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Abstract

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ON PERTURBATION DETERMINANTS AND THE TRACE FORMULA FOR UNITARY AND SELF-ADJOINT OPERATORS

(Presented by Academician V. I. Smirnov on 5 I 1962)

1. In what follows $\mathfrak{H}$ denotes a separable Hilbert space, $\mathfrak{R}$ the linear ring of all bounded operators acting in $\mathfrak{H}$, and $\mathfrak{S}$ the two-sided ideal in $\mathfrak{R}$ consisting of all nuclear operators, i.e., of all completely continuous operators A such that

$$\operatorname{Sp}|A| = \operatorname{Sp}(A^*A)^{1/2} < \infty.$$

For $A \in \mathfrak{S}$ the two functionals $\operatorname{Sp} A$ and $\det(I + A)$ are meaningful.

If G is a domain in the complex plane, A_z $(z \in G)$ is a holomorphic operator-valued function with values in $\mathfrak{S}$, and $\Delta(z) = \det(I + A_z)$, then at any point $z \in G$ for which $\Delta(z) \neq 0$ the formula

$$\Delta'(z)/\Delta(z) = \operatorname{Sp}[(I + A_z)^{-1}(dA_z/dz)]$$

holds.

Let A be a linear operator with domain of definition $\mathfrak{D}(A) \subset \mathfrak{H}$ and with nonempty set $\rho(A)$ of all regular points (i.e., all complex points z for which there exists a resolvent $R_z(A) = (A - zI)^{-1} \in \mathfrak{R}$). If B is another linear operator with $\mathfrak{D}(B) = \mathfrak{D}(A)$ and, at least at one point $z \in \rho(A)$, the condition

$$(B - A)R_z(A) \in \mathfrak{S}$$

is satisfied, then this condition will be satisfied for all $z \in \rho(A)$, and for these z the perturbation determinant is meaningful:

$$\Delta_{B/A}(z) = \det[(B - zI)(A - zI)^{-1}] = \det[I + (B - A)R_z(A)], \tag{1}$$

which is a holomorphic function on each connected component of $\rho(A)$. From formula (1) it follows that at points $z \in \rho(A)$ for which $\Delta_{B/A}(z) \neq 0$:

$$\frac{d}{dz}\Delta_{B/A}(z)/\Delta_{B/A}(z) = \operatorname{Sp}[R_z(A) - R_z(B)] \quad \text{for } z \in \rho(A) \cap \rho(B). \tag{2}$$

Perturbation determinants for various pairs of operators A, B have been used in various works of the author (^{1,2}). Apparently, without knowing of these works, Sh. T. Kuroda (^{3}) came to the consideration of perturbation determinants. He considered the properties of $\Delta_{B/A}(z)$ for the case of two closed linear operators A, B, for which $\mathfrak{D}(A) = \mathfrak{D}(B)$ is dense in $\mathfrak{H}$. In this case one may assert (^{4}) that if certain connected components $G(A) \subset \tilde{\rho}(A)$ and $G(B) \subset \tilde{\rho}(B)$ have a common point, then $G(A) = G(B)$, and on $G(A)$ the function $\Delta_{B/A}(z)$ is a meromorphic function, where the order of $\Delta_{B/A}(z)$ at any point $z \in G(A)$ is computed in a natural way (^{1,3}). Here $\tilde{\rho}(A)$ ($\tilde{\rho}(B)$) denotes the set of complex points consisting of $\rho(A)$ ($\rho(B)$) and all isolated points of the spectrum of the operator A (B) that are eigenvalues of A (B) of finite algebraic multiplicity.

In a plenary lecture at the IV All-Union Mathematical Congress (6 VII 1961) the author indicated that in known cases the notion of a generalized perturbation determinant $\widetilde{\Delta}_{B/A}(z)$ may be introduced. For example, this is possible when the operators A and B are **resolvent comparable**, i.e., when the set $\rho = \rho(A) \cap \rho(B)$ is nonempty and, at least for one point $z \in \rho$ (and then for all $z \in \rho$),

$$R_z(B) - R_z(A) \in \mathfrak{S}.$$

In this case, choosing

arbitrary $z_0 \in \rho$, one may set $\widetilde{\Delta}_{B/A}(z) = \Delta_{B_0/A_0}(z)$, where $A_0 = R_{z_0}(A)$, $B_0 = R_{z_0}(B)$.

It is not difficult to show that, up to a multiplicative constant, the determinant $\Delta_{B/A}(z)$ does not depend on the choice of the point $z_0 \in \rho$; for $z \in \rho$, (2) will again hold with Δ replaced by $\widetilde{\Delta}$.

2. All assertions of Theorem 1 were established already in (^{2}), except for the last of them, which contains a positive answer to the question posed in (^{2}) (p. 618).

Theorem 1. *Let H_1 be a self-adjoint operator, $V \in \mathfrak{S}$, $H_2 = H_1 + V$, and $\Delta(z) = \Delta_{H_2/H_1}(z)$. Then, under the corresponding definition of* $\ln \Delta(z)$*,*

$$\ln \Delta(z) = \int_{-\infty}^{\infty} \frac{\xi(\lambda)}{\lambda - z}\, d\lambda \qquad (\operatorname{Im} z \neq 0), \tag{3}$$

where $\xi(\lambda)$ is a real measurable function, and moreover

$$1) \int_{-\infty}^{\infty} |\xi(\lambda)|\, d\lambda \leq \operatorname{Sp} |V|; \qquad 2) \int_{-\infty}^{\infty} \xi(\lambda)\, d\lambda = \operatorname{Sp} V. \tag{4}$$

If the operator V has in all p positive (in all q negative) eigenvalues, then almost everywhere $\xi(\lambda) \leq p$ ($\xi(\lambda) \geq -q$). In particular, if the operator V is nonnegative, then almost everywhere $\xi(\lambda) \geq 0$. For any complex-valued continuously differentiable function $\Phi(\lambda)$ $(-\infty < \lambda < \infty)$ such that

$$\Phi(\lambda) = \int_{-\infty}^{\infty} e^{i\lambda t}\, d\omega(t), \qquad \int_{-\infty}^{\infty} |t|\, |d\omega(t)| < \infty, \tag{5}$$

one always has $\Phi(H_2) - \Phi(H_1) \in \mathfrak{S}$, *and the trace formula is valid*

$$\operatorname{Sp}\,[\Phi(H_2) - \Phi(H_1)] = \int_{-\infty}^{\infty} \xi(\lambda)\Phi'(\lambda)\, d\lambda. \tag{6}$$

Formula (3) was first discovered by I. M. Lifshits (^{5}) in connection with certain questions in the quantum theory of crystals (see also his survey (^{6})). In deriving this formula, the author mentioned assumed that V is a finite-dimensional operator, and imposed a number of smoothness requirements on the spectral function $E(\lambda)$ of the operator H_1 (moreover, when a discrete spectrum appeared in H_2, I. M. Lifshits wrote formula (3) in another form).

3. All assertions of Theorem 1 have their analogues in the theory of unitary operators. In particular, the following holds:

Theorem 2. *Let* U_1 *and* U_2 *be two unitary operators, with* $U_2 - U_1 \in \mathfrak{S}$. *Then, up to an additive constant, there exists a unique real function* $\eta(t) \in L_1(-\pi, \pi)$ *such that*

$$\operatorname{Sp}\,[\Psi(U_2) - \Psi(U_1)] = \int_{-\pi}^{\pi} \eta(t)\, d\Psi(e^{it}), \tag{7}$$

where $\Psi(\xi)$ $(|\xi| = 1)$ *is any function admitting an expansion*

$$\Psi(\xi) = \sum_{n=-\infty}^{\infty} c_n \xi^n, \qquad \sum_{n=-\infty}^{\infty} |nc_n| < \infty. \tag{8}$$

The function $\eta(t)$ *can be obtained from the formula*

$$\eta(t) = \frac{1}{\pi} \lim_{\rho \uparrow 1} \arg \Delta_{U_2/U_1}(\rho e^{it}) + \text{const} \quad \text{(almost everywhere).} \tag{9}$$

We shall give some explanations concerning the proof of the theorem. If $U_2 - U_1 \in \mathfrak{S}$, then $U_2 = U_1(I + T)$, where $T \in \mathfrak{S}$. Since $I + T$ is a unitary operator, it follows that $T = \sum t_j P_j$, where $P_j = (\,\cdot\,, \varphi_j)\varphi_j$ $(j \in J)$ is a certain finite or infi-

an infinite sequence of pairwise orthogonal projectors, and $1 + \tau_j = \exp(i\theta_j)$ $(-\pi < \theta_j \leqslant \pi)$ are points of the unit circle, with $\operatorname{Sp}|T| = \sum |\tau_j| < \infty$. Thus,

$$U_2 = U_1 \left(I + \sum_{j \in J} \tau_j P_j \right) = U_1 \prod_{j \in J} (I + \tau_{jP} j),$$

$$\operatorname{Sp}\left|\ln_0(U_1^{-1}U_2)\right| = \sum_{j\in J}|\theta_j| < \infty,$$

where by $\ln_0(U_1^{-1}U_2)$ we denote that operator value of $\ln(U_1^{-1}U_2)$ whose spectrum lies in the interval $(-\pi i, \pi i]$, open on the left.

Let us first consider the case of a one-dimensional perturbation, i.e., when $U_2 = U_1(I + \tau(\,\cdot\,,\varphi)\varphi)$, where $\|\varphi\| = 1$, $1+\tau = \exp(i\theta)$ $(-\pi < \theta < \pi)$. In this case it is easily shown that

$$\Delta_{U_2/U_1}(z) = e^{i\frac{\theta}{2}}\left[\cos\frac{\theta}{2} + i\sin\frac{\theta}{2}\int_{-\pi}^{\pi}\frac{e^{it}+z}{e^{it}-z}\,d(E(t)\varphi,\varphi)\right] \qquad (|z|\neq 1),$$

where $E(t)$ is the spectral function of the operator U_1. Hence it is already not difficult to conclude that

$$\ln\Delta_{U_2/U_1}(z) = i\frac{\theta}{2} + i\int_{-\pi}^{\pi}\frac{e^{it}+z}{e^{it}-z}\eta_1(t)\,dt, \qquad \int_{-\pi}^{\pi}\eta_1(t)\,dt = \frac{\theta}{2},$$

where $|\eta_1(t)| \leqslant 1$ and $\operatorname{sign}\theta\cdot\eta_1(t) \geqslant 0$ $(-\pi \leqslant t \leqslant \pi)$. Recalling relation (2), we verify for the case under consideration the validity of (7) with $\eta(t) = \eta_1(t)$ and $\Psi(\zeta) = \Psi_z(\zeta) = (\zeta - z)^{-1}$ $(|z| \neq 1)$. Since the trace formula has been obtained for the family of functions $\Psi_z(\zeta)$ $(|z|\neq 1)$, its extension to the entire class of functions $\Psi(\zeta)$ indicated in Theorem 2 presents no particular difficulty.

In the case of the general relation (9), the function $\eta(t)$ in (7) can be obtained (cf. (2), § 4) in the form of a sum $\sum\eta_j(t)$ convergent in the $L_1(-\pi,\pi)$ metric, where $\eta_j(t)$ $(j = 1, 2, \ldots)$, obtained in the manner indicated above, is the function from the trace formula for the unitary operators $U^{(j)}$ and $U^{(j+1)}$, with

$$U^{(j+1)} = U^{(j)}(I + \tau_{jP}j) \quad (j = 1, 2, \ldots;\ U^{(1)} = U_1).$$

This way of establishing the trace formula (7) is also interesting because it supplies a function $\eta(t)$ possessing the following two properties:

$$\int_{-\pi}^{\pi}|\eta(t)|\,dt \leqslant \operatorname{Sp}\left|\ln_0(U_1^{-1}U_2)\right|, \qquad i\int_{-\pi}^{\pi}\eta(t)\,dt = \operatorname{Sp}\ln_0(U_1^{-1}U_2). \tag{10}$$

The last equality uniquely determines the function $\eta(t)$ in the trace formula (7). This equality may be regarded as the requirement that formula (7) be valid for the function $\Psi(\zeta) = \ln_0\zeta$, if in doing so the expression $\operatorname{Sp}[\ln_0 U_2 - \ln_0 U_1]$ is understood as $\operatorname{Sp}[\ln_0(U_1^{-1}U_2)]$. The function $\eta(t)$, normalized by equality (10), will be called the **spectral shift function** of the ordered pair of unitary operators U_1, U_2. From its construction it also follows that, if the operator $U_1^{-1}U_2$

has in all p eigenvalues in the closed half-plane $\operatorname{Im} z \geqslant 0$ (in all q eigenvalues in the open half-plane $\operatorname{Im} z < 0$), then almost everywhere $\eta(t) \leqslant p$ ($\eta(t) \geqslant -q$).

4. It is easy to see that two self-adjoint operators H_1 and H_2 are resolvent comparable if and only if the difference of their Cayley transforms $U_k = (iI - H_k)(iI + H_k)^{-1}$ ($k = 1, 2$) is nuclear: $U_2 - U_1 \in \mathfrak{S}$.

From Theorem 2 and the other assertions concerning the function $\eta(t)$ there follows

Theorem 3. *To every ordered pair of resolvent-comparable self-adjoint operators H_1, H_2 there corresponds, up to an additive constant,*

of the summand a unique real measurable function $\xi(\lambda)$ ($-\infty < \lambda < \infty$) such that $(1 + \lambda^2)^{-1}\xi(\lambda) \in L_1(-\infty, \infty)$ and

$$\operatorname{Sp}\left[(H_1 - zI)^{-1} - (H_2 - zI)^{-1}\right] = \int_{-\infty}^{\infty} \frac{\xi(\lambda)}{(\lambda - z)^2}\, d\lambda \quad (z \in \rho(H_1) \cap \rho(H_2)). \tag{11}$$

If one sets $\Delta(z) = \widetilde{\Delta}_{H_2/H_1}(z)$ and chooses a single-valued harmonic branch $\arg \Delta(z)$ ($\operatorname{Im} z > 0$), then the required function $\xi(\lambda)$ can be obtained from the formula

$$\xi(\lambda) = \frac{1}{\pi} \lim_{\varepsilon \downarrow 0} \arg \Delta(\lambda + i\varepsilon) + \text{const} \quad \text{(almost everywhere)}.$$

The function $\xi(\lambda)$ will be semibounded from below, provided the following conditions are satisfied: 1) $\mathfrak{D}(H_1) = \mathfrak{D}(H_2)$; 2) the form $((H_2 - H_1)f, f)$ ($f \in \mathfrak{D}(H_1)$) has a finite number of negative squares; and 3) there exist constants α, β ($0 \leq \alpha < 1,\ \beta \geq 0$) such that

$$\|(H_2 - H_1)f\| \leq \alpha \|H_1 f\| + \beta \|f\|$$

for all $f \in \mathfrak{D}(H_1)$.

In proving the last assertion one has to invoke a lemma which, as the author has found, is useful in various questions of perturbation theory.

If the spectra of the unitary operators U_k ($k = 1, 2$) lie respectively on the arcs $\zeta = \exp(i\theta)$ ($\alpha_k \leq \theta \leq \beta_k;\ k = 1, 2$), then the spectrum of their product $U_1 U_2$ lies on the arc $\zeta = \exp(i\theta)$ ($\alpha_1 + \alpha_2 \leq \theta \leq \beta_1 + \beta_2$).

We note that the totality of conditions 1) and 3) was used for another purpose in the paper (^{7}).

Of course, the function $\xi(\lambda)$, defined by (11), makes it possible to write the trace formula (6), which will be valid for the corresponding class of functions $\Phi(\lambda)$.

5. If H_1 is a semibounded operator (or, more generally, an operator having a certain spectral gap), then every self-adjoint operator H_2 resolvent-comparable with H_1 will also be such. In these cases the first two assertions of Theorem 3 can easily be obtained from Theorem 1 by passing from the operators H_1 and H_2 to their resolvents $R_a(H_1)$ and $R_a(H_2)$, where a is some real point regular for H_1 and H_2. Moreover, for the case when, for example, both operators H_1 and H_2 are semibounded from below, the trace formula for them can be obtained (on the basis of Theorem 3) under the condition
$$R_a^\nu(H_2) - R_a^\nu(H_1) \in \mathfrak{S},$$
where $\nu > 0$ and a is some* real point lying to the left of the spectra of H_1 and H_2 (concerning this condition, see ([8],[9])).

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* The validity of the condition does not depend on the choice of the point a, and its strength decreases as ν increases.

Note: Figure translations are in progress. See original paper for figures.

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