Certain Explicit Relationships between Phase Shift and Scattering Potential

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An intuitive account is given of recent important results of Gelfand and Levitan for the determination of the potential in the one-dimensional Schrödinger equation from the S-phase shift, the bound states, and certain normalizing parameters.

The method is then used to obtain the first variation in the potential corresponding to a small change in the phase shift, bound states, and normalizing parameters.

I.

THE determination of the potential from a given S-phase shift has been considered in a number of recent papers. For particulars see the introduction and references of Jost and Kohn.[1] The method of Jost and Kohn for constructing a potential from a phase shift has much to commend it. However, as the authors point out, it has a limited range of convergence, and of necessity is ambiguous in case bound states occur.

Here methods developed recently by Gelfand and Levitan[2] for the determination of the potential from the spectral function will be presented in intuitive form. These methods introduce a number of quite new ideas which are of great interest in themselves.

The problem may be described as follows. The Schrödinger equation,

$$\phi''+k^2\phi=V(r)\phi, \tag{1}$$

is considered over the interval $0<r<\infty$. It is assumed that

$$\int_0^\infty r^j|V(r)|dr<\infty, \quad j=1,2.$$

Let $\phi(k,r)$ be the resolution of (1) satisfying $\phi(k,0)=0$, $\phi'(k,0)=1$. It is well known that as $r\to\infty$ and for real $k>0$

$$\phi(k,r)\sim\frac{|f(k)|}{k}\sin[kr+\eta(k)], \tag{2}$$

where $\eta(k)$ is the phase function and $f(k)$ is $f(k,0)=g(k)$ as given in Jost and Kohn.[1] Let $ik_1, \cdots, ik_m$ denote the values of k for which there are bound states of energy $-k_1^2, \cdots, -k_m^2$. That m is finite has been shown by Levinson.[3] The eigenfunctions associated with the bound states are $\phi(ik_j,r)$, $j=1, \cdots, m$, and will be denoted by $\phi_j(r)$.

The expansion theorem associated with the eigenvalue problem states that, for any suitably restricted function $F(r)$,

$$F(r)=\sum_{j=1}^n c_j\phi_j(r)\left[\int_0^\infty F(r)\phi_j(r)dr\right] +\frac{2}{\pi}\int_0^\infty \frac{k^2}{|f(k)|^2}\phi(k,r)\left[\int_0^\infty F(r)\phi(k,r)dr\right]dk, \tag{3}$$

where $f(k)$ is as given in Eq. (2) and the $c_j^{\frac{1}{2}}$ are the normalizing factors for $\phi_j(r)$.

Let $k^2=\lambda$ and let $\phi(k,r)=\phi(\sqrt{\lambda},r)$ be denoted by $y(\lambda,r)$. Let $\rho(\lambda)$ be a monotone nondecreasing function which for $\lambda<0$ is constant except for jumps at $\lambda=-k_j^2$, the magnitude of each jump being c_j. Let $\rho(0)=0$ and let

$$\rho(\lambda)=\frac{1}{\pi}\int_0^\lambda \frac{\lambda^{\frac{1}{2}}}{|f(\lambda^{\frac{1}{2}})|^2}d\lambda$$

for $\lambda>0$. Then Eq. (3) becomes

$$F(r)=\int_{-\infty}^\infty y(\lambda,r)\left(\int_0^\infty F(r)y(\lambda,r)dr\right)d\rho(\lambda). \tag{4}$$

The problem of determining $V(r)$ when $\eta(k)$ is given has been shown by Bargmann[4] not to have a unique solution. It has been shown by Levinson[3] that if no bound states exist $\eta(k)$ does determine $V(r)$ uniquely. Jost and Kohn[1] showed that this uniqueness proof could be extended to the case where bound states exist, providing the normalizing factors $c_1, \cdots c_m$ are also given.

Suppose now that $\eta(k)$, ik_j, and c_j, $j=1, \cdots, m$ are given. Then proceeding as in Jost and Kohn,[1] §2, $f(k)$ may be found. Once $f(k)$ is known, $\rho(\lambda)$ as defined below Eq. (3) is completely determined. The function $\rho(\lambda)$ is known as the spectral function. It will be shown how $\rho(\lambda)$ determines $V(r)$ explicitly and uniquely.

II.

This section will develop the motivation for the method of Gelfand and Levitan.[2]

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4 V. Bargmann, Phys. Rev. **75**, 301 (1949); Revs. Modern Phys. **21**, 488 (1949).

The function $\phi(k, r)=y(\lambda, r)$ is written in the form

$$\phi(k, r)=\frac{\sin kr}{k}+\int_0^r K(r, \xi)\frac{\sin k\xi}{k}d\xi. \tag{5}$$

It must now be shown that $K(r, \xi)$ exists. Integrating Eq. (5) by parts twice yields

$$k^2\phi=k\sin kr-K(r, r)\cos kr+K(r, 0)+\frac{\partial K(r, r)}{\partial \xi}\frac{\sin kr}{r}-\int_0^r\frac{\partial^2 K}{\partial \xi^2}\frac{\sin k\xi}{k}d\xi.$$

Computing ϕ'' directly from Eq. (5) and using the above result, it is found that

$$\phi''+k^2\phi=2\frac{\sin kr}{k}\frac{dK(r, r)}{dr}+K(r, 0)+\int_0^r\left(\frac{\partial^2 K(r, \xi)}{\partial r^2}-\frac{\partial^2 K(r, \xi)}{\partial \xi^2}\right)\frac{\sin k\xi}{k}d\xi.$$

By Eqs. (1) and (5) the right side above must be equal to

$$V(r)\frac{\sin kr}{r}+V(r)\int_0^r K(r, \xi)\frac{\sin k\xi}{k}d\xi.$$

This will be true if, for $0\leq\xi\leq r$,

$$\partial^2 K/\partial r^2-\partial^2 K/\partial \xi^2=V(r)K(r, \xi), \tag{6}$$

and the boundary conditions

$$K(r, 0)=0, \quad K(r, r)=\tfrac{1}{2}\int_0^r V(r)dr, \tag{7}$$

hold. If the range $0\leq\xi\leq r$ is replaced by $-r\leq\xi\leq r$, $r\geq 0$ and the boundary conditions by

$$K(r, r)=-K(r, -r)=\tfrac{1}{2}\int_0^r V(r)dr,$$

then the problem is the standard one of solving a linear hyperbolic partial differential equation with boundary conditions prescribed on two intersecting characteristic curves. Thus $K(r, \xi)$ is determined.

In case $V(r)\equiv 0$ then it is readily seen that the $\rho(\lambda)$ in (4) becomes $2\lambda^{3/2}/(3\pi)$ for $\lambda\geq 0$ and zero for $\lambda<0$. The $\rho(\lambda)$ for (1) is written as

$$\begin{aligned}\rho(\lambda)&=2\lambda^{3/2}/3\pi+\sigma(\lambda), \quad \lambda\geq 0\\ \rho(\lambda)&=\sigma(\lambda), \quad \lambda<0.\end{aligned} \tag{8}$$

In much the same way as Eq. (5) is justified it can be shown that there exists a $K_0(r_1, \xi)$ such that

$$\frac{\sin kr_1}{k}=\phi(k, r_1)+\int_0^{r_1}K_0(r_1, \xi)\phi(k, \xi)d\xi. \tag{9}$$

Recalling that $k^2=\lambda$, and that

$$\int_{-\infty}^{\infty}\phi(k, r_1)\phi(k, r)d\rho(\lambda)=\delta(r-r_1),$$

where δ is the Dirac function, it is seen that

$$\int_{-\infty}^{\infty}\phi(k, r)\phi(k, r_1)d\rho(\lambda)=0, \quad r\neq r_1.$$

If this is used in Eq. (9) there results for $r>r_1\geq 0$

$$\int_{-\infty}^{\infty}\frac{\sin kr_1}{k}\phi(k, r)d\rho(\lambda)=0.$$

Then if one refers to Eq. (5), this implies that for $r>r_1\geq 0$

$$\int_{-\infty}^{\infty}\frac{\sin kr\sin kr_1}{k^2}d\rho(\lambda)+\int_0^x K(r, \xi)d\xi\int_{-\infty}^{\infty}\frac{\sin k\xi\sin kr_1}{k^2}d\rho(\lambda)=0.$$

If Eq. (8) is used in the above equation in conjunction with the fact that

$$\int_0^{\infty}\frac{\sin kr\sin kr_1}{k^2}d\left(\frac{2\lambda^{3/2}}{3\pi}\right)=\delta(r-r_1),$$

there results for $r>r_1\geq 0$,

$$\int_{-\infty}^{\infty}\frac{\sin kr\sin kr_1}{k^2}d\sigma(\lambda)+\int_0^r K(r, \xi)d\xi\int_{-\infty}^{\infty}\frac{\sin k\xi\sin kr_1}{k^2}d\sigma(\lambda)+K(r, r_1)=0. \tag{10}$$

Let

$$\frac{1}{2}\int_{-\infty}^{\infty}\frac{1-\cos ku}{k^2}d\sigma(\lambda)=\Phi(u). \tag{11}$$

Then

$$\Phi(r+r_1)-\Phi(r-r_1)=P(r, r_1)=\int_{-\infty}^{\infty}\frac{\sin kr\sin kr_1}{k^2}d\sigma(\lambda). \tag{12}$$

Thus (10) becomes

$$P(r, r_1)+\int_0^r K(r, \xi)P(\xi, r_1)d\xi+K(r, r_1)=0. \tag{13}$$

From continuity considerations this holds for $0\leq r_1\leq r$. It is (13) which forms the point of departure for the determination of $V(r)$ from $\rho(\lambda)$. It is clear from (12) that $P(r, r_1)=P(r_1, r)$.

III.

Suppose now that $\rho(\lambda)$ is given. Then $\sigma(\lambda)$ is determined by (8), and thus $P(r, r_1)$ from (11) and (12). It is clearly the case that for each fixed $r>0$, Eq. (13) is a Fredholm equation with $K(r, r_1)$ as an unknown function of r_1.

It will now be shown that the homogeneous equation,

$$\int_0^r P(r_1, \xi)h(\xi)d\xi + h(r_1) = 0,$$

has only the null solution, $h\equiv 0$.

Let

$$I=\int_0^r\int_0^r P(r_1, \xi)h(\xi)h(r_1)d\xi dr_1 + \int_0^r h^2(r_1)dr_1.$$

Clearly $I=0$. By using (12), it is found that

$$P(r_1, \xi)=\int_{-\infty}^{\infty}\frac{\sin kr_1 \sin k\xi}{k^2}d\sigma(\lambda)$$
$$=\int_{-\infty}^{\infty}\frac{\sin kr_1 \sin k\xi}{k^2}d\rho(\lambda)-\delta(r_1-\xi).$$

Thus

$$I=\int_0^r\int_0^r h(\xi)h(r_1)d\xi dr_1\int_{-\infty}^{\infty}\frac{\sin kr_1 \sin k\xi}{k^2}d\rho(\lambda)$$
$$-\int_0^r\int_0^r h(\xi)h(r_1)\delta(r_1-\xi)d\xi dr_1 + \int_0^r h^2(r_1)dr_1.$$

Or, since the last two integrals are equal,

$$I=\int_{-\infty}^{\infty}\left(\int_0^r\frac{h(\xi)\sin k\xi}{k}d\xi\right)^2 d\rho(\lambda).$$

Since

$$\frac{1}{k}\int_0^r h(\xi)\sin k\xi d\xi \tag{14}$$

is an entire function of λ and since $\rho(\lambda)$ has a continuous spectrum for $\lambda>0$, it follows that $I>0$ unless (14) is identically zero. This last implies $h(\xi)\equiv 0$ so that indeed the homogeneous equation has only the null solution, and thus by the Fredholm theorem the nonhomogeneous integral equation (13) has a unique solution, $K(r, r_1)$. If it is assumed that $\Phi''(u)$ exists, then it can be shown that the first and second partial derivatives of $K(r, r_1)$ exist. As suggested by (7) let $V(r)=2dK(r, r)/dr$. Then $\phi(k, r)$ given by (5) satisfies (1), and $\rho(\lambda)$ is the spectral function of (1) with boundary condition $\phi(k, 0)=0$.

In summarizing, it is found that a knowledge of the phase function $\eta(k)$, the bound states $k_1, \cdots k_m$, and the normalizing factors $c_1, \cdots c_m$ determines the spectral function $\rho(\lambda)$. By Eq. (8) this determines $\sigma(\lambda)$. From $\sigma(\lambda)$, $\Phi(u)$ is determined in Eq. (11), and $P(r, r_1)$ by Eq. (12). The function $K(r, r_1)$ is then determined from the Fredholm equation (13) for $0\le r_1\le r$. The variable r appears in the Fredholm equation as a parameter, and thus the determination of $K(r, r_1)$ computationally may be a long process. Once $K(r, r_1)$ is found, $V(r)$ is given by $2dK(r, r)/dr$.

IV.

Suppose the potential $V(r)$ corresponding to a given spectral function $\rho(\lambda)$ is sought. Let $\rho_0(\lambda)$ be another spectral function, and suppose its potential function $V_0(r)$ is known or has been determined. Then what is the relationship between $V(r)-V_0(r)$ and $\rho(\lambda)-\rho_0(\lambda)$? The case treated above corresponds to $V_0(r)\equiv 0$.

Let $\phi_0(k, r)$ denote the solutions of Eq. (1) where V is replaced by V_0. Let $\rho(\lambda)-\rho_0(\lambda)=\sigma(\lambda)$. Then the same argument as used above, for the case $V_0(r)\equiv 0$, shows that

$$V(r)-V_0(r)=2dK(r, r)/dr, \tag{15}$$

where K is the solution of

$$K(r, r_1)+P_0(r, r_1)+\int_0^r K(r, \xi)P_0(\xi, r_1)d\xi=0, \tag{16}$$

and

$$P_0(r, r_1)=\int_{-\infty}^{\infty}\phi_0(k, r)\phi_0(k, r_1)d\sigma(\lambda).$$

If $\rho(\lambda)-\rho_0(\lambda)$ is small, then P_0 is small and as a *first approximation*, Eq. (16) yields

$$K(r, r_1)\sim -P_0(r, r_1).$$

In Eq. (15) this gives

$$V(r)-V_0(r)\sim -4\int_{-\infty}^{\infty}\phi_0(k, r)\phi_0'(k, r)d\sigma(\lambda),$$

or, if $V-V_0=\delta V$ and $\rho-\rho_0=\delta\rho$, then

$$\delta V(r)\sim -4\int_{-\infty}^{\infty}\phi(k, r)\phi'(k, r)d(\delta\rho(\lambda)).$$

These formulas are, of course, only approximations which neglect terms of higher order than the first in $\delta\rho(\lambda)$.