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Phase-Shift Method for One-Dimensional Scattering

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The phase-shift method is developed for the problem of the scattering of a one-dimensional wave by a symmetric potential. Reflection and transmission coefficients are expressed in terms of the phase shifts of odd and even solutions of the Schrödinger equation in the asymptotic range. Integral equations are established for the phase shifts and some approximate methods investigated.

I. INTRODUCTION

THIS paper applies the method of phase shifts to the problem of quantum-mechanical scattering in one dimension. Reflection and transmission coefficients are expressed in terms of phase shifts of basic real wave functions which satisfy simple boundary conditions. The method is amenable to approximate procedures.

The author's interest in problems of one dimension arose from a study of the scattering of electrons in solids by ionized impurities, in the presence of a strong magnetic field. In that situation,[1] the magnetic field influences the dynamics of an electron so that the motion parallel to the field is essentially one-dimensional free motion, while its transverse motion is bounded. The use of time dependent perturbation theory for scattering by impurities with the magnetic field present leads to divergent scattering rates,[2] and approximate methods related to the present type of approach are necessary.

In the following sections the phase shifts are defined and the scattering problem formulated in terms of them. Integral equations for the phase shifts are produced and approximate methods for solution discussed.

II. FORMULATION OF THE SCATTERING PROBLEM

We consider the scattering of an incoming wave e^{ikx} by a potential $V(x)$.[3] $V(x)$ is assumed symmetric about the origin and of finite range. Upon letting $v(x)=2mV(x)/\hbar^2$, the Schrödinger equation for this problem is written

$$(d^2\psi/dx^2)+k^2\psi=v(x)\psi. \tag{1}$$

We require a solution which satisfies the boundary conditions

$$\begin{aligned}\psi(x)&\rightarrow e^{ikx}+re^{-ikx} \quad \text{as} \quad x\rightarrow-\infty\\ \psi(x)&\rightarrow te^{ikx} \quad \text{as} \quad x\rightarrow+\infty,\end{aligned} \tag{2}$$

where r and t are reflection and transmission amplitudes. The quantities of ultimate interest, the reflection and transmission coefficients, are given by the absolute squares of the respective amplitudes.

Instead of working directly with the function ψ, we introduce two new functions $\phi_+(x)$ and $\phi_-(x)$, real solutions to Eq. (1) which are even and odd in x, respectively, and form a complete set. We have

$$\phi_+'(0)=0 \tag{3a}$$

$$\phi_-(0)=0. \tag{3b}$$

For $|x|\gg a$, the range of the potential, the ϕ's must go over into linear combinations of the sine and cosine solutions of Eq. (1) for $v=0$. We

[1] A. H. Kahn and H. P. R. Frederikse, Advances in Solid State Phys. **9**, 257 (1959).
[2] A. H. Kahn, Phys. Rev. **119**, 1189 (1960).

[3] Specific examples of this type of problem are given in the texts: L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), 1st ed., Chap. V; and L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon Press, New York, 1958), pp. 72–77. In this treatment the problem is given in more general form.

write these asymptotic forms as

$$\left.\begin{aligned}\phi_+(x) &\to \frac{\cos(kx+\delta_+)}{\cos\delta_+} = \cos kx - \tan\delta_+ \sin kx\\ \phi_-(x) &\to \frac{\sin(kx+\delta_-)}{\sin\delta_-} = \sin kx + \tan\delta_- \cos kx\end{aligned}\right\} x \to +\infty$$
$$\left.\begin{aligned}\phi_+(x) &\to \frac{\cos(kx-\delta_+)}{\cos\delta_+} = \cos kx + \tan\delta_+ \sin kx\\ \phi_-(x) &\to \frac{\sin(kx-\delta_-)}{\sin\delta_-} = \sin kx - \tan\delta_- \cos kx\end{aligned}\right\} x \to -\infty. \qquad (4)$$

In Eq. (4) the choices of sign of the phases $\delta_\pm$ are taken to assure the proper symmetries of the ϕ's about the origin; the denominators provide convenient normalization. If the potential $v(x)$ were to vanish, ϕ_+ and ϕ_- would be the functions $\cos kx$ and $\sin kx$, respectively. The $\sin kx$ component of ϕ_+ and the $\cos kx$ component of ϕ_-, for large x, represent the effect of the scattering potential. We now expand the ψ function as a linear combination of the ϕ functions. We set

$$\psi = A\phi_+(x) + B\phi_-(x). \qquad (5)$$

The constants A and B are determined by requiring ψ to satisfy the asymptotic boundary conditions (2), while employing the forms [see Eq. (4)] for the asymptotic values of the ϕ's. The results are that $A=\cos\delta_+ \exp(i\delta_+)$ and $B=i\sin\delta_- \exp(i\delta_-)$. Then we find $r=\frac{1}{2}[\exp(2i\delta_+)\times\exp(2i\delta_-)]$ and $t=\frac{1}{2}[\exp(2i\delta_+)+\exp(2i\delta_-)]$. Finally, the reflection coefficient R and the transmission coefficient T are obtained:

$$\begin{aligned}R&=\sin^2(\delta_+-\delta_-)\\ T&=\cos^2(\delta_+-\delta_-).\end{aligned} \qquad (6)$$

We observe that $R+T=1$, as is required.

We have thus reduced the problem of finding the scattering coefficients to that of calculating the asymptotic phase shifts of the even and odd solutions of Eq. (1). This is analogous to expressing the differential scattering cross section, for a spherically symmetric scatterer, in terms of the phase shifts of the radial functions corresponding to the various angular momenta. In fact, our solution ϕ_- satisfies a differential equation and boundary conditions identical to those of the s-wave radial function in three-dimensional spherically symmetric scattering.[4]

III. GREEN'S FUNCTIONS

In the following section, the Schrödinger equation with boundary conditions of Eqs. (3a) or (3b) will be converted into integral equations. This procedure will lead to useful approximate methods. For this purpose, we introduce the Green's functions which satisfy the equation

$$[d^2K(x,x')/dx^2]+k^2K(x,x')=\delta(x-x'), \qquad (7)$$

with boundary conditions to be specified later. Upon integrating Eq. (7) over x, across a small region including x', we find that the Green's functions have a discontinuity in derivative given by

$$\lim_{\epsilon\to 0}\left[\left.\frac{dK(x,x')}{dx}\right|_{x=x'+\epsilon} - \left.\frac{dK(x,x')}{dx}\right|_{x=x'-\epsilon}\right]=1. \qquad (8)$$

Let us find the Green's function $K_+(x,x')$ for the boundary condition in Eq. (3a), satisfying

$$\left.\frac{dK_+(x,x')}{dx}\right|_{x=0,\ x'>x}=0. \qquad (9)$$

Since this will be needed for the representation of the scattering part of ϕ_+, we require

$$K_+(x,x') \propto \sin kx \quad (\text{for } x>x'). \qquad (10)$$

[4] See, for example, N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, New York, 1950), 2nd ed., Chap. II.

We write K_+ in the following form:

$$K_+(x,x')=\begin{cases} A\cos kx+B\sin kx & x\leq x' \\ C\cos kx+D\sin kx & x\geq x'. \end{cases}$$

Applying the boundary conditions, we evaluate the constants in Eq. (11). We find

$$K_+(x,x')=\begin{cases} (1/k)\sin kx'\cos kx & x\leq x' \\ (1/k)\cos kx'\sin kx & x\geq x'. \end{cases} \quad (12)$$

Similarly, for K_- we must satisfy, in addition to Eq. (8), the conditions

$$\begin{aligned} K_-(0,x') &= 0 \quad (\text{for } x'>0) \\ K_-(x,x') &\propto \cos kx \quad (\text{for } x>x'). \end{aligned} \quad (13)$$

In like manner, we obtain

$$K_-(x,x')=\begin{cases} -(1/k)\cos kx'\sin kx & x\leq x' \\ -(1/k)\sin kx'\cos kx & x\geq x', \end{cases} \quad (14)$$

which is the same as in three-dimensional s-wave scattering.[5]

IV. INTEGRAL EQUATIONS FOR THE PHASE SHIFTS

The solutions $\phi_\pm$ may be written as superpositions of the solutions of Eq. (7), by using the appropriate $K_\pm$, with the addition of a suitable solution of the homogeneous part of Eq. (1). Since the unknown appears in the inhomogeneous term, the result will be an integral equation.

For the basic ϕ functions we find

$$\begin{aligned} \phi_+ &= \cos kx+\int_0^\infty K_+(x,x')v(x')\phi_+(x')dx' \\ \phi_- &= \sin kx+\int_0^\infty K_-(x,x')v(x')\phi_-(x')dx'. \end{aligned} \quad (15)$$

In the limit of large x, we obtain

$$\begin{aligned} \phi_+(x) &\approx \cos kx+\sin kx \times\int_0^\infty \frac{1}{k}\cos kx'v(x')\phi_+(x')dx' \\ \phi_-(x) &\approx \sin kx-\cos kx \times\int_0^\infty \frac{1}{k}\sin kx'v(x')\phi_-(x')dx'. \end{aligned} \quad (16)$$

[5] J. M. Blatt and J. D. Jackson, Phys. Rev. **76**, 18 (1949).

Upon comparing with Eq. (4), we make the identifications

$$\begin{aligned} \tan\delta_+ &= -(1/k)\int_0^\infty \cos kx'v(x')\phi_+(x')dx' \\ \tan\delta_- &= -(1/k)\int_0^\infty \sin kx'v(x')\phi_-(x')dx'. \end{aligned} \quad (17)$$

V. APPROXIMATE METHODS

Perhaps, the simplest method of finding an approximate solution for the scattering coefficients in a one-dimensional problem is to perform the numerical integrations of the Schrödinger equations for ϕ_+ and ϕ_-. From the asymptotic forms one may find the phase shifts and obtain the results directly.

In the case of scattering by a square barrier, as treated by Schiff,[6] an exact solution is more easily obtained by the phase-shift method, avoiding a certain amount of tedious matching of incident and scattered waves at the boundaries of the scattering potential. This is performed in the Appendix.

At first glance, one might have tried to find a direct approximation to the reflection coefficient, without appeal to the phase-shift method, by employing golden rule #2,[7] i.e., first-order time-dependent perturbation theory.[8] According to this method, the probability per unit time for a reflective transition from state k to state $-k$ is given by

$$w_{k\to -k}=(2\pi/\hbar)|\langle -k|V(x)|k\rangle|^2\rho_f, \quad (18)$$

where $\langle -k|V|k\rangle$ is the matrix element of the scattering potential between initial and final states, and ρ_f is the density of final states per unit energy range. If the initial and final state wave functions are e^{ikx} and e^{-ikx}, respectively, we find the reflection coefficient given by the transition probability per unit time divided by the incident current:

$$R=w_{k\to -k}/(\hbar k/m). \quad (19)$$

For typical potentials the matrix element is finite for all energies. However, the density of

[6] L. I. Schiff, footnote 3.

[7] E. Fermi, *Nuclear Physics* (University of Chicago Press, Chicago, Illinois, 1940), p. 142.

[8] See L. I. Schiff, footnote 3, p. 193.

states for free one-dimensional motion is given by

$$\rho_f = m/2\pi\hbar^2 k. \quad (20)$$

Therefore, for slow incoming particles, as k approaches zero, this approximation yields an infinite reflection coefficient, in violation of probability conservation. Techniques which maintain normalized wave functions must be used.

If v may be considered small, the Born approximation may be applied to the calculation of phase shifts. This is the first iteration of Eqs. (14), i.e., in the integrals we take

$$\begin{aligned} \phi_+(x) &\approx \cos kx \\ \phi_-(x) &\approx \sin kx. \end{aligned} \quad (21)$$

Then, from Eqs. (17), we find

$$\begin{aligned} \tan\delta_+ &\approx -(1/k)\int_0^\infty \cos^2 kx v(x) dx \\ \tan\delta_- &\approx -(1/k)\int_0^\infty \sin^2 kx v(x) dx. \end{aligned} \quad (22)$$

Whether the Born approximation is valid or not, the results of Eqs. (22), when substituted into Eqs. (6), will always yield a reflection coefficient no greater than unity. Thus, this approximation may have value in qualitative estimates

Some insight concerning the failure of the use of Eq. (18) can be obtained by considering the Born approximation for the phase shifts. If $v(x)$ may be considered small, we take $\tan\delta_\pm \approx \sin\delta_\pm \approx \delta_\pm$. Then, in the limit $k \to 0$ we obtain

$$\delta_- = 0, \quad \delta_+ \approx -(1/k)\int_0^\infty v(x)dx.$$

Finally, we find

$$R \approx (1/k^2)\left[\int_0^\infty v(x)dx\right]^2.$$

For sufficiently small k, the reflection coefficient not only will exceed unity, but will diverge as $1/k^2$, exactly as in Eq. (20). This result emphasizes the fact that for low energies one cannot replace $\tan\delta_+$ by δ_+ and even a weak potential cannot be considered small.

More advanced techniques, such as the Schwinger variational principle,[5] are easily adapted to this problem.

APPENDIX. SCATTERING BY A SQUARE WELL

We consider scattering by a square well potential, i.e., one for which

$$v(x) = \begin{cases} -k_0^2 & |x| < a/2 \\ 0 & |x| > a/2, \end{cases} \quad (A.1)$$

where k_0 is constant. Let $k'^2 = k^2 + k_0^2$. We now proceed to find ϕ_+ and the phase shift δ_+. With constant v, the Schrödinger equaton is solved easily; the solution is of the form

$$\phi_+(x) = \begin{cases} A \cos k'x & |x| < a/2 \\ B \cos(kx + \delta_+) & x > a/2. \end{cases} \quad (A.2)$$

The conditions of continuity of ϕ_+ and ϕ_+' at $x = a/2$ enable us to find δ_+. We obtain

$$\delta_+ = \tan^{-1}\left(\frac{k'}{k}\tan\frac{k'a}{2}\right) - \frac{ka}{2}. \quad (A.3)$$

In similar fashion, we find ϕ_- and the phase shift:

$$\delta_- = \tan^{-1}\left(\frac{k}{k'}\tan\frac{k'a}{2}\right) - \frac{ka}{2}. \quad (A.4)$$

The reflection coefficient is obtained from Eq. (6). After some manipulation of trigonometric relations, we find

$$\begin{aligned} R &= [1 + \cot^2(\delta_+ - \delta_-)]^{-1} \\ &= \left[1 + \frac{4k^2(k^2 + k_0^2)}{k_0^4 \sin^2 ka}\right]^{-1}, \end{aligned} \quad (A.5)$$

a formula which is in agreement with that of Schiff.[3]

It may be of some interest to compare the result of Born approximation for the phase shifts and reflection coefficient with the exact result of Eq. (A.5). Upon using the potential (A.1) and the approximations of Eqs. (22), we obtain

$$\tan\delta_\pm \approx k_0^2(ka \pm \sin ka)/4k^2 \quad (A.6)$$

$$R \approx \left\{1 + \frac{[2k^2 + k_0^4(k^2a^2 - \sin^2 ka)/k^2]^2}{k_0^4 \sin^2 ka}\right\}^{-1}. \quad (A.7)$$

The result (A.7) is qualitatively very similar to (A.5). For $ka = n\pi$, both formulas yield $R = 0$, i.e., transparency of the obstacle. Also, (A.7) has the correct dependence on k for small k, even though Born approximation is valid only for large k.