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# Calculation of a Perturbing Central Field of Force from the Elastic Scattering Phase Shift

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It has been shown that the interaction potential between two particles can be uniquely determined from the supposed knowledge of the observed phase shifts for the whole energy range, but for only one particular angular momentum. Coulomb forces between charged particles, as well as all kinds of inelastic scattering, have so far not been considered.

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It is well known that the fraction of particles scattered by an angle $\vartheta$ through a unit solid angle by a central field of force is given by the expression

$$|(1/k)\sum_l(2l+1)P_l(\cos\vartheta)e^{i\eta_l}\sin\eta_l|^2, \tag{1}$$

where $\eta_l$ is the so-called phase shift defined by the asymptotic behavior of the radial wave functions

$$\begin{aligned} c_1r^{l+1}&\leftarrow v_1\rightarrow\sin(kr-l(\pi/2)+\eta_l),\\ c_2r^{-l}&\leftarrow v_2\rightarrow\cos(kr-l(\pi/2)+\eta_l),\\ 0&\leftarrow r\;\rightarrow\infty, \end{aligned}\tag{2}$$

$v_1$ and $v_2$ being themselves solutions of the radial wave equation for angular momentum $l$,

$$\begin{aligned} &\{L+V(r)\}v=0,\\ &L=(d^2/dr^2)-[l(l+1)/r^2]+k^2,\\ &k=(2\pi/h)p=2\pi/\lambda. \end{aligned}\tag{3}$$

As we see the phase shift $\eta_l$ is uniquely determined by the interaction potential $V(r)$. Suppose, on the other hand, that the phase shift for a given $l$ is known from scattering measurements for the whole (or at least the major) part of the energy range from zero to infinity, the question arises whether, conversely, the interaction potential is uniquely determined by the phase shift. The true answer to this question, of course, must be of some importance to the judgment of the expected usefulness or necessity of introducing the so-called $S$-matrix method in quantum mechanics.

On the suggestion of W. Pauli the problem has been successfully, but rather incompletely, dealt with by C. E. Fröberg[1] in the form of solution of a certain integral equation. Because of the lack of any convergence proof, or even a clear formulation of the method itself in higher approximations, his treatment of the problem can scarcely be considered more than a first approximation, corresponding to the Born approximation in scattering theory.

In this paper we shall try to give a detailed method for calculation of the interaction potential. The starting point is the phase shift as a function of the energy expressed by a definite integral over the potential function. Since the leading idea has been to consider this phase shift as analogous to the Fourier transform of a coordinate function in the ordinary theory of Fourier integrals, we shall start with some preliminary considerations which, I hope, will make the understanding easier.

Consider the Fourier transformations:

$$\begin{aligned} F(r)&=(4/\pi)\int_0^\infty G(k)\,\sin 2krdk,\\ G(k)&=\int_0^\infty F(r)\,\sin 2krdr. \end{aligned}\tag{4}$$

We can find the condition for the validity of these transformations in the whole region $0\leq r\leq\infty$, $0\leq k\leq\infty$, of the variables by introducing one of the transformations into the other. We shall then find that some improper product integrals have to be $\delta$-functions. For instance, the integral

$$\begin{aligned} &\lim_{K\to\infty}(4/\pi)\int_0^K \sin 2kr\,\sin 2kr'dk\\ &\quad=\lim_{K\to\infty}\left\{\frac{\sin 2K(r-r')}{\pi(r-r')}-\frac{\sin 2K(r+r')}{\pi(r+r')}\right\}\\ &\quad=\delta(r-r')-\delta(r+r') \end{aligned}\tag{5}$$

[1] Carl-Erik Fröberg, Phys. Rev. 72, 519 (1947).

is a difference of two δ-functions, the second of them being insignificant in the case of positive values of $r$. For $r=0$, however, the two terms are equal, leading to a zero value of the function $F(r)$ represented by the Fourier integral. This of course also follows directly from Eqs. (4).

Now introducing

$$f(r) = -F'(r), \quad F(r) = \int_r^\infty f(r)dr, \tag{6}$$

$f(r)$ being an integrable function in the region $r\to\infty$, we get

$$f(r) = -(4/\pi)\int_0^\infty G(k)(d/dr)\sin 2krdk,$$

$$kG(k) = \int_0^\infty f(r)\sin^2 krdr. \tag{7}$$

These transformations, of course, are equivalent to ordinary Fourier cosine integrals in the case of

$$F(0) = \int_0^\infty f(r)dr = 0.$$

In the case of $F(0)\neq 0$, the transformations may give rise to some improper integrals. Therefore, when applying analogous formulae from the theory that is to follow one should examine separately the convergence of the integrals.

By introducing the expressions

$$\begin{aligned} &u_1 = v_1 = \sin kr, \quad u_2 = v_2 = \cos kr, \\ &Y_k(r) = u_1 v_1, \quad Z_k(r) = u_1 v_2 + u_2 v_1, \end{aligned} \tag{8}$$

the transformations (7) obviously can be written

$$f(r) = -(4/\pi)\int_0^\infty G(k)Z_k'(r)dk,$$

$$kG(k) = \int_0^\infty f(r)\,Y_k(r)dr, \tag{9}$$

and this is the form we shall meet in the following transformations of a potential function to its scattering phase shift and *vice versa*.

We now make use of the solutions

$$\begin{aligned} &C_1 r^{l+1} \leftarrow u_1 \rightarrow \sin(kr - l(\pi/2) + \xi(k)), \\ &C_2 r^{-l} \leftarrow u_2 \rightarrow \cos(kr - l(\pi/2) + \xi(k)), \\ &0 \leftarrow r \rightarrow \infty, \end{aligned} \tag{10}$$

of an auxiliary equation,

$$\{L+U\}u = 0, \tag{11}$$

with some approximate potential function $U(r)$. With a good starting function the calculations would be easier. Usually, however, we shall have to start with the function $U=0$.

From Eqs. (3) and (11) we now easily obtain

$$k\sin(\eta-\xi) = \int_0^\infty (V-U)\,Y_k(r)dr, \quad Y_k = u_1 v_1, \tag{12}$$

an equation which is well known and frequently quoted in the case of $U=0$ and $\xi=0$. Comparison with (9) suggests the existence of an inverted equation

$$\begin{aligned} &V-U = -(4/\pi)\int_0^\infty \sin(\eta-\xi)Z_k'(r)dk, \\ &Z_k(r) = u_1 v_2 + u_2 v_1. \end{aligned} \tag{13}$$

The condition for the validity of Eqs. (12) and (13) may be written

$$-(4/\pi)\int_0^\infty (1/k)\,Y_k(r)Z_{k'}'(r)dr = \delta(k-k') \tag{14}$$

or

$$-(4/\pi)\int_0^\infty (1/k)\,Y_k(r')Z_k'(r)dk = \delta(r-r'). \tag{15}$$

The equations are obviously equivalent, but so far it has not been possible to prove directly the validity of (15). Hence, we should have to prove Eq. (14), but we shall rather prove the equation

$$(4/\pi)\int_0^\infty (1/k)\,Y_k'(r)Z_{k'}'(r)dr = \delta(k-k'), \tag{16}$$

which differs from (14) only by the term

$$\lim_{R\to\infty}\left\{-\frac{4}{\pi}\frac{1}{k}Y_k(R)\sin(2k'R - l\pi + \eta(k') + \xi(k'))\right\}.$$

This term makes no difference because an integration with respect to $dk'$ gives zero.

## PROOF OF THE COMPLETENESS RELATION

The proof of Eq. (16) is based exclusively upon the differential equations (3) and (11), defining the functions $u$ and $v$ together with the asymptotic values of the functions when $r\rightarrow\infty$. In this way we avoid all kinds of complicated transformation theorems analogous to those already established, as for instance in the theory of Bessel functions.

To clarify the idea, consider once more the simplest case of $U=V=0$, $l=0$,

$$\begin{aligned} &Y_k'''+4k^2Y_k'=0, \quad (1/k)Y_k'\rightarrow\sin 2kr, \\ &Z_k''+4k^2Z_k=0, \qquad Z_k\rightarrow\sin 2kr, \\ &\qquad\qquad r\rightarrow\infty. \end{aligned} \tag{17}$$

If we replace $k$ by $k'$ in the last equation, multiply by $Z_{k'}$ and $Y_k$, respectively, subtract, and integrate, we obtain

$$\begin{aligned} \frac{4}{\pi}\int_0^R \frac{1}{k}Y_k'Z_{k'}dr &= \frac{Y_k'(R)Z_{k'}'(R)-Y_k''(R)Z_{k'}(R)}{\pi k(k^2-k'^2)} \\ &= \frac{\sin 2R(k-k')}{\pi(k-k')}-\frac{\sin 2R(k+k')}{\pi(k+k')} \\ &= \delta(k-k')-\delta(k+k'), \text{ when } R\rightarrow\infty. \end{aligned} \tag{18}$$

In the general case of arbitrary $U$, $V$, and $l$ the functions $Y_k$ and $Z_k$ are obeying third-order equations only when $U=V$. When $U\neq V$ and, hence, $u_1$, $u_2$ is different from $v_1$, $v_2$, it can be shown that

$$\begin{aligned} &MY_k'+[4l(l+1)/r^3]Y_k+(U'+V')Y_k \\ &\qquad -(V-U)(u_1v_1'-u_1'v_1)=0, \\ &MZ_k+(u_1v_2''+u_1''v_2-2u_1'v_2'+u_2v_1'' \\ &\qquad +u_2''v_1-2u_2'v_1')=0, \\ &M=(d^2/dr^2)-[4l(l+1)/r^2]+2(U+V)+4k^2. \end{aligned} \tag{19}$$

We shall also have use for the equations

$$\begin{aligned} &(V-U)Y_k+(d/dr)(u_1v_1'-u_1'v_1)=0, \\ &(V-U)Z_k+(d/dr)(u_1v_2'-u_1'v_2 \\ &\qquad +u_2v_1'-u_2'v_1)=0, \end{aligned} \tag{20}$$

$$\begin{aligned} &Y_k\left[\frac{d}{dr}(MZ_k)-\frac{4l(l+1)}{r^3}Z_k-(U'+V')Z_k\right] \\ &\quad =[u_1v_2'-u_1'v_2+u_2v_1'-u_2'v_1](V-U)Y_k. \end{aligned}$$

We now change $k$ into $k'$ in $Z_k$ and corresponding product functions with different subscripts, like $u_1v_2$. If we combine Eqs. (19) in the same way as Eqs. (17), we obtain, after some rearrangements,

$$\begin{aligned} &4(k^2-k'^2)Y_k'Z_{k'}+(d/dr)[Y_k''Z_{k'}-Y_k'Z_{k'}'] \\ &\quad -(d/dr)[Y_k(u_1v_2''+u_1''v_2-2u_1'v_2' \\ &\qquad +u_2v_1''+u_2''v_1-2u_2'v_1')] \\ &\quad +(d/dr)[(u_1v_1'-u_1'v_1)(u_1v_2'-u_1'v_2 \\ &\qquad +u_2v_1'-u_2'v_1)]. \end{aligned} \tag{21}$$

Upon integration from $r=0$ to $r=R$, and as $R\rightarrow\infty$, the two last terms disappear and we are left with an equation rather similar to Eq. (18). In fact, we get

$$\begin{aligned} &\frac{4}{\pi}\int_0^\infty \frac{1}{k}Y_k'Z_{k'}dr \\ &\quad =\lim_{R\rightarrow\infty}\left\{\frac{\sin(2R(k-k')+\eta_k+\xi_k-\eta_{k'}-\xi_{k'})}{\pi(k-k')}\right. \\ &\qquad \left.-\frac{\sin(2R(k+k')+\eta_k+\xi_k+\eta_{k'}+\xi_{k'})}{\pi(k+k')}\right. \\ &\quad =\delta(k-k')-\delta(k+k'). \end{aligned} \tag{22}$$

Hence, the completeness of the product functional system and the validity of Eq. (13) have been proved.

## METHOD OF SOLUTION

Starting from Eqs. (11) and (13), we introduce a known potential $U=V_0$, which may be equal to zero, and solve Eq. (11), obtaining thereby the approximate wave functions $u_1$ and $u_2$ with the approximate phase shift $\xi$. Now we replace the unknown functions $v_1$ and $v_2$ in Eq. (13) by $u_1$ and $u_2$, thus finding an approximate value of the potential difference $V-U$. By calling this $V_1-U$ we have a first approximation $V_1$ of the unknown potential $V$.

In the next approximation we put $U=V_1$, and by solving anew Eq. (11), we obtain better approximate functions $u_1$, $u_2$ and a better approximate phase shift $\xi$. Writing again $v_1=u_1$ and $v_2=u_2$ in Eq. (13) we obtain an approximate value $V_2-V_1$ of the potential difference $V-V_1$ and so on.

This, of course, is an iteration method and we should have to prove its convergence or at least apply it to some elementary problem in order to illustrate how it works. Unfortunately, there is no simple potential law to which it could be applied without entering into calculations containing non-elementary functions and integrals. However, there is an improper potential law to which the method—with some precautions—might be applied without leading to non-elementary calculations. This is the inverse-square distance law for the potential which, for convenience, we write in the form

$$V = -(2l+1+\epsilon)\epsilon/r^2 \tag{23}$$

so that the solutions of the wave equation (3)—apart from a factor $(\pi kr/2)^{\frac{1}{2}}$—are Bessel functions of $kr$ with index numbers $\pm(l+\frac{1}{2}+\epsilon)$. The true phase shift now is $\eta = -(\pi/2)\epsilon$. Similarly, we may use an auxiliary potential

$$U = -(2l+1+\delta)\delta/r^2$$

corresponding to the approximate phase shift $\xi = -(\pi/2)\delta$.

The integral (13), of course, is then an improper, non-convergent integral. It can be made convergent, however, by the introduction of a convergence factor in the integrand. This amounts to the same as averaging over a great number of different values of the upper limit, $k=K$, of the integral when all these values tend to infinity. In this way we only eliminate oscillating terms with respect to the upper limit of the integral. With respect to the lower limit, $k\rightarrow 0$, the integral is convergent only if $|\epsilon-\delta|<2$, that is when the phase shift difference is smaller than $\pi$.

Putting now in the $(n+1)$th approximation $r^2U = r^2V_n = -(2l+1+\epsilon_n)\epsilon_n$, we find from (13) by making $\epsilon\rightarrow\epsilon_n$, that

$$\begin{aligned} r^2(V_n - V_{n+1}) &= (2l+1+2\epsilon_n)(2/\pi)\sin(\pi/2)(\epsilon-\epsilon_n) \\ &\approx (2l+1+2\epsilon_n)(\epsilon-\epsilon_n). \end{aligned} \tag{24}$$

On the other hand,

$$r^2(V_n - V) + (2l+1+\epsilon+\epsilon_n)(\epsilon-\epsilon_n). \tag{25}$$

Hence,

$$\begin{aligned} r^2(V_{n+1} - V) &= (2l+1+\epsilon+\epsilon_{n+1})(\epsilon-\epsilon_{n+1}) \\ &\approx (\epsilon-\epsilon_n)^2. \end{aligned} \tag{26}$$

By starting now from $U=V_0=0$, $\epsilon_0=0$, we obtain from (26)

$$\begin{aligned} &r^2(V_1 - V) \approx \epsilon^2, && \epsilon-\epsilon_1 \approx \epsilon^2/(2l+1), \\ &r^2(V_2 - V) \approx \epsilon^4/(2l+1)^2, && \epsilon-\epsilon_2 \approx \epsilon^4/(2l+1)^3, \\ &r^2(V_3 - V) \approx \epsilon^8/(2l+1)^6, && \epsilon-\epsilon_3 \approx \epsilon^8/(2l+1)^7, \\ &r^2(V_4 - V) \approx \epsilon^{16}/(2l+1)^{14}, \text{ etc.} \end{aligned} \tag{27}$$

These results show clearly that the convergence is extremely good in all cases where the phase difference at the starting point is not too close to the very limit of convergence.

Now in the case of an ordinary integrable potential we may argue that if it is numerically smaller than a given inverse-square potential of the form (23) the convergence will be even better than in the case considered above in (27).

Hence if an approximate starting potential $U$ can be found giving a phase shift difference $\eta-\xi$ numerically smaller than some given number in the entire energy region, we may be safe that the method outlined above is convergent. Thus it has been proved that a perturbing central field of force can be uniquely determined from the observed scattering phase shift.