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Abstract

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TRACE FORMULAS FOR THE SCHRÖDINGER OPERATOR IN THREE-DIMENSIONAL SPACE

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In the present work trace formulas are obtained for the Schrödinger operator H in three-dimensional space. These formulas relate certain characteristics of the scattering problem (expressed in terms of the scattering amplitude) to the eigenvalues of the operator H. The method of deriving the formulas is analogous to that used earlier in the consideration of a similar problem for the Schrödinger operator on the half-line ([1]).

1. The self-adjoint operator H is given by the differential expression

$$(Hu)(x) = -\Delta u(x) + q(x)u(x), \qquad x = \{x_i,\ i = 1,2,3;\ -\infty < x_i < \infty\}. \quad (1)$$

We shall assume that $q(x)$ is an infinitely differentiable function and, for simplicity, suppose that $q(x)$ and all its derivatives, as $|x| \to \infty$, decrease faster than any power of $|x|^{-1}$.

The spectrum of the operator H consists of a continuous spectrum on the half-line $[0,\infty]$ and a finite number of eigenvalues λ_l ($\lambda_l \leq 0,\ l = 1,2,\dots,M$), each of finite multiplicity m_l. We shall additionally assume that all eigenvalues are negative ($\lambda_l < 0,\ l = 1,2,\dots,M$).

Let R_λ be the resolvent of H, and R^0_λ the resolvent of the operator $(-\Delta)$. Outside the points of the spectrum of the operator H there exists $\mathrm{Sp}(R_\lambda - R^0_\lambda)$, which in the complex λ-plane with a cut $\lambda \geq 0$ is an analytic function; the limiting values on the shores of the cut are continuous, and moreover

$$\lim_{\varepsilon\downarrow 0} \mathrm{Sp}(R_{\lambda+i\varepsilon} - R^0_{\lambda+i\varepsilon}) = \lim_{\varepsilon\uparrow 0} \mathrm{Sp}(R_{\lambda+i\varepsilon} - R^0_{\lambda+i\varepsilon}) \quad (\lambda \geq 0);$$

at the points λ_l there are simple poles with residues $(-m_l)$.

The behavior of the function $\mathrm{Sp}(R_\lambda - R^0_\lambda)$ as $|\lambda| \to \infty$ can be obtained from the following theorem, which is perhaps also of independent interest.

Theorem 1. As $|\lambda| \to \infty$, the kernel $R_\lambda(x,x')$ of the integral operator R_λ has a uniform asymptotic expansion with respect to $\arg\lambda$

$$R_\lambda(x,x') \underset{\lambda\to\infty}{\sim} \frac{e^{i\sqrt{\lambda}|x-x'|}}{4\pi|x-x'|} \sum_{n=0}^{\infty} (-1)^n \left(\frac{1}{2i\sqrt{\lambda}}\right)^n \sum_{m=0}^{n} |x-x'|^m \Omega_n^{(m)}(x,x'). \quad (2)$$

The coefficients $\Omega_n^{(m)}(x,x')$ can be found from the recurrence formulas

$$\Omega_{n+1}^{(m+1)}(x,x') = 2(m+1)\Omega_n^{(m+2)}(x,x') + \frac{1}{2}\int_{-1}^{1} d\eta \left(\frac{1}{2}(-\eta)\right)^m \times$$

$$\times \left\{\Delta_y \Omega_n^{(m)}(y,x') - q(y)\Omega_n^{(m)}(y,x') - m(m+1)\Omega_n^{(m+2)}(y,x')\right\}, \quad (3)$$

where

$$y = \frac{1}{2}(1-\eta)x + \frac{1}{2}(1+\eta)x' \quad (n = 0,1,\dots;\ m = 0,1,\dots,n),$$

$$\Omega_0^{(0)} = 1 \quad \text{and, in addition,} \quad \Omega_{n+1}^{(0)} = 0 \quad (n = 0,1,\dots).$$

From the recurrence formulas (3) it follows that

$$\Omega_{2s}^{2t+1}(x,x') = \Omega_{2s-1}^{2t}(x,x') = 0 \quad (s = 1,2,\dots;\ t = 0,1,\dots).$$

From Theorem 1 one can derive the following asymptotics (needed for obtaining the trace formulas)

$$\mathrm{Sp}\,(R_\lambda - R_\lambda^0) \underset{|\lambda|\to\infty}{\sim} \sum_{n=1}^{\infty} (-1)^n \left(\frac{1}{2i\sqrt{\lambda}}\right)^n \frac{1}{4\pi} \int dx\, \Omega_n^{(1)}(x,x). \quad (4)$$

2. In paper ([1]), for the case of a half-line, a connection was established between $\mathrm{Sp}(R_\lambda - R_\lambda^0)$ and the limiting phase (of scattering). The corresponding result in the three-dimensional case is given by:

Theorem 2. Let $S_\lambda(\alpha,\beta)$ (α,β are points on the unit sphere in three-dimensional space) be the kernel of the unitary scattering operator

$$S_\lambda(\alpha,\beta) = \delta(\alpha-\beta) + \frac{i\sqrt{\lambda}}{2\pi} f_\lambda(\alpha,\beta), \qquad \lambda \geqslant 0 \quad (5)$$

($f_\lambda(\alpha,\beta)$ is the scattering amplitude, see (10)); then

$$\operatorname{Im}\lim_{\varepsilon\downarrow 0}\operatorname{Sp}(R_{\lambda+i\varepsilon}-R^0_{\lambda+i\varepsilon})=-\frac{i}{2}\int d\beta\int d\alpha\,\overline{S_\lambda(\beta,\alpha)}\,\frac{\partial}{\partial\lambda}S_\lambda(\beta,\alpha). \tag{6}$$

The result of the theorem can be formally rewritten as follows:

$$\operatorname{Im}\lim_{\varepsilon\downarrow 0}\operatorname{Sp}(R_{\lambda+i\varepsilon}-R^0_{\lambda+i\varepsilon})=-\frac{i}{2}\frac{d}{d\lambda}\operatorname{Sp}\ln S_\lambda=-\frac{i}{2}\frac{d}{d\lambda}\ln\det S_\lambda; \tag{7}$$

hence we obtain (in the absence of a discrete spectrum)

$$\ln\det{}'(E+qK_\lambda)=\frac{1}{\pi}\int_0^\infty\frac{dz}{z-\lambda}\,\frac{i}{2}\left[\ln\det S_z+\frac{\sqrt{z}}{2\pi i}\int dx\,q(x)\right]. \tag{8}$$

The symbol $\ln\det{}'(E+qR_\lambda)$ means that the divergent determinant is regularized by subtracting from its logarithm a certain infinite term.

Formula (8) was communicated to the author by L. D. Faddeev, who had obtained it earlier by another method (see also ([2])).

For the proof of the theorem the following representation is used ([3])

$$\operatorname{Im}\lim_{\varepsilon\downarrow 0}R_{\lambda+i\varepsilon}(x,x)=\left(\frac{1}{2\pi}\right)^3\frac{\pi\sqrt{\lambda}}{2}\int d\alpha\,|\psi_\alpha(x,\lambda)|^2. \tag{9}$$

In this formula $\psi_\alpha(x,\lambda)$ are the eigenfunctions of the operator H—solutions of the scattering problem determined by the asymptotic behavior

$$\psi_\alpha(x,\lambda)\underset{|x|\to\infty}{\sim}e^{i\sqrt{\lambda}x\alpha}+\frac{e^{i\sqrt{\lambda}|x|}}{|x|}f_\lambda\left(\alpha,\frac{x}{|x|}\right). \tag{10}$$

Representation (9) reduces the proof to the computation of the integral

$$\int dx\int d\alpha\,(|\psi_\alpha(x,\lambda)|^2-1),$$

which should be transformed by means of the formula

$$\int_{|x|<R}dx\,|\psi_\alpha(x,\lambda)|^2=\int_{|x|=R}dS_x\left\{\frac{\partial}{\partial\lambda}\psi_\alpha(x,\lambda)\frac{\partial}{\partial|x|}\overline{\psi_\alpha(x,\lambda)}-\overline{\psi_\alpha(x,\lambda)}\frac{\partial^2}{\partial\lambda\,\partial|x|}\psi_\alpha(x,\lambda)\right\}. \tag{11}$$

3. To derive the trace formulas it now suffices to use the simple auxiliary proposition:

Lemma. Let the function $f(\lambda)$ of the complex variable λ have the following properties: 1) $f(\lambda)$ is analytic in the λ-plane with a cut $\lambda \geqslant 0$ and with simple poles $\tilde{\lambda}_l$ ($\tilde{\lambda}_l < 0,\ l = 1, 2, \ldots, \widetilde{M}$); 2) on the banks of the cut $f(\lambda)$ uniformly assumes continuous and bounded (for $\lambda > 0$) limiting values; 3) $f(\lambda + i0) = \overline{f(\lambda - i0)}$, $\lambda \geqslant 0$; 4) $\operatorname{Res} f(\lambda)\big|_{\lambda=\tilde{\lambda}l} = -\widetilde{m}_l$; 5) as $\lambda \sim 0$, $f(\lambda)$ may tend to infinity no faster than $\lambda^{-1/2}$; 6) as $|\lambda| \to \infty$ the uniform asymptotic formula holds

$$f(\lambda) \underset{|\lambda|\to\infty}{\sim} \sum_{l=1}^{\infty} (-1)^l \frac{(-l/2)}{\lambda} \left(\frac{1}{2i\sqrt{\lambda}}\right)^l Q_l, \tag{12}$$

(Q_l are real). Denote

$$\eta(\lambda) \equiv \int_0^{\infty} d\lambda \ \operatorname{Im} f(\lambda + i0) \quad (\lambda \geqslant 0). \tag{13}$$

Then:

a)

$$\sum_{l=1}^{\widetilde{M}} \widetilde{m}_l = -\frac{1}{\pi}\eta(+0); \tag{14}$$

b) for $\mu = 1, 2, 3, \ldots$

$$\sum_{l=1}^{\widetilde{M}} \widetilde{m}_l \tilde{\lambda}_l^{\mu} + \frac{\mu}{\pi} \int_0^{\infty} d\lambda\, \lambda^{\mu-1} \left[\eta(\lambda) - \sum_{l=0}^{\mu-1} \frac{(-1)^{l+1} Q_{2l+1}}{(2\sqrt{\lambda})^{2l+1}}\right] = (-1)^{\mu} \frac{\mu Q_{2\mu}}{2^{2\mu}}. \tag{15}$$

4. We now obtain the trace formulas if, in the conditions of the lemma, we put

$$f(\lambda) = \operatorname{Sp}(R_\lambda - R_\lambda^0) - \frac{1}{2i\sqrt{\lambda}} \frac{1}{4\pi} \int dx\, q(x), \tag{16}$$

$$\tilde{\lambda}_l = \lambda_l, \qquad \widetilde{M} = M, \qquad \widetilde{m}_l = m_l;$$

in this case

$$\eta(\lambda) = \frac{1}{2i} \int_\lambda^{\infty} d\lambda \left\{ \iint d\beta\, d\alpha\, \overline{S_\lambda(\beta, \alpha)} \frac{\partial}{\partial \lambda} S_\lambda(\beta, \alpha) - \frac{1}{2i\sqrt{\lambda}} \frac{1}{2\pi} \int dx\, q(x) \right\}; \tag{17}$$

$$Q_{2\mu} = 0, \qquad Q_{2\mu-1} = -\frac{1}{2(2\mu-1)}\frac{1}{4\pi}\int dx\,\Omega^{(1)}_{2\mu+1}(x,x). \tag{18}$$

$Q_{2\mu-1}$ can be computed with the aid of Theorem 1.

Formulas (14) and (15), for $\mu = 1$, for example, then give

$$\sum_{l=1}^{M} m_l = -\frac{1}{2\pi i}\int_0^\infty d\lambda\left\{\iint d\beta\,d\alpha\,\overline{S_\lambda(\beta,\alpha)}\frac{\partial}{\partial\lambda}S_\lambda(\beta,\alpha) - \frac{1}{2i\sqrt{\lambda}}\frac{1}{2\pi}\int dx\,q(x)\right\}; \tag{19}$$

$$\sum_{l=1}^{M} m_l\lambda_l + \frac{1}{\pi}\int_0^\infty d\lambda\left\{\frac{1}{2i}\int_\lambda^\infty dt\left[\iint d\beta\,d\alpha\,\overline{S_t(\beta,\alpha)}\frac{\partial}{\partial t}S_t(\beta,\alpha) - \frac{1}{2i\sqrt{t}}\frac{1}{2\pi}\int dx\,q(x)\right] + \frac{1}{2\sqrt{\lambda}}\frac{1}{8\pi}\int dx\,q^2(x)\right\} = \tag{20}$$

5. Formula (6) makes it possible to establish the connection between the scattering amplitude and M. G. Krein' s function $\xi(t)$, defined by the representation [4,5]

$$\mathrm{Sp}(R_\lambda - R_\lambda^0) = -\int_{-\infty}^{\infty}\xi(t)\,d\frac{1}{t-\lambda} \tag{21}$$

and also arising in the theory of perturbation determinants [5]. In our case the function $\xi(t)$ can be written as follows:

$$\xi(t) = \begin{cases} -\displaystyle\int_{-\infty}^{t}\sum_l m_l\delta(z-\lambda_l)\,dz, & t<0,\\[2ex] \dfrac{1}{\pi}\eta(t) + \dfrac{\sqrt{t}}{(2\pi)^2}\displaystyle\int dx\,q(x), & t>0.\end{cases} \tag{22}$$

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