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Scattering from a separable, non-local potential†

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Abstract. The problem of elastic scattering from a separable, complex, non-local potential has been investigated, and expressions for the phase shifts have been obtained for all orders of scattering.

During the past several years considerable attention has been given to the problem of scattering from a non-local potential (Perey and Buck 1962, Mulligan 1964, Tabakin 1965). In particular, a number of authors have examined the special class of non-local interactions which are separable (Yamaguchi 1954, Nichols 1965). In this paper we wish to investigate the scattering from a separable, complex, non-local potential and to obtain the phase shifts for all orders of scattering.

The Schrödinger equation appropriate for a non-local interaction is

$$\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+E\psi(\mathbf{r}) = \int K(\mathbf{r},\mathbf{r}')\psi(\mathbf{r}')\,d\mathbf{r}' \tag{1}$$

where m is the reduced mass of the projectile–target system, E is the centre-of-mass energy of the incident particle and $K(\mathbf{r}, \mathbf{r}')$ is the interaction kernel.

The solution of equation (1) can be obtained by introducing the appropriate Green function $\mathrm{G}(\mathbf{r}, \mathbf{r}')$. If we set

$$Q(\mathbf{r}) = \int K(\mathbf{r},\mathbf{r}')\psi(\mathbf{r}')\,d\mathbf{r}'$$

then equation (1) becomes

$$\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+E\psi(\mathbf{r}) = Q(\mathbf{r})$$

and we can write the desired solution $\psi(\mathbf{r})$ as

$$\psi(\mathbf{r}) = \psi_{\mathrm{H}}(\mathbf{r})+\int \mathrm{G}(\mathbf{r},\mathbf{r}')Q(\mathbf{r}')\,d\mathbf{r}' \tag{2}$$

where

$$\left(\frac{\hbar^2}{2m}\nabla^2+E\right)\psi_{\mathrm{H}}(\mathbf{r}) = 0 \tag{3}$$

and

$$\mathrm{G}(\mathbf{r},\mathbf{r}') = 4\pi i K_0 \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \mathrm{j}_l(K_0 r_<)\mathrm{h}_l^{(1)}(K_0 r_>)Y_l^{m*}(\theta',\phi')Y_l^m(\theta,\phi). \tag{4}$$

Here $K_0 = (2mE/\hbar^2)^{1/2}$, $\mathrm{j}_l(\rho)$ and $\mathrm{h}_l^{(1)}(\rho)$ are, respectively, spherical Bessel and Hankel functions, $Y_l^m(\theta, \phi)$ is a normalized spherical harmonic and $r_>$ $(r_<)$ is the greater (lesser) of r and r'. If we now introduce for $\psi(\mathbf{r})$ and $K(\mathbf{r}, \mathbf{r}')$ the expansions

$$\psi(\mathbf{r}) = \sum_{l=0}^{\infty} a_l \frac{u_l(r)}{r}\mathrm{P}_l(\cos\theta) \tag{5}$$

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where

$$a_l = \frac{(2l+1)i^l}{(2\pi)^{3/2}} \exp(i\delta_l) \tag{6}$$

and δ_l is the phase shift for the lth partial wave,

$$K(\mathbf{r}, \mathbf{r}') = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} g_l(r, r') Y_l^{m*}(\theta', \phi') Y_l^m(\theta, \phi) \tag{7}$$

and substitute equations (4), (5) and (7) into the right-hand side of equation (2), this latter equation becomes, after some algebra,

$$\psi(\mathbf{r}) = \psi_{\mathrm{H}}(\mathbf{r}) - \frac{2miK_0}{\hbar^2} \int_0^\infty \int_0^\infty \sum_{l=0}^{\infty} \mathrm{j}_l(K_0 r_<) \mathrm{h}_l^{(1)}(K_0 r_>)$$
$$\times g_l(r', r'') u_l(r'') a_l r'^2 r'' \, dr' \, dr'' \, \mathrm{P}_l(\cos\theta). \tag{8}$$

The solution of the homogeneous equation (equation (3)) can be expanded in terms of partial waves as follows:

$$\psi_{\mathrm{H}}(\mathbf{r}) = (2\pi)^{-3/2} \sum_{l=0}^{\infty} (2l+1) i^l \mathrm{j}_l(K_0 r) \mathrm{P}_l(\cos\theta). \tag{9}$$

If equations (5) and (9) are substituted into equation (8) and use is made of the expression for a_l in equation (6), then equating corresponding terms on both sides of the resulting equation leads to

$$\frac{u_l(r)}{r} = \exp(-i\delta_l) \mathrm{j}_l(K_0 r) - \frac{2miK_0}{\hbar^2} \int_0^\infty \int_0^\infty \mathrm{j}_l(K_0 r_<) \mathrm{h}_l^{(1)}(K_0 r_>)$$
$$\times g_l(r', r'') u_l(r'') r'^2 r'' \, dr' \, dr''. \tag{10}$$

Equation (10) is the fundamental equation for the non-local interaction. It is readily verified that in the limit

$$g_l(r', r'') \to V(r')\delta(r' - r'')/r'^2$$

equation (10) reduces to the usual integral equation for the scattering phase shifts associated with a local potential $V(r)$.

If we now introduce the restriction that the function $g_l(r, r')$ is separable, i.e. that

$$g_l(r, r') = q_l(r) q_l(r') \tag{11}$$

equation (10) becomes

$$\frac{u_l(r)}{r} = \exp(-i\delta_l) \mathrm{j}_l(K_0 r) - \frac{2miK_0}{\hbar^2} B_l \int_0^\infty \mathrm{j}_l(K_0 r_<) \mathrm{h}_l^{(1)}(K_0 r_>) q_l(r') r'^2 \, dr' \tag{12}$$

where

$$B_l = \int_0^\infty q_l(r'') u_l(r'') r'' \, dr''. \tag{13}$$

Equation (12) is a general expression for the radial part of the wave function for the non-local scattering problem under the assumption of the 'separability' condition of equation (11).

Having obtained the general solution given by equation (12), we now turn to the problem of evaluating this expression for the scattering phase shifts δ_l. We begin by introducing the assumption that the function $q_l(r)$ is non-zero only in the region $0 \leqslant r \leqslant a$. The infinite upper limit of integration appearing in equation (12) may therefore be replaced by the cut-off value a. With this in mind, it is not difficult to see that the scattering problem has separated into two parts, one part relating to the solution in the region $0 \leqslant r \leqslant a$ and the other for $r > a$.

For the region $r > a$ we must certainly have $r > r'$, and therefore equation (12) becomes

$$\frac{u_l(r)}{r} = \exp(-i\delta_l)\mathrm{j}_l(K_0 r) - \frac{2miK_0}{\hbar^2} B_l \mathrm{h}_l^{(1)}K(_0 r) \times \int_0^a \mathrm{j}_l(K_0 r')q_l(r')r'^2\,dr' \qquad (r > a). \tag{14}$$

For the region $r \leqslant a$ the situation is slightly more complicated. In this region both r and r' vary over the same values, and thus the designation of $r_>$ and $r_<$ will change over the interval of integration. To take this into account we write for $r \leqslant a$

$$\frac{u_l(r)}{r} = \exp(-i\delta_l)\mathrm{j}_l(K_0 r) - \frac{2miK_0}{\hbar^2} B_l\Big\{\mathrm{h}_l^{(1)}(K_0 r)\int_0^r \mathrm{j}_l(K_0 r')q_l(r')r'^2\,dr' + \mathrm{j}_l(K_0 r)\int_r^a \mathrm{h}_l^{(1)}(K_0 r')q_l(r')r'^2\,dr'\Big\} \qquad (r \leqslant a). \tag{15}$$

The complete solution to the problem may now be written by combining equations (14) and (15).

The constant B_l can be evaluated in the following manner. We multiply both sides of equations (14) and (15) by $q_l(r)r^2$ and integrate from 0 to ∞ (or, more precisely, from 0 to a because of the fact that $q_l(r) = 0$ for $r > a$). The left-hand side of each of these expressions is, by definition, B_l. On the right-hand side we see that the contribution from that part of the solution valid for $r > a$ vanishes because the integration from a to ∞ of any function containing $q_l(r)$ will be zero. We thus find

$$B_l = \Big\{\int_0^a q_l(r)\exp(-i\delta_l)\mathrm{j}_l(K_0 r)r^2\,dr\Big\}\Big[1 + \frac{2miK_0}{\hbar^2} \times \Big\{\int_0^a q_l(r)\mathrm{h}_l^{(1)}(K_0 r)r^2 \int_0^r \mathrm{j}_l(K_0 r')q_l(r')r'^2\,dr'\,dr + \int_0^a q_l(r)\mathrm{j}_l(K_0 r)r^2\int_r^a \mathrm{h}_l^{(1)}(K_0 r')q_l(r')r'^2\,dr'\,dr\Big\}\Big]. \tag{16}$$

Now that the complete solution to the problem is known in both regions of interest we can proceed to obtain an expression for the phase shifts δ_l. This can be accomplished by taking equation (14) in the limit $r \to \infty$ and solving the resulting expression for δ_l. If we set

$$A_l = \frac{2mK_0}{\hbar^2} B_l \int_0^a \mathrm{j}_l(K_0 r')q_l(r')r'^2\,dr'$$

then equation (14) becomes

$$\frac{u_l(r)}{r} = \exp(-i\delta_l)\mathrm{j}_l(K_0 r) - iA_l\mathrm{h}_l^{(1)}(K_0 r) \tag{17}$$

and in the limit $r \to \infty$ we have, upon replacing the functions of equation (17) by their appropriate asymptotic forms,

$$\frac{\sin(K_0 r - \frac{1}{2}l\pi + \delta_l)}{K_0 r} = \frac{\cos(K_0 r - \frac{1}{2}l\pi - \frac{1}{2}\pi)}{K_0 r} - iA_l\frac{\exp\{i(K_0 r - \frac{1}{2}l\pi - \frac{1}{2}\pi)\}}{K_0 r}.$$

After some algebra we finally find

$$\tan\delta_l = \frac{-\frac{2mK_0}{\hbar^2}B_l'\int_0^a \mathrm{j}_l(K_0 r')q_l(r')r'^2\,dr'}{1 - \frac{2miK_0}{\hbar^2}B_l'\int_0^a \mathrm{j}_l(K_0 r')q_l(r')r'^2\,dr'} \tag{18}$$

where

$$B_l' = \exp(i\delta_l)B_l. \tag{19}$$

Equations (18) and (19) constitute a complete solution to the scattering problem for a separable, non-local potential. The interesting feature of this result is that the expression for the phase shifts can be written entirely in terms of known functions, a situation which is in sharp contrast with the one found for local potentials, where the equation for the phase shifts involves integrations over the (unknown) wave function $u_l(r)$. It should also be noted that no assumption has been made regarding the reality of the functions $q_l(r)$.

Calculations involving the scattering of neutrons from a separable, complex, non-local potential have been made and these results will be presented in a future publication.

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