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On the Phase Shifts in Scattering Problems

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竹原敏夫：散乱問題における位相のずれについて

Let us consider a collision between two particles in three dimensions. The problem of the non-relativistic motion of two particles is reduced to the relative motion in the center-of-mass coordinate system, when the interaction depends on their relative positions. We calculate the result of a collision process in the center-of-mass system in which a particle of reduced mass m and an initial positive kinetic energy E collides with a fixed scattering center. If the potential energy is spherically symmetric, so that the interaction $V(r)$ depends only on the distance r from the origin, the Schrödinger wave equation can be separated in spherical coordinates.

The radial equation may be written in the form

$$\frac{d^2\chi_l}{dr^2}+\left[k^2-U(r)-\frac{l(l+1)}{r^2}\right]\chi_l=0 \tag{1}$$

where $\quad k^2=\frac{2mE}{\hbar^2}, \qquad U(r)=\frac{2mV(r)}{\hbar^2}$

It will be assumed that $U(r)$ is negligible for r greater than some distance a, provided that $U(r)$ falls off more rapidly than $1/r$; in cases of practical interest, a may be small enough so that l term in (1) is not negligible. For large r, therefore, Eq. (1) becomes

$$\frac{d^2\chi_l^2}{dr^2}+\left[k^2-\frac{l(l+1)}{r^2}\right]\chi_l=0 \tag{2}$$

The solutions of Eq. (2) may be written

$$f_l^+(r)=\sqrt{\frac{\pi kr}{2}}\,J_{l+\frac{1}{2}}(kr),$$
$$f_l^-(r)=\sqrt{\frac{\pi kr}{2}}\,J_{-l-\frac{1}{2}}(kr) \tag{3}$$

$J_{\pm(l+\frac{1}{2})}(kr)$ being ordinary Bessel functions of half-odd-integer order. f_l^+ vanishes as r^{l+1} at $r=0$, while f_l^- has a singularity as r^{-l}.

From a physical point of view, we interest the solution of Eq. (1) that vanishes at $r=0$. The boundary condition at $r=0$ that χ_l vanishes determines the asymptotic form. The asymptotic form of χ_l can then be written

$$\chi_l(r)\cong\sin(kr-\tfrac{1}{2}l\pi+\delta_l) \tag{4}$$

where the phase shift δ_l of lth partial wave depends on k, l, and the interaction $V(r)$. The phase shifts completely determine the scattering.

The phase shift δ_l is computed exactly by the following integral equation

$$\sin\delta_l=-\frac{1}{k}\int_0^\infty f_l^+(r)\,U(r)\,\chi_l(r)\,dr \tag{5}$$

A proof for this expression is found according to the relation

$$\sin\delta_l=\sin(kr-\tfrac{1}{2}l\pi+\delta_l)\cos(kr-\tfrac{1}{2}l\pi)-\cos(kr-\tfrac{1}{2}l\pi+\delta_l)\sin(kr-\tfrac{1}{2}l\pi)$$

noting that the asymptotic relation

$$\chi_l(r)\cong\sin(kr-\tfrac{1}{2}l\pi+\delta_l),\quad f_l^+(r)\cong\sin(kr-\tfrac{1}{2}l\pi),$$

$$\frac{1}{k}\;\frac{d\chi_l}{dr}\cong\cos(kr-\tfrac{1}{2}l\delta+\delta_l),\qquad \frac{1}{k}\;\frac{df_l^-}{dr}\cong\cos(kr-\tfrac{1}{2}l\pi),$$

and vanishing properties of χ_l and f_l^+ at $r=0$. Thus, we obtain

$$\sin\delta_l=\frac{1}{k}\Big[\chi_l\frac{df_l^+}{dr}-f_l^+\frac{d\chi_l}{dr}\Big]_0^\infty \tag{6}$$

Now, by means of Eqs. (2) and (3), we have

$$\chi_l\Big(\frac{d^2f_l^+}{dr^2}+k^2f_l^+-\frac{l(l+1)}{r^2}f_l^+\Big)-f_l^+\Big(\frac{d^2\chi_l}{dr^2}+k^2\chi_l-U(r)\chi_l-\frac{l(l+1)}{r^2}\chi_l\Big)$$

$$=\chi_l\frac{d^2f_l^+}{dr^2}-f_l^+\frac{d^2\chi_l}{dr^2}+f_l^+U(r)\chi_l=0$$

which is integrated over r to give

$$-\int_0^\infty f_l^+U(r)\chi_l dr=\int_0^\infty\Big(\chi_l\frac{d^2f_l^+}{dr^2}-f_l^+\frac{d^2\chi_l}{dr^2}\Big)dr=\Big[\chi_l\frac{df_l^+}{dr}-f_l^+\frac{d\chi_l}{dr}\Big]_0^\infty \tag{7}$$

From (6) and (7), we get Eq. (5).

Further, χ_l and $\chi'_{l'}$ are solutions of (1) ; δ_l and $\delta'_{l'}$ the phase shifts for the same k, but different interactions U and U', respectively. Then, it is seen by analogy

$$\sin(\delta'_{l'}-\delta_l-\tfrac{1}{2}(l'-l)\pi)$$

$$=\sin(kr-\tfrac{1}{2}l'\pi+\delta'_{l'})\cos(kr-\tfrac{1}{2}l\pi+\delta_l)-\cos(kr-\tfrac{1}{2}l'\pi+\delta'_{l'})\sin(kr-\tfrac{1}{2}l\pi+\delta_l)$$

$$=\frac{1}{k}\Big[\chi'_{l'}\frac{d\chi_l}{dr}-\chi_l\frac{d\chi'_{l'}}{dr}\Big]_0^\infty$$

Hence

$$\sin(\delta'_{l'}-\delta_l-\tfrac{1}{2}(l'-l)\pi)=-\frac{1}{k}\int_0^\infty\chi'_{l'}\Big[U'+\frac{l'(l'+1)}{r^2}-U-\frac{l(l+1)}{r^2}\Big]\chi_l dr \tag{8}$$

If now we set $l'=l$ and the difference $U'-U=\delta U$, the corresponding change of the phase shift $\delta'_{l'}-\delta_l=\delta\delta_l$ is given by

$$\delta\delta_l=-\frac{1}{k}\int_0^\infty\chi_l^2\delta U dr \tag{9}$$

Equation (9) provides the first order perturbation for the phase shifts.

If the whole interaction is taken as a perturbation, substitution of (9) into the scattering amplitude gives the Born approximation. If we put $U=U'=0$, Eq. (8) gives

$$\sin\Big((l'-l)\frac{\pi}{2}\Big)=-\frac{1}{k}\int_0^\infty f_{l'}^+\Big[\frac{l'(l'+1)}{r^2}-\frac{l(l+1)}{r^2}\Big]f_l^+dr \tag{10}$$

Eq. (10) corresponds to an integral formula in the theory of Bessel functions:

$$\int_0^\infty J_\mu(at)\,J_\nu(at)\frac{dt}{t}=\frac{2}{\pi}\;\frac{\sin\frac{1}{2}(\nu-\mu)\pi}{\nu^2-\mu^2}$$

A singular solution $f_l^-(r)$ at $r=0$ is used also to calculate the phase shifts instead of $f_l^+(r)$. Analogous to $f_l^+(r)$, the following relation is easily written

$$f_l^-\frac{d^2\chi_l}{dr^2}-\chi_l\frac{d^2f_l^-}{dr^2}=f_l^-U(r)\chi_l$$

which may be integrated to be

$$\Big[f_l^-\frac{d\chi_l}{dr}-\chi_l\frac{df_l^-}{dr}\Big]_0^\infty=\int_0^\infty f_l^-U(r)\chi_l dr \tag{11}$$

The leading terms for small r are

$$f_l^-(r) \cong A_{-l}(kr)^{-l}, \qquad A_{-l}=\sqrt{\frac{\pi}{2}}\,\frac{2^{l+\frac{1}{2}}}{\Gamma(-l+\frac{1}{2})} \tag{12}$$

$$\chi_l(r) \cong C_{l+1}(kr)^{l+1}, \qquad C_{l+1}=\sqrt{\frac{\pi}{2}}\,\frac{a}{2^{l+\frac{1}{2}}\Gamma(-l+\frac{3}{2})} \tag{13}$$

a being a constant determined for given U, and if $U=0$, $\chi_l=f_l^+$, and it is shown that $a=1$ by the properties of Bessel functions. We thus obtain for small r

$$f_l^-\frac{d\chi_l}{dr}-\chi_l\frac{df_l^-}{dr} \cong (2l+1)kA_{-l}C_{l+1}=(-1)^l ka \tag{14}$$

For large r, we take into account the asymptotic form of (4) and for f_l^- in the following form

$$f_l^-(r) \cong \cos(kr+\tfrac{1}{2}l\pi)$$

so that the left side of Eq. (11) becomes

$$\left[f_l^-\frac{d\chi_l}{dr}-\chi_l\frac{df_l^-}{dr}\right]_0^\infty=(-1)^l k\cos\delta_l-(-1)^l ka$$

Consequently the following formula is obtained

$$\cos\delta_l=a+\frac{(-1)^l}{k}\int_0^\infty f_l^- U(r)\chi_l dr \tag{15}$$

where $\quad a=\chi_l/f_l^+\Big|_{r\to\infty}$

Formulae (5) and (15) will be made use of in checking the phase shifts obtained by another methods.

References

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