I+B)]\\ &\quad=\lim_{n\to\infty}\det[(I+P_nAP_n)(I+P_nBP_n)]\end{aligned}$$

$$= \lim_{n\to\infty} \det[(P_n + P_nAP_n)(P_n + P_nBP_n)]$$

$$= \lim_{n\to\infty} \det(P_n + P_nAP_n)\det(P_n + P_nBP_n)$$

$$= \lim_{n\to\infty} \det(I + P_nAP_n)\det(I + P_nBP_n)$$

$$= \det(I + A)\det(I + B),$$

which proves (iii). By (A.1), and the inequality $1 + x < e^x$ for $x > 0$, we get

$$|\det(I + A)| \leqslant \prod_{j=1}^{\infty} (1 + |\lambda_j(A)|)$$

$$\leqslant \exp\left(\sum_{j=1}^{\infty} |\lambda_j(A)|\right)$$

$$\leqslant e^{\|A\|_1}.$$

Since $\sigma(A) = \sigma(SAS^{-1})$ for any unitary operator S, part (v) follows from (A.1). ■

Next we define the perturbation determinants for two explicit cases and study some of their properties.

Case I. Let H be a self-adjoint operator in $\mathscr{H}$. Assume that V_1 and V_2 are two trace class self-adjoint operators, so that $H_j = H + V_j$ are self-adjoint for $j = 1, 2$. For $\operatorname{Im} z \neq 0$, define the perturbation determinants

$$\left.\begin{aligned} \Delta_j(z) &\equiv \det[I + V_j(H - z)^{-1}] \quad \text{for } j = 1, 2, \\ \Delta_{2,1}(z) &\equiv \det[I + (V_2 - V_1)(H_1 - z)^{-1}]. \end{aligned}\right\} \tag{A.5}$$

Case II. Let U, U_1 and U_2 be three unitary operators in $\mathscr{H}$ such that $U_j - U \in \mathscr{B}_1$ for $j = 1, 2$. For complex ω with $|\omega| < 1$ define the perturbation determinants

$$\left.\begin{aligned} \Delta_j(\omega) &\equiv \det[I + (U_j - U)(U - \omega)^{-1}] \quad \text{for } j = 1, 2, \\ \Delta_{2,1} &\equiv \det[(I + (U_2 - U_1)(U_1 - \omega)^{-1}]. \end{aligned}\right\} \tag{A.6}$$

We start with the following abstract result.

Lemma A.4. *Let $z \to A(z)$ be a $\mathscr{B}_1$-valued analytic function in some domain D in* C. *Then $\det(I + A(z))$ is analytic in D. For all z for which $(I + A(z))^{-1} \in \mathscr{B}(\mathscr{H})$, $\ln\det(I + A(z))$ is an analytic function and*

$$\frac{\mathrm{d}}{\mathrm{d}z} \ln\det(I + A(z)) = \operatorname{Tr}\left\{(I + A(z))^{-1} \frac{\mathrm{d}A(z)}{\mathrm{d}z}\right\}.$$

Proof. As in the proof of theorem A.3, we choose an increasing sequence of finite dimentional projections $\{P_n\}$ and view $P_n + P_nA(z)P_n$ as acting in $P_n\mathscr{H}$. Then for every $z \in D$,

$$\begin{aligned}\Delta(z) &= \det(I + A(z)) \\ &= \lim_{n\to\infty} \det(I + P_n A(z) P_n) \\ &= \lim_{n\to\infty} \det(P_n + P_n A(z) P_n) \\ &\equiv \lim_{n\to\infty} \Delta_n(z).\end{aligned}$$

Since $A(z)$ is $\mathscr{B}_1$-analytic in D, $\Delta_n(z)$ is analytic for each n and by theorem A.3 (iv), $|\Delta_n(z)| \leqslant \exp(\|A(z)\|_1) \leqslant M$. This and Cauchy's integral formula implies equicontinuity of $\{\Delta_n(z)\}$, and by Ascoli's theorem (relabelling the consequent subsequence) we conclude that $\Delta_n(z)$ converges to $\Delta(z)$ as $n \to \infty$ uniformly in z in compact subsets of D and consequently $\Delta(z)$ is analytic.

Set $A_n(z) = P_n A(z) P_n$ and let $(I + A(z_0))^{-1} \in \mathscr{B}(\mathscr{H})$ for some $z_0 \in D$. Then there is an open ball $\mathscr{U}$ about z_0 such that $(I + A(z))^{-1} \in \mathscr{B}(\mathscr{H})$ for all $z \in \mathscr{U}$. Thus $\Delta(z) \neq 0$ and hence $\ln \Delta(z)$ is analytic in $\mathscr{U}$. Since $\Delta_n(z)$ converges to $\Delta(z)$ uniformly in $\tilde{\mathscr{U}}$ (a closed ball in $\mathscr{U}$), $\Delta_n(z) \neq 0$ for $z \in \tilde{\mathscr{U}}$ and $n > N$ (depending on $\tilde{\mathscr{U}}$ only). By the spectral theory of compact operators, we have that $(I + A_n(z))^{-1} \in \mathscr{B}(\mathscr{H})$ or equivalently $(P_n + A_n(z))^{-1} \in \mathscr{B}(P_n \mathscr{H})$ and therefore $\ln \Delta_n(z)$ is analytic for such n and z. For finite dimensional determinants, the formula in this lemma is well known and we have for all n and z as above,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}z} \ln \Delta_n(z) &= \frac{\Delta_n'(z)}{\Delta_n(z)} \\ &= \mathrm{Tr}\left[(P_n + A_n(z))^{-1} \frac{\mathrm{d}A_n(z)}{\mathrm{d}z}\right] \\ &= \mathrm{Tr}\left[(I + A_n(z))^{-1} \frac{\mathrm{d}A_n(z)}{\mathrm{d}z}\right].\end{aligned} \tag{A.7}$$

For such z and n one has the identity:

$$(I + A_n(z))^{-1} - (I + A(z))^{-1} = (I + A_n(z))^{-1}\{A(z) - A_n(z)\}(I + A(z))^{-1}.$$

This implies that for fixed $z \in \tilde{\mathscr{U}}$, $\|(I + A_n(z))^{-1}\| \leqslant M(z)$ and $(I + A_n(z))^{-1}$ converges to $(I + A(z))^{-1}$ as $n \to \infty$ in $\mathscr{B}_1$. Since $\frac{\mathrm{d}A(z)}{\mathrm{d}z} \in \mathscr{B}_1$, it follows that $\frac{\mathrm{d}A_n(z)}{\mathrm{d}z}$ converges to $\frac{\mathrm{d}A(z)}{\mathrm{d}z}$ in $\mathscr{B}_1$ and hence the right hand side of (A.7) converges pointwise in $\tilde{\mathscr{U}}$ to $\mathrm{Tr}\left[(I + A(z))^{-1} \frac{\mathrm{d}A(z)}{\mathrm{d}z}\right]$. As for the left hand side of (A.7) we need only to use Cauchy's integral formula to conclude that $\Delta_n'(z)$ converges to $\Delta'(z)$ as $n \to \infty$. ■

Theorem A.5. (i) *Let $\Delta_{2,1}(z)$, $\Delta_j(z)$ $(j=1,2)$ be the perturbation determinants given by (A.5). Then they are analytic for $\mathrm{Im}\, z \neq 0$ and have no zeroes there. Furthermore $\Delta_{2,1}(z)\Delta_1(z) = \Delta_2(z)$ and*

$$\frac{\mathrm{d}}{\mathrm{d}z} \ln \Delta_j(z) = -\operatorname{Tr}\{(H_j - z)^{-1} - (H-z)^{-1}\} \tag{A.8}$$

for $j = 1, 2$.

(ii) *The perturbation determinants $\Delta_{2,1}(\omega)$, $\Delta_j(\omega)$, $(j=1,2)$, given by (A.6) are analytic for all complex number ω with $|\omega| < 1$ and have no zeros. Furthermore $\Delta_{2,1}(\omega)\Delta_1(\omega) = \Delta_2(\omega)$ and*

$$\frac{\mathrm{d}}{\mathrm{d}\omega} \ln \Delta_j(\omega) = -\operatorname{Tr}[(U_j - \omega)^{-1} - (U-w)^{-1}] \tag{A.9}$$

for $j = 1, 2$.

Proof. We shall only prove (i) since the proof of (ii) is identical.

Since for $\mathrm{Im}\, z \neq 0$, $(H-z)^{-1}$ is analytic in $\mathscr{B}(\mathscr{H})$, so $V_j(H-z)^{-1}$ is analytic in $\mathscr{B}_1$. Hence by lemma A.4, $\Delta_j(z)$ is analytic in the same domain. Furthermore for $\mathrm{Im}\, z \neq 0$ and $f \in \mathscr{H}$, $[I + V_j(H-z)^{-1}]f = (H_j - z)(H-z)^{-1} f = 0$ implies $f = 0$ since z belongs to $\rho(H) \cap \rho(H_j)$. Thus, $\Delta_j(z)$ has no zeros there. Hence by theorem A.4, $\ln \Delta_j(z)$ is analytic for $\mathrm{Im}\, z \neq 0$, and

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}z} \ln \Delta_j(z) &= \operatorname{Tr}\left[[1 + V_j(H-z)^{-1}]^{-1} \frac{\mathrm{d}}{\mathrm{d}z} \{V_j(H-z)^{-1}\} \right] \\
&= \operatorname{Tr}[\{I - V_j(H_j - z)^{-1}\} V_j(H-z)^{-2}] \\
&= \operatorname{Tr}[(H-z)^{-1}\{I - V_j(H_j - z)^{-1}\} V_j(H-z)^{-1}] \\
&= \operatorname{Tr}[(H_j - z)^{-1} V_j(H-z)^{-1}] \\
&= -\operatorname{Tr}\{(H_j - z)^{-1} - (H-z)^{-1}\}.
\end{aligned}$$

Next by theorem A.3 (iii),

$$\begin{aligned}
&\Delta_{2,1}(z)\Delta_1(z) \\
&= \det[I + (V_2 - V_1)(H_1 - z)^{-1}] \cdot \det[I + V_1(H-z)^{-1}] \\
&= \det[\{I + (V_2 - V_1)(H_1 - z)^{-1}\}\{I + V_1(H-z)^{-1}\}] \\
&= \det[I + (V_2 - V_1)\{(H_1 - z)^{-1} + (H_1 - z)^{-1} V_1(H-z)^{-1}\} + V_1(H-z)^{-1}] \\
&= \det[I + (V_2 - V_1)(H-z)^{-1} + V_1(H-z)^{-1}] \\
&= \det[1 + V_2(H-z)^{-1}] \\
&= \Delta_2(z).
\end{aligned}$$

■

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