Phase Series

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An expansion theorem for the calculation of the parameters occurring in the scattering cross sections has been developed. The series converges exponentially and is expressible in terms of known functions, provided the interactions are expressed as a power series in r and $1/r$.

INTRODUCTION

THE solution of problems involving the scattering of one particle by another is attended by extreme difficulties. In general, evaluation of cross sections can be obtained only in infinite series, each term of such a series containing a parameter (phase), which must be determined from a linear differential equation of the second order. The evaluation of this parameter must proceed, usually, by numerical integration of this equation. Such calculations are excessively laborious and are, furthermore, subject to numerous errors. It has seemed desirable, therefore, to derive an expansion for the phases, in series form, the convergence of which could be accurately determined. Such an expansion possesses a particular advantage which lies in the latitude permissible in the choice of function to represent the interaction between particles. This is of special importance in the evaluation of integrals involving the interaction potential and other known functions. Such integrals invariably arise, as the distortion of the wave function of one particle by another involves the values of the interaction for all distances of separation. Apart from the points mentioned, however, a series solution holds little practical superiority over the numerical integration of the differential equation.

1. First approximations

The problem to be solved is, then, the determination of $I(\theta)d\omega$, the number of particles scattered into a given solid angle $d\omega$ per unit time, when the incident beam is such that one particle crosses unit area per unit time. The series expansion for $I(\theta)$ then has the form:[1,2]

$$I(\theta)=|f(\theta)|^2, \tag{1a}$$

where

$$f(\theta)=(1/2ik)\sum(2l+1)\times[\exp(2i\delta_l)-1]P_l(\cos(\theta)), \tag{1b}$$

$$k^2=4\pi^2m^2v^2/h^2=8\pi^2mE/h^2, \tag{1c}$$

and δ_l is a constant to be determined from the equation,

$$\frac{d^2(r\psi)}{dr^2}+\left(k^2-\frac{8\pi^2mV(r)}{h^2}-\frac{(l)(l+1)}{r^2}\right)(r\psi)=0. \tag{2}$$

One selects that solution finite at the origin (or that solution of lower order singularity at the origin,[3] and determines δ_l from its behavior at infinity. δ_l is then defined by the asymptotic solution,

$$\psi\sim(1/r)\sin(kr-\tfrac{1}{2}l\pi+\delta_l). \tag{3}$$

The determination of δ_l is then the immediate point of attack. Various formulae have been given for δ_l which are due, in order, to Born,[4] Jeffreys,[5] and Massey and Mohr.[6]

$$\delta_l=-\frac{4\pi^3m}{h^2}\int_0^\infty V(r)J^2_{l+\frac{1}{2}}(kr)rdr, \tag{4}$$

$$\delta_l=\tfrac{1}{4}\pi+\tfrac{1}{2}l\pi-kr_0+\int_{r_0}^\infty(F^{\frac{1}{2}}-k)dr, \tag{5}$$

$$\delta_l=\int_{r_0'}^\infty\left[F+\frac{8\pi^2m}{h^2}V(r)\right]^{\frac{1}{2}}dr-\int_{r_0}^\infty F^{\frac{1}{2}}dr \quad (6),$$

[1] H. Faxén and J. Holtsmark, Zeits. f. Physik **45**, 307 (1927).
[2] N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions* (Clarendon Press, Oxford, 1933), first edition, p. 24.
[3] Reference 2, p. 30.
[4] Reference 2, p. 28.
[5] Jeffreys, Proc. London Math. Soc., Series 2, **23**, Part 6; or reference 2, p. 92.
[6] H. S. W. Massey and C. B. O. Mohr, Proc. Roy. Soc. **A144**, 202 (1934).

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where

$$F(r)=(8\pi^2m/h^2)(E-V(r))-l(l+1)/r^2.$$

Formula (4) is valid for small phases, that of (5) for large phases and for (6) Massey and Mohr claim accuracy for both large and small phases. Actually, all three expressions must be regarded as first approximations, not valid generally for large phases. An exact solution of (2) in finite terms has never been given, except for special choice of $V(r)$. Moreover, any expression of the solution of (2) by a simple integral of some function of $V(r)$, may be seen by actual substitution to solve this equation for $V(r)$ replaced by a function of $V(r)$ and $dV(r)/dr$. The accuracy of (5) and (6) for large phases is then dependent on the choice of $V(r)$, and unless one has some independent criterion for their accuracy, their use in calculations is somewhat hazardous. It is possible, however, to give a series for δ_l, the first term of which is the expression (4).

2. Derivation of the first-order equations

Let us suppose, considering one dimension only, that it be required to determine the conditions necessary that a function f of variables r, ξ, η satisfy Eq. (2). ξ and η are functions of ψ so chosen that

$$f(r,\xi,\eta)=r\psi; \tag{7}$$

$$\partial f(r,\xi,\eta)/\partial r=\partial(r\psi)/\partial r \tag{8}$$

for $r=r_1$ and $r=r_1+\Delta r_1$. ξ, η must then possess first derivatives defined by the following system:[7]

$$\frac{\partial f}{\partial\xi}\frac{d\xi}{dr}+\frac{\partial f}{\partial\eta}\frac{d\eta}{dr}=0, \tag{9}$$

$$\frac{\partial^2 f}{\partial\xi\partial r}\frac{d\xi}{dr}+\frac{\partial^2 f}{\partial\eta\partial r}\frac{d\eta}{dr}=-\left(\frac{\partial^2 f}{\partial r^2}+H_\psi f\right), \tag{10}$$

where $H_\psi(r)$ has been set for the coefficient of $(r\psi)$ in (2). In particular, if one takes f as a linear function of ξ and η,

$$f=\xi\varphi_1+\eta\varphi_2, \tag{11}$$

where φ_1 and φ_2 both satisfy the condition

$$\partial^2\varphi/\partial r^2=-(H_\varphi)(\varphi), \tag{12}$$

one has the system

$$d\xi/dr-(\varphi_1\varphi_2\xi+\varphi_2{}^2\eta)(H_\psi-H_\varphi)/W(\varphi)=0, \tag{13}$$

$$d\eta/dr+(\varphi_1{}^2\xi+\varphi_1\varphi_2\eta)(H_\psi-H_\varphi)/W(\varphi)=0, \tag{14}$$

where $W(\varphi)$ indicates the Wronskian of φ_1, φ_2,

$$W(\varphi)=\varphi_1(\partial\varphi_2/\partial r)-\varphi_2(\partial\varphi_1/\partial r). \tag{15}$$

The Wronskian, under the condition (12), is a constant for all values of r[8].

It is a simple matter to confirm that (11) does actually satisfy (2) provided that also (12) and (13) are satisfied.

Equations (13) and (14) may, for convenience, be written in matrix form.

$$\begin{pmatrix}\xi\\ \eta\end{pmatrix}-\int_c^r\begin{pmatrix}\varphi_1\varphi_2, & \varphi_2{}^2\\ -\varphi_1{}^2, & -\varphi_1\varphi_2\end{pmatrix}\times\left(\frac{H_\psi-H_\varphi}{W(\varphi)}\right)\begin{pmatrix}\xi\\ \eta\end{pmatrix}dr=\begin{pmatrix}\xi_c\\ \eta_c\end{pmatrix}, \tag{16}$$

where ξ_c and η_c are arbitrary values assigned to ξ and η for $r=c$.

3. Solution of the integral equation

Equation (16) is a Volterra integral equation, of the second kind, for the unknowns ξ and η. If one denotes the unknown matrix by y, the constant matrix by $g(c)$, the solution is given by the series:[9]

$$y=g(c)+\sum_1^\infty K_jg(c), \tag{17}$$

where K is so defined that

$$K_j=\int_c^r K(r_j)dr_j\int_c^{r_j}K(r_{j-1})dr_{j-1}\cdots\times\int_c^{r_2}K(r_1)dr_1 \tag{18}$$

and K denotes the four-component matrix of (16).

[7] This procedure has some resemblance to that of A. Schuchowitzky and M. Olewsky, Physik. Zeits. Sowjetunion, 11.5 pp. 498–512 (1937). They however, use finite intervals, and after determining some parameters so as to assure continuity of the wave function, the remainder are evaluated by use of the variational principle.

[8] The derivative vanishes identically.

[9] Gerhard Kowalewski, *Integral Gleichungen* (Walter de Gruyter and Co., Berlin, 1930), first edition, pp. 49–90. See also E. G. C. Poole, *Theory of Linear Differential Equations* (Oxford Clarendon Press, 1936), Chapter I, for discussions on the convergence and uniqueness of the expansion.

One may easily demonstrate the convergence of (17) as follows: If φ_1 and φ_2 are finite in the interval r to c, let us replace each element of the matrix by M^2 where M exceeds both φ_1 and φ_2 over the entire interval. Also, let us take the absolute value of $H_\psi - H_\varphi$ at every point in the interval. One then obtains a series, term by term larger than (17), of the form,

$$\begin{pmatrix}\xi_c\\ \eta_c\end{pmatrix}+\sum_{j=1}^{\infty}\frac{1}{j!}\left[\int_c^r\left|\frac{H_\psi-H_\varphi}{W(\varphi)}\right|\right.\times 2M^2\begin{pmatrix}1\\1\end{pmatrix}\left(\frac{\xi_c+\eta_c}{2}\right). \quad (19)$$

The series (17) thus is absolutely convergent and summable in any order,[10] provided $|(H_\psi)-(H_\varphi)|$ is integrable in the interval c, r. The series likewise will still converge as r approaches infinite values, provided the integral converges.

4. Differential equation for δ_l

In order to evaluate the series (17) it is convenient to use a vector representation instead of a matrix representation. One then considers the pair as a two-component vector and the matrix of four elements as a product (dyadic) of two two-component vectors, which are

$$\varphi \equiv (\varphi_1, \varphi_2); \quad \bar{\varphi} \equiv (\varphi_2, -\varphi_1). \quad (20), (21)$$

φ and $\bar{\varphi}$ are thus mutually perpendicular.

If one denotes the vector ξ, η by P, then corresponding to (13) and (14), one has,

$$dP/dr - \bar{\varphi}(\varphi\cdot P)(H_\psi - H_\varphi)/W(\varphi) = 0, \quad (22)$$

where $\varphi\cdot P$ denotes the scalar product $\varphi_1\xi + \varphi_2\eta$.

One may set P equal to the product of a scalar and a unit vector of components $\cos\gamma$ and $\sin\gamma$. The resulting equation for γ is,

$$\frac{d\gamma}{dr}+\frac{(\varphi_1^2+\varphi_2^2)(H_\psi-H_\varphi)}{W(\varphi)}\sin^2(\gamma+\alpha)=0, \quad (23)$$

where $\tan\alpha \equiv \varphi_1/\varphi_2$.

γ may be identified with the phase angle δ_l, depending on asymptotic behavior of φ_1 and φ_2 at infinity. As a particular example, if $\varphi_1 = \sin(kr)$, $\varphi_2 = \cos(kr)$, then $\gamma_{r\to\infty} = \delta_l + l\pi/2$.

From (23), one may derive the perturbation formula

$$\gamma=\gamma_0-\exp\{-G_1\}\int\exp\{+G_1\}G_2(H_\psi-H_\psi{}^0)dr, \quad (24)$$

where

$$G_1=\int\left(\frac{\varphi_1^2+\varphi_2^2}{W(\varphi)}\right)(H_\psi{}^0-H_\varphi)\sin 2(\gamma_0+\alpha)dr;$$

$$G_2=\left(\frac{\varphi_1^2+\varphi_2^2}{W(\varphi)}\right)\sin^2(\gamma_0+\alpha)$$

by setting γ equal to $\gamma_0+(\gamma-\gamma_0)$, where γ_0 satisfies (23) for the potential $V(r^0)$. The Born formula (4) is a less accurate expression, obtained by equating γ_0 to zero, and retaining only term linear in V. Another perturbation formula could be obtained by using the Picard second approximation[11] on (23).

One may also formulate the eigenvalue problem from (23), for δ_l by requiring the solution of the following equation to approach zero as r approaches infinity:

$$\frac{d\gamma}{dr}+\frac{1}{k}\left(\frac{8\pi^2 m}{h^2}V(r)+\frac{l(l+1)}{r^2}\right)\times\sin^2\left\{\gamma+kr-\frac{l\pi}{2}+\delta_l\right\}=0. \quad (25)$$

It is not the only solution as the addition of any multiple of π to the solution of (25) is also an acceptable solution.

5. Explicit series for δ_l

Using (22), one may write (17) in the following manner,

$$\xi=\xi_c+\sum_{j=1}^{\infty}\int_c^r dr_j\cdots dr_2\int_c^{r_2}\varphi_2(r_j)\{\varphi_1\xi_c+\varphi_2\eta_c\}\prod^{j\to1}\Gamma(s)\cdot\prod^{j\to2}\{\varphi_1(r_s)\varphi_2(r_{s-1})-\varphi_2(r_s)\varphi_1(r_{s-1})\}dr_1, \quad (26)$$

$$\eta=\eta_c-\sum_{j=1}^{\infty}\int_c^r dr_j\cdots dr_2\int_c^{r_2}\{\varphi_1\xi_c+\varphi_2\eta_c\}\varphi_1(r_j)\prod^{j\to1}\Gamma(s)\cdot\prod^{j\to2}\{\varphi_1(r_s)\varphi_2(r_{s-1})-\varphi_2(r_s)\varphi_1(r_{s-1})\}dr_1, \quad (27)$$

[10] E. T. Whittaker and G. N. Watson, *Modern Analysis* (Cambridge University Press, 1935), fourth edition, pp. 18–28.
[11] E. G. C. Poole, reference 9.

where $\Gamma(s)=[H_\psi(r_s)-H_\varphi(r_s)]/W(\varphi)$ and the following inequalities hold,

$$r_j>r_{j-1}>r_{j-2}\cdots>r_2>r_1. \tag{27a}$$

The ratio of ξ to η then determines the phase δ_l. In the event ξ_c and η_c are not specified, and φ_1 is bounded at the origin, ξ_c and η_c are replaced by 1 and 0, and c is taken to be zero. This procedure is permissible, however, only when the series still converges. In general this will hold provided $H_\psi-H_\varphi$ is everywhere finite, and decreases faster than $1/r$ as r approaches infinity.[12]

If one employs the functions $r^{\frac{1}{2}}J_{l+\frac{1}{2}}(kr)$ and $r^{\frac{1}{2}}J_{-l-\frac{1}{2}}(kr)$ for φ_1 and φ_2 in (26) and (27), the Wronskian of φ becomes $(-1)^{l+1}(2/\pi)$, and $H_\psi-H_\varphi$ becomes $-8\pi^2 mV(r)/h^2$. To terms of the second order, then, one has for δ_l, with $c=0$, $\xi_0=1$, $\eta_0=0$,

$$\begin{aligned}\delta_l=&-\frac{4\pi^3m}{h^2}\int_0^\infty J^2_{l+\frac{1}{2}}(kr)rV(r)dr+(-1)^l\frac{16\pi^2m^2}{h^4}\int_0^\infty J^2_{l+\frac{1}{2}}(kr)rV(r)dr\int_0^\infty J_{-l-\frac{1}{2}}(kr)J_{l+\frac{1}{2}}(kr)rV(r)dr\\&+(-1)^{l+1}\frac{16\pi^2m^2}{h^2}\int^\infty dr_2\int_0^{r_2}\{J_{l+\frac{1}{2}}(kr_2)J_{-l-\frac{1}{2}}(kr_1)-J_{-l-\frac{1}{2}}(kr_2)J_{l+\frac{1}{2}}(kr_1)\}\cdot J_{l+\frac{1}{2}}(kr_2)J_{-l-\frac{1}{2}}(kr_1)\{r_2r_1V(r_2)V(r_1)dr_1\}.\end{aligned} \tag{28}$$

In general, for the choice of functions given above, one may write for tan δ_l, the following quotient,

$$\tan\delta_l=(-1)^l\frac{(-1)^{l+1}\dfrac{4\pi^3m}{h^2}\displaystyle\int_0^\infty J^2_{l+\frac{1}{2}}(kr)drrV(r)+\sum_{j=2}^\infty a_j}{1+(-1)^l\dfrac{4\pi^3m}{h^2}\displaystyle\int_0^\infty J_{-l-\frac{1}{2}}(kr)J_{l+\frac{1}{2}}(kr)rV(r)dr+\sum_{j=2}^\infty b_j}, \tag{29}$$

where

$$\begin{aligned}a_j=-\left[(-1)^l\frac{4\pi^3m}{h^2}\right]^j\int_0^\infty dr_j\cdots dr_2\int_0^{r_2}\prod^{j\to2}\{J_{l+\frac{1}{2}}(kr_s)J_{-l-\frac{1}{2}}(kr_{s-1})-J_{-l-\frac{1}{2}}(kr_s)J_{l+\frac{1}{2}}(kr_{s-1})\}\\\cdot\prod^{j\to1}\{r_sV(r_s)\}J_{l+\frac{1}{2}}(kr_j)J_{l+\frac{1}{2}}(kr_1)dr_1\end{aligned} \tag{30}$$

and

$$\begin{aligned}b_j=\left[(-1)^l\frac{4\pi^3m}{h^2}\right]^j\int_0^\infty dr_j\cdots dr_2\int_0^{r_2}\prod^{j\to2}\{J_{l+\frac{1}{2}}(kr_s)J_{-l-\frac{1}{2}}(kr_{s-1})-J_{-l-\frac{1}{2}}(kr_s)J_{l+\frac{1}{2}}(kr_{s-1})\}\\\cdot\prod^{j\to1}\{r_sV(r_s)\}J_{-l-\frac{1}{2}}(kr_j)J_{l+\frac{1}{2}}(kr_1)dr_1.\end{aligned} \tag{31}$$

If the range of the potential $V(r)$ is not too great, one may use an approximation for $\varphi_1(r_s)\varphi_2(r_{s-1})-\varphi_2(r_s)\varphi_1(r_{s-1})$, obtained by expanding the functions φ_1 and φ_2 of r_{s-1}, about the point $r=r_s$. Retaining only the first term, one has,

$$\varphi_1(r_s)\varphi_2(r_{s-1})-\varphi_2(r_s)\varphi_1(r_{s-1})=-(r_s-r_{s-1})W(\varphi), \tag{32}$$

where the Wronskian $W(\varphi)$ is a constant.

Three factors limit the magnitude of (30) and (31): the inequalities (27a), the range of $V(r)$, and the form of the integrand, (32). The range is a constant, and one may easily see that the approximation (32) is less serious the higher the order of a_j or b_j.

[12] The asymptotic form of the wave function is periodic with respect to ($kr-$const.$\times\log r$). Reference 2, Chapter III; reference 10, Chapter XVI, for $V\sim 1/r$.

6. Application to various models

When the interaction potential is such that ξ_c and η_c of (26) and (27) can be determined ($c>0$), it is possible to use simpler functions than those employed in (29). A more convenient set is r^{l+1} and r^{-l}. With this choice one finds that $H_\psi - H_\varphi = k^2 - 8\pi^2 m V/h^2$. Now if $V(r)=\infty$, $0<r<c$. $V(r)=\sum \mu_j r^{-v_j}$, $c<r<d$ then one may set $\xi_c = c^{-l-1}$, $\eta_c = -c^l$ and calculate $\xi\cdot\eta$, $\partial\xi/\partial r$, and $\partial\eta/\partial r$, in known functions for $r=d$. At this point the solution may be joined to that given by the functions $r^{\frac{1}{2}}J_{l+\frac{1}{2}}(kr)$ and $r^{\frac{1}{2}}J_{-l-\frac{1}{2}}(kr)$ and again one may determine from the asymptotic behavior at infinity, the phase δ_l.

Instead of taking $V(r)$ to be infinite for $0<r<c$, one may also assume $V(r)=\sum G_j r^j$, $0<r<c$. Again the functions r^{l+1}, r^{-l} may be employed to determine ξ_c and η_c, repeating the previous analysis.

It is possible to show that the series (26) and (27), with the above choice of functions, is absolutely convergent, being less than the corresponding series, near the origin

$$\sum 2^j \frac{\left[\int_0^r \left| k^2 - \frac{8\pi^2 m}{h^2} V(r) \right| r dr\right]^j}{j!(2l+1)^j}. \tag{33}$$

One may, therefore, treat potentials, with these functions, which are singular at the origin, provided such singularities are of an order less than the inverse square.