Determination of the Potential from Scattering Data*

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(Received December 1, 1955)

It is shown that in classical mechanics a spherically symmetric repulsive potential can be determined from the differential scattering cross section for particles of a single energy E. The potential is determined explicitly, but only outside the radius of closest approach at energy E. Higher energies are required to probe closer to the center. The results are compared with related quantum-mechanical results.

INTRODUCTION

SUPPOSE that a particle of energy E is scattered by a spherically symmetric scatterer. According to classical mechanics the particle will be scattered through an angle θ which depends upon the potential $V(r)$, the energy E, and the impact parameter b. We will show how $V(r)$ can be uniquely determined from the knowledge of θ as a function of b for a single energy E, if $V(r)$ is repulsive, i.e., is a positive monotonic decreasing function of r, and if $V(0)>E$. $V(r)$ cannot be determined for all values of r, but only for $r>r_{\min}(E)$, where $r_{\min}(E)$ is the distance of closest approach at energy E, i.e., the largest root of $V(r_{\min})=E$. This limitation is to be expected since the potential inside $r_{\min}$ does not affect the scattering of particles of energy E, and therefore scattering data at energy E cannot determine the potential inside $r_{\min}$. It would be necessary to use a higher energy to probe nearer the center of the potential.

In scattering experiments the measured quantity is the differential scattering cross section $\sigma(\theta)=-(b/\sin\theta)(db/d\theta)$ rather than $\theta(b)$. However, from the differential cross section and its definition we can determine $\theta(b)$ by integration. Since $\theta=\pi$ when $b=0$, we obtain

$$\int_\theta^\pi \sigma(\theta)\,\sin\theta d\theta=b^2/2. \tag{1}$$

Thus we can restate our result as follows: given the differential scattering cross section $\sigma(\theta)$ at a single energy E, we can uniquely determine $V(r)$ for $r>r_{\min}(E)$.

It is interesting to compare this result with related quantum-mechanical results.[1] The latter require knowledge of the scattered wave for all energies E and they determine V for all r. On the other hand, they do not require the whole function $\sigma(\theta)$ but only the phase shift for any one angular momentum l. However, the potential is not uniquely determined unless there are no bound states with this value of l. Otherwise a number of parameters equal to the number of bound states must also be known in order to determine the potential uniquely. Our result is restricted to decreasing potentials, for which there are not bound states. If V is not monotonically decreasing, or if $V(0)<E$, additional data must also be given in order to determine V uniquely.[2] Wheeler,[3] using the W.K.B. method, has shown that in the quantum-mechanical problem $V(r)$ can be determined from *all* the phase shifts for a *single* E. This result is similar to ours, since we require $\sigma(\theta)$ for *all* θ and a *single* E. This similarity is to be expected because of the relation between classical mechanics and the W.K.B. approximation in quantum mechanics.

METHOD OF SOLUTION

In classical mechanics, θ is related to b and $V(r)$ by the equation

$$\theta(b)=\pi-2\int_{r_0}^\infty \frac{dr}{r^2[b^{-2}-r^{-2}-V(r)E^{-1}b^{-2}]^{\frac{1}{2}}}. \tag{2}$$

In (2) r_0 is the largest root of the denominator. It is convenient to introduce the new variables $x=b^{-2}$ and $u=r^{-1}$ and to regard θ as a function of x, and V as a function of u. Then (2) becomes

$$\theta(x)=\pi-2\int_0^{u_0} \frac{du}{[x(1-VE^{-1})-u^2]^{\frac{1}{2}}}. \tag{3}$$

We now define the functions $v(u)$ and $w(u)$ by

$$v(u)=1-V(u)E^{-1},\quad w=u^2v^{-1}. \tag{4}$$

In terms of v and w, (3) becomes

$$\frac{\pi-\theta(x)}{2}=\int_0^x \frac{g(w)dw}{(x-w)^{\frac{1}{2}}}, \tag{5}$$

* The research reported in this article has been made possible through support and sponsorship extended by the U. S. Air Force, Air Force Cambridge Research Center.

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where $g(w)=v^{-\frac{1}{2}}du/dw$. In (5), to determine the lower limit, we have made use of the fact that the potential vanishes at $r=\infty$, that is, at $u=0$.

Equation (5) may be considered to be an integral equation for the determination of $g(w)$. Since it is of Abel type, it can be solved explicitly with the result

$$g(w)=\frac{d}{dw}\left[\frac{1}{2\pi}\int_0^w \frac{\pi-\theta(x)}{(w-x)^{\frac{1}{2}}}dx\right]. \tag{6}$$

Now, from (4), the relation between v and $g(w)$ is given by

$$v^{-\frac{1}{2}}\frac{du}{dw}=\frac{1}{2\sqrt{w}}+\frac{\sqrt{w}}{2v}\frac{dv}{dw}=g(w).$$

Solving this equation for v in terms of $g(w)$, noting that $v=1$ when $w=0$, we obtain

$$v=\exp\int_0^w\left[\frac{2g(w)}{\sqrt{w}}-\frac{1}{w}\right]dw. \tag{7}$$

Since $g(w)$ is given by (6), we see that (7) yields v in terms of w. Then (4) yields the potential $V(u)$ in the following parametric form, with w as parameter:

$$V=E[1-v]; \quad u=(wv)^{\frac{1}{2}}. \tag{8}$$

Thus to determine V we obtain θ as a function of $x=b^{-2}$ from (1), use this result in (6) to compute $g(w)$, insert $g(w)$ into (7) to get v in terms of w, and finally compute u and V from (8).

This calculation can be simplified by integrating by parts in (6), which yields

$$g(w)=\frac{d}{dw}\left[w^{\frac{1}{2}}-\frac{1}{\pi}\int_0^w (w-x)^{\frac{1}{2}}\theta'(x)dx\right]$$
$$=\frac{1}{2\sqrt{w}}+\frac{1}{2\pi}\int_0^w\frac{\theta'(x)}{(w-x)^{\frac{1}{2}}}dx. \tag{9}$$

Now changing the integration variable to θ, and noting that $\theta(0)=0$, we obtain

$$g(w)=\frac{1}{2\sqrt{w}}+\frac{1}{2\pi}\int_0^{\theta(w)}\frac{d\theta}{[w-x(\theta)]^{\frac{1}{2}}}. \tag{10}$$

Thus (7) becomes

$$v=\exp\frac{1}{\pi}\int_0^w\frac{1}{\sqrt{w'}}\int_0^{\theta(w')}\frac{d\theta}{[w'-x(\theta)]^{\frac{1}{2}}}dw'. \tag{11}$$

Now to determine V we merely compute $x(\theta)$ from (1), then $v(w)$ from (11), and finally obtain u and V from (8).

It should be observed that if $(wv)^{\frac{1}{2}}$ in (8) never exceeds some upper bound $u_{\max}$, then V is determined by (8) only for values of $u<u_{\max}$; i.e., for $r>r_{\min}=1/u_{\max}$. This occurs if the integral in (7) has a limit as $w\to\infty$ which is the case if $\pi-\theta(x)$ decreases faster than $x^{-\frac{1}{2}}=b$ as $b\to 0$.

Two examples of the use of our result will now be presented.

Example I. Rutherford Scattering

Consider the Rutherford scattering formula,

$$\sigma(\theta)=\frac{A}{4\sin^4(\theta/2)}, \tag{12}$$

where $A=e^2/4E^2$. From (1) we obtain

$$x=A^{-1}\tan^2(\theta/2), \quad \theta=2\tan^{-1}[(Ax)^{\frac{1}{2}}]. \tag{13}$$

Now using (13) in (11) yields

$$v=\exp\frac{1}{\pi}\int_0^w\frac{1}{\sqrt{w'}}\times\int_0^{2\tan^{-1}[(Aw')^{\frac{1}{2}}]}\frac{d\theta}{[w'-A^{-1}\tan^2(\theta/2)]^{\frac{1}{2}}}dw'. \tag{14}$$

To evaluate the θ integral, we introduce the new variable ϕ by

$$\tan(\theta/2)=(Aw')^{\frac{1}{2}}\sin\phi. \tag{15}$$

Then we have

$$\int_0^{2\tan^{-1}[(Aw')^{\frac{1}{2}}]}\frac{d\theta}{[w'-A^{-1}\tan^2(\theta/2)]^{\frac{1}{2}}}=2A^{\frac{1}{2}}\int_0^{\pi/2}\frac{d\phi}{1+Aw'\sin^2\phi}=\frac{\pi\sqrt{A}}{(1+Aw')^{\frac{1}{2}}}. \tag{16}$$

Using (16) in (14) yields, upon integration,

$$v=1+2Aw+2[Aw(2+Aw)]^{\frac{1}{2}}. \tag{17}$$

If we use (17) in (8), we can eliminate v and then solve for v in terms of u; thus we obtain

$$V=2EA^{\frac{1}{2}}u=eu=e/r. \tag{18}$$

This is, of course, the Coulomb potential from which (12) was obtained.

Example II. Inverse Square Potential

Let us now consider the cross section

$$\sigma(\theta)=\frac{e[1-(\theta/\pi)]}{\pi E\sin\theta(\theta/\pi)^2[2-(\theta/\pi)]^2}. \tag{19}$$

Inserting this into (1) yields

$$x=\frac{E}{e}\left[\left(1-\frac{\theta}{\pi}\right)^{-2}-1\right],\quad \theta=\pi\left[1-\left(1+\frac{ex}{E}\right)^{-\frac{1}{2}}\right]. \tag{20}$$

Upon substituting (20) into (11), we obtain

$$v=\exp\frac{1}{\pi}\int_0^w \frac{1}{\sqrt{w'}} \times\int_0^{\pi[1-(1+ew'/E)^{-\frac{1}{2}}]} \frac{d\theta}{\{w-(E/e)[(1-\theta/\pi)^{-2}-1]\}^{\frac{1}{2}}}dw'. \tag{21}$$

After evaluating the θ integral, we have

$$v=\exp\int_0^w \frac{(e/E)dw}{1+(ew/E)} =\exp\left[\log\frac{1}{1+(ew/E)}\right]=\frac{1}{1+(ew/E)}. \tag{22}$$

Now from (8), $w=u^2v^{-1}$, so (22) yields

$$v=1-(e/E)u^2. \tag{23}$$

Then, using (8) again, we have

$$V=E(1-v)=eu^2=e/r^2. \tag{24}$$

The inverse square potential (24) is just the one from which the cross section (19) was originally obtained.

PHYSICAL REVIEW VOLUME 102, NUMBER 2 APRIL 15, 1956

Calculation of the Scattering Potential from Reflection Coefficients*

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(Received November 17, 1955)

It is shown how the scattering potential can be calculated from suitably defined reflection coefficients in the case of the one- and three-dimensional reduced wave equations by means of a formal series expansion. The more general problem of calculating scattering potentials from elements of the scattering operator is also discussed and it is shown that to calculate the scattering potential it is often sufficient to prescribe the representation in which it is to be diagonal.

1. INTRODUCTION AND SUMMARY

JOST and Kohn[1] have developed a procedure for finding spherically symmetric potentials from scattering phases. This problem is simplified by the fact that the solutions of the radial equation are not degenerate.

It has been found possible to generalize their procedure to cases where the outgoing eigenfunctions are degenerate. One is able to show that in many cases the scattering potential can be obtained from certain elements of the scattering operator, provided one specifies the representation in which V is to be diagonal.

In the present paper the method is applied to the one- and three-dimensional scattering problems, where the scattering potential V is assumed to be a function (not necessarily symmetric) of the space variables. It is shown that in the one-dimensional case, the potential can be obtained from the reflection coefficient at one end. The potential is calculated explicitly to the first two orders in the reflection coefficient where it is shown that the results are the same as those obtained using the Gelfand-Levitan procedure.[2,3]

In the three-dimensional case it is shown that the potential can be obtained from the amplitudes of the spherical waves reflected back along the rays on which the incident plane waves are sent, the totality of such rays being those pointing out at right angles to a hemisphere whose center is at the origin.

The general procedure for obtaining the scattering potential from the scattering operator is also discussed. It is shown that one must specify the representation in which V is diagonal to get a unique answer.

We restrict our discussion to cases in which the unperturbed and perturbed Hamiltonians have purely continuous spectra which coincide. However, it is possible to generalize the results to cases where the

* The research reported in this article was done at the Institute of Mathematical Sciences, New York University, and has been made possible through support and sponsorship extended by Geophysics Research Directorate, Air Force Cambridge Research Center.

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