OPTICAL POTENTIALS AND EIKONAL APPROXIMATIONS

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Abstract

An intermediate and high energy scattering approximation is developed by approximating the sum of intermediate states of the target system and expanding the free particle propagator. The resulting expression plays the role of an optical potential and reduces to the eikonal approximation if the average of the excitation energy for the intermediate states is negligible in comparison with the energy of the incident particle.

I. Introduction

The eikonal approximation and the use of optical potentials are closely related to one another and both have found wide applications in scattering theory. In using the eikonal approximation one assumes that the interaction potential is undistorted and the wavefunctions are distorted plane waves, while optical potential methods assume the converse. A scattering problem is formulated here using the T-matrix formalism and the free particle propagator is expanded in terms of the momentum transfer to intermediate states. The approximation shows how one may find an expression for the optical potential and how this is related to the eikonal approximation if the average excitation energy of the intermediate states is much smaller than the energy of the incident particle. As exchange effects and coupling between intermediate states are neglected, the approximation should give reasonable results only for intermediate and high energies. The technique may be used to calculate elastic or inelastic cross sections.

The general formulation of the problem is developed in Section II. In Section III the first-order solution obtained is shown to reduce to the eikonal and Born approximation, and applications to a square well and Coulomb potential are discussed. Section IV is devoted to conclusions.

II. General Formulation

Consider a non-interacting incident particle and target system described by the equations

$$H\,|\,m\rangle = E\,|\,m\rangle \qquad \text{and} \qquad h\,|\,k\rangle = e_k\,|\,k\rangle\,. \tag{1}$$

When the two interact with a potential V_0 then the state $|\,\psi\rangle$ which describes the composite system is a solution to

$$(H+h+V_0)\,|\,\psi\rangle = E\,|\,\psi\rangle\,. \tag{2}$$

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The outgoing wave solution is given by

$$|\psi^{+}\rangle = |0k\rangle + G_0^{+} V_0 |\psi^{+}\rangle, \tag{3}$$

where $G_0^{+} = (E-H-h+i\eta)^{-1}$ and $|0k\rangle$ indicates the ground state of the target system and the initial momentum of the incident particle. The T-matrix element for a scattering process from the state $|0k\rangle$ to the state $\langle mk_f|$ is given by

$$T_{if} = \langle mk_f | T | 0k\rangle. \tag{4}$$

The T-operator plays the role of an effective potential and is a solution to the operator equation

$$T = V_0 + V_0 G_0^{+} T. \tag{5}$$

Expanding T on the coordinate space representation of the non-interacting eigenstates, we have

$$\langle \boldsymbol{r}, \boldsymbol{r}_1 | T | 0k\rangle = V_0(\boldsymbol{r}, \boldsymbol{r}_1)\,\phi_0(\boldsymbol{r}_1)\,\Phi_k(\boldsymbol{r}) + \frac{1}{4\pi^3} V_0(\boldsymbol{r}, \boldsymbol{r}_1) \sum_n \phi_n(\boldsymbol{r}_1) \int \mathrm{d}\boldsymbol{r}'\,\mathrm{d}\boldsymbol{r}_1'\, \phi_n^{*}(\boldsymbol{r}_1') \langle \boldsymbol{r}'\boldsymbol{r}_1' | T | 0k\rangle \int \frac{\mathrm{d}\boldsymbol{p}\, \exp\{\mathrm{i}\boldsymbol{p}\,.\,(\boldsymbol{r}-\boldsymbol{r}')\}}{k_n^2 - p^2 + \mathrm{i}\eta}, \tag{6}$$

where $\boldsymbol{r}$ and $\boldsymbol{r}_1$ denote the coordinates of the incident particle and the target respectively, $\phi_0(\boldsymbol{r}_1) = \langle \boldsymbol{r}_1 | 0\rangle$, $\Phi_k(\boldsymbol{r}) = \langle \boldsymbol{r} | k\rangle$, $k_n^2 = k^2 + (E_0 - E_n)$, and the summation includes the continuum states. We have assumed that V_0 is a local potential.

The summation in (6) may be done using the closure relation if we replace the energy difference of the intermediate states by an average energy difference Δ_n^2. Then

$$k_n^2 = k^2 + (E_0 - E_n) \approx k^2 - \Delta_n^2, \qquad k_n = k(1 - \Delta_n^2/k^2)^{\frac{1}{2}},$$

or to first order

$$k - k_n \approx \Delta_n^2/2k \tag{7}$$

for $\Delta_n^2/k^2 < 1$. Using this approximation to carry out the summation and introducing a normalized t-function†

$$t(\boldsymbol{r}, \boldsymbol{r}_1) = \frac{\langle \boldsymbol{r}\boldsymbol{r}_1 | T | 0k\rangle}{V_0(\boldsymbol{r}, \boldsymbol{r}_1) \langle \boldsymbol{r}\boldsymbol{r}_1 | 0k\rangle}, \tag{8}$$

we find

$$t(\boldsymbol{r}, \boldsymbol{r}_1) = 1 + \frac{1}{4\pi^3} \int \mathrm{d}\boldsymbol{r}'\, V_0(\boldsymbol{r}', \boldsymbol{r}_1) \exp\{\mathrm{i}\boldsymbol{k}\,.\,(\boldsymbol{r}'-\boldsymbol{r})\}\, t(\boldsymbol{r}', \boldsymbol{r}_1) \int \frac{\mathrm{d}\boldsymbol{p}\, \exp\{\mathrm{i}\boldsymbol{p}\,.\,(\boldsymbol{r}-\boldsymbol{r}')\}}{k_n^2 - p^2 + \mathrm{i}\eta}. \tag{9}$$

† The normalized t-function defined here is related to the wave operator as

$$T = V_0 \Omega^{(+)}, \qquad \langle \boldsymbol{r}\boldsymbol{r}_1 | T | 0k\rangle = \langle \boldsymbol{r}\boldsymbol{r}_1 | V_0 \Omega^{(+)} | 0k\rangle.$$

For local potentials

$$\langle \boldsymbol{r}\boldsymbol{r}_1 | T | 0k\rangle = V_0(\boldsymbol{r}, \boldsymbol{r}_1) \langle \boldsymbol{r}\boldsymbol{r}_1 | \Omega^{(+)} | 0k\rangle$$

and then

$$t(\boldsymbol{r}, \boldsymbol{r}_1) = \frac{\langle \boldsymbol{r}\boldsymbol{r}_1 | T | 0k\rangle}{V_0(\boldsymbol{r}, \boldsymbol{r}_1) \langle \boldsymbol{r}\boldsymbol{r}_1 | 0k\rangle} = \frac{\langle \boldsymbol{r}\boldsymbol{r}_1 | \Omega^{(+)} | 0k\rangle}{\langle \boldsymbol{r}\boldsymbol{r}_1 | 0k\rangle}.$$

The T-matrix element is now given by

$$T_{\mathrm{if}} = \langle \phi_n(\boldsymbol{r}_1)\exp(\mathrm{i}\boldsymbol{k}_{\mathrm{f}}\,.\,\boldsymbol{r}),\, t(\boldsymbol{r},\boldsymbol{r}_1)\, V_0(\boldsymbol{r},\boldsymbol{r}_1)\,\phi_0(\boldsymbol{r}_1)\exp(\mathrm{i}\boldsymbol{k}\,.\,\boldsymbol{r})\rangle\,. \tag{10}$$

Let $\boldsymbol{q} = \boldsymbol{p} - \boldsymbol{k}_n$ and consider the integral

$$\begin{aligned} I &= \int \frac{\mathrm{d}\boldsymbol{p}\,\exp\{\mathrm{i}\boldsymbol{p}\,.\,(\boldsymbol{r}-\boldsymbol{r}')\}}{k_n^2 - p^2 + \mathrm{i}\eta} \\ &= -\exp\{\mathrm{i}\boldsymbol{k}_n\,.\,(\boldsymbol{r}-\boldsymbol{r}')\}\int \frac{\mathrm{d}\boldsymbol{q}\,\exp\{\mathrm{i}\boldsymbol{q}\,.\,(\boldsymbol{r}-\boldsymbol{r}')\}}{2\boldsymbol{q}\,.\,\boldsymbol{k}_n - \mathrm{i}\eta}\left[1 + \frac{q^2}{2\boldsymbol{q}\,.\,\boldsymbol{k}_n - \mathrm{i}\eta}\right]^{-1}. \end{aligned} \tag{11}$$

If q^2 is less than $2\boldsymbol{q}\,.\,\boldsymbol{k}_n$ then the term in square brackets in (11) may be expanded. Since k_n is of order k, q is approximately the momentum transfer and the expansion is valid for the range of energies and small angles we wish to consider. Then

$$I = -\exp\{\mathrm{i}\boldsymbol{k}_n\,.\,(\boldsymbol{r}-\boldsymbol{r}')\}\sum_{j=0} I_j\,,$$

where

$$I_j = (-1)^j \int \mathrm{d}\boldsymbol{q}\, \frac{q^{2j}\exp\{\mathrm{i}\boldsymbol{q}\,.\,(\boldsymbol{r}-\boldsymbol{r}')\}}{(2\boldsymbol{q}\,.\,\boldsymbol{k}_n - \mathrm{i}\eta)^{j+1}} = \int \mathrm{d}\boldsymbol{q}\, \frac{\nabla_{r'}^{2j}(\exp\{\mathrm{i}\boldsymbol{q}\,.\,(\boldsymbol{r}-\boldsymbol{r}')\})}{(2q_z k_n - \mathrm{i}\eta)^{j+1}}. \tag{12}$$

In equation (12) we have chosen $\boldsymbol{k}_n$ to define the q_z axis. Substitution of this expression for I into equation (9) and carrying out the $2j$ partial integrations over $\boldsymbol{r}'$ gives

$$\begin{aligned} t(\boldsymbol{r},\boldsymbol{r}_1) = 1 - \frac{1}{4\pi^3}\sum_{j=0}\int \mathrm{d}\boldsymbol{r}'\ \nabla_{r'}^{2j}(V_0(\boldsymbol{r}',\boldsymbol{r}_1)\,t(\boldsymbol{r}',\boldsymbol{r}_1)\exp\{\mathrm{i}(\boldsymbol{k}_n - \boldsymbol{k})\,.\,(\boldsymbol{r}-\boldsymbol{r}')\}) \\ \times \int \mathrm{d}\boldsymbol{q}\,\frac{\exp\{\mathrm{i}\boldsymbol{q}\,.\,(\boldsymbol{r}-\boldsymbol{r}')\}}{(2q_z k_n - \mathrm{i}\eta)^{j+1}}. \end{aligned} \tag{13}$$

The above procedure for linearizing the propagator has been given by Schiff (1956) and allows one to carry out the integrations over $\boldsymbol{q}$ in a systematic manner. The propagator becomes

$$\int \mathrm{d}\boldsymbol{q}\,\frac{\exp\{\mathrm{i}\boldsymbol{q}\,.\,(\boldsymbol{r}-\boldsymbol{r}')\}}{(2q_z k_n - \mathrm{i}\eta)^{j+1}} = (2\pi)^2\,\delta(\boldsymbol{b}-\boldsymbol{b}')\int \mathrm{d}q_z\,\frac{\exp\mathrm{i}\{q_z(z-z')\}}{(2q_z k_n - \mathrm{i}\eta)^{j+1}}$$

or

$$\lim_{\eta\to 0^+}\int \mathrm{d}\boldsymbol{q}\,\frac{\exp\{\mathrm{i}\boldsymbol{q}\,.\,(\boldsymbol{r}-\boldsymbol{r}')\}}{(2q_z k_n - \mathrm{i}\eta)^{j+1}} = \frac{(2\pi)^3\mathrm{i}}{2\,|\,k_n\,|\,j!}\left(\frac{\mathrm{i}(z-z')}{2\,|\,k_n\,|}\right)^j \delta(\boldsymbol{b}-\boldsymbol{b}')\,\theta(z-z')\,. \tag{14}$$

In these expressions $\boldsymbol{b}$ represents the coordinates perpendicular to $\hat{\boldsymbol{k}}_n$ and $\theta(z-z')$ is the step function, that is, $\theta(z-z') = 0$ for $z < z'$ and $\theta(z-z') = 1$ for $z > z'$. Substitution of the expression (14) into equation (13) and carrying out the $\boldsymbol{b}$-integrals, where $\boldsymbol{r}' = (\boldsymbol{b}', z')$, we find

$$\begin{aligned} t(\boldsymbol{r},\boldsymbol{r}_1) = 1 - \frac{\mathrm{i}}{|\,k_n\,|}\sum_{j=0}\Bigg(\frac{\mathrm{i}^j}{j!(2\,|\,k_n\,|)^j}\int_{z_0}^{z}\mathrm{d}z'\ (z-z')^j \\ \times \nabla_{r'}^{2j}(V_0(\boldsymbol{r}',\boldsymbol{r}_1)\,t(\boldsymbol{r}',\boldsymbol{r}_1)\exp\{\mathrm{i}(\boldsymbol{k}_n - \boldsymbol{k})\,.\,(\boldsymbol{r}-\boldsymbol{r}')\})_{\boldsymbol{b}'=\boldsymbol{b}}\Bigg). \end{aligned} \tag{15}$$

z_0 is the lower range of the interaction potential V_0 and $\nabla_{r'}^0 = 1$.

III. First-order Solution

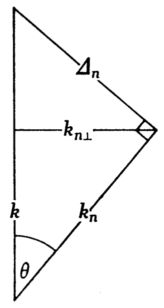

Fig. 1.—Relation between k, k_n, Δ_n, and $k_{n\perp}$.

In order to use the expansion (15) for a calculation we must examine the relative size of the contributions to $t(\boldsymbol{r}, \boldsymbol{r}_1)$ as a function of the incident energy. Figure 1 shows how k, k_n, Δ_n, and $k_{n\perp}$, the perpendicular components of k_n, are related. From this figure it can be seen that

$$\sin\theta = k_{n\perp}/k_n = \Delta_n/k$$

or

$$k_{n\perp} = (k_n/k)\Delta_n\,,$$

so that in the lowest order $k_{n\perp} \sim \Delta_n$. We will now use this result and that of equation (7) to examine the first three terms in the expression for $t(\boldsymbol{r}, \boldsymbol{r}_1)$.

Supressing the $\boldsymbol{b}$ and $\boldsymbol{r}_1$ variables for the moment we find from equation (15) that

$$t(z) = 1 - \frac{\mathrm{i}}{|k_n|}\int_{z_0}^{z} \mathrm{d}z'\; V_0(z')\,t(z')\exp\{\mathrm{i}(k_n-k)_z\,(z-z')\}$$

$$+\frac{1}{2\,|k_n|^2}\int_{z_0}^{z} \mathrm{d}z'\;(z-z')\nabla^2_{r'}\big(V_0(z')\,t(z')\exp\{\mathrm{i}(\boldsymbol{k}_n-\boldsymbol{k})\,.\,(\boldsymbol{r}-\boldsymbol{r}')\}\big)_{b'=b}\,. \qquad (16)$$

This is a Volterra integral equation which may be converted to a differential equation subject to the boundary condition $t(z_0) = 1$. For simplicity we write it as

$$t(z) = 1 - t_1 + t_2$$

and then

$$\partial t/\partial z = -\partial t_1/\partial z + \partial t_2/\partial z\,.$$

We find

$$\frac{\partial t_1}{\partial z} = \frac{\mathrm{i}}{|k_n|}\,V_0(z)\,t(z) - \frac{(k_n-k)_z}{|k_n|}\int_{z_0}^{z}\mathrm{d}z'\;V_0(z')\,t(z')\exp\{\mathrm{i}(k_n-k)_z\,(z-z')\}$$

$$= \frac{\mathrm{i}}{|k_n|}\,V_0(z)\,t(z) + \mathrm{i}(k_n-k)_z\{1-t(z)\} + \mathrm{i}(k_n-k)_z\,t_2$$

and

$$\frac{\partial t_2}{\partial z} = \frac{1}{2\,|k_n|^2}\int_{z_0}^{z}\mathrm{d}z'\;\nabla^2_{r'}\big(V_0(z')\,t(z')\exp\{\mathrm{i}(\boldsymbol{k}_n-\boldsymbol{k})\,.\,(\boldsymbol{r}-\boldsymbol{r}')\}\big)_{b'=b} - (k_n-k)_z^2\,t_2\,.$$

Thus,

$$\frac{\partial t}{\partial z} = -\frac{\mathrm{i}}{|k_n|}\,V_0(z)\,t(z) - \mathrm{i}(k_n-k)_z\{1-t(z)\} - \mathrm{i}(k_n-k)_z\,t_2 - (k_n-k)_z^2\,t_2$$

$$+\frac{1}{2\,|k_n|^2}\int_{z_0}^{z}\mathrm{d}z'\;\nabla^2_{r'}\big(V_0(z')\,t(z')\exp\{\mathrm{i}(\boldsymbol{k}_n-\boldsymbol{k})\,.\,(\boldsymbol{r}-\boldsymbol{r}')\}\big)_{b'=b}\,. \qquad (17)$$

Examination of the last three terms in (17) shows that they may be neglected to order k^{-1}, since $k-k_n \sim \Delta_n^2/2k$ and $k_{n\perp} \sim \Delta_n$. The resulting expression is

$$\partial t/\partial z = -(\mathrm{i}/k)V_0(z)\,t(z) - \mathrm{i}(k_n-k)\{1-t(z)\}, \tag{18}$$

with the solution

$$t(\boldsymbol{r},\boldsymbol{r}_1) = \left(1+\mathrm{i}\frac{\Delta_n^2}{2k}\int_{z_0}^{z}\mathrm{d}z'\,\exp\{\mathrm{i}g(z',z_0)\}\right)\exp\{-\mathrm{i}g(z,z_0)\}, \tag{19}$$

where

$$g(\xi,\eta) = \frac{\Delta_n^2}{2k}(\xi-\eta)+\frac{1}{k}\int_{\eta}^{\xi}\mathrm{d}\xi'\,V_0(\boldsymbol{b},\xi',\boldsymbol{r}_1). \tag{20}$$

The solution reduces to that given by the eikonal or Glauber (1959) approximation in the limit $k = k_n$, since then we have

$$g(\xi,\eta) = k^{-1}\int_{\eta}^{\xi}\mathrm{d}\xi'\,V_0(\boldsymbol{b},\xi',\boldsymbol{r}_1), \tag{21}$$

$$t(\boldsymbol{r},\boldsymbol{r}_1) = \exp\left(-\frac{\mathrm{i}}{k}\int_{z_0}^{z}\mathrm{d}z'\,V_0(\boldsymbol{b},z',\boldsymbol{r}_1)\right), \tag{22}$$

and

$$T_{\mathrm{if}} = \Big\langle \phi_n(\boldsymbol{r}_1)\exp(\mathrm{i}\boldsymbol{k}_\mathrm{f}\,.\,\boldsymbol{r}), \\ V_0(\boldsymbol{r},\boldsymbol{r}_1)\exp\left(-\frac{\mathrm{i}}{k}\int_{z_0}^{z}\mathrm{d}z'\,V_0(\boldsymbol{b},z',\boldsymbol{r}_1)\right)\phi_0(\boldsymbol{r}_1)\exp(\mathrm{i}\boldsymbol{k}\,.\,\boldsymbol{r})\Big\rangle. \tag{23}$$

This in turn reduces to the Born approximation if

$$\left|k^{-1}\int_{z_0}^{z}\mathrm{d}z'\,V_0(\boldsymbol{b},z',\boldsymbol{r}_1)\right| \ll 1,$$

as may be seen by expanding the exponential term. Our approximation may be viewed as giving the eikonal phase correction terms discussed by Schiff (1956).

If we consider a constant potential of finite range, namely

$$\begin{aligned} V_0(\boldsymbol{r},\boldsymbol{r}_1) &= V_0 \qquad \text{for} \qquad |\boldsymbol{r}-\boldsymbol{r}_1| \leqslant a, \\ &= 0 \qquad\qquad\qquad |\boldsymbol{r}-\boldsymbol{r}_1| > a, \end{aligned}$$

then an analytic form for the normalized t-function may be found. In this case

$$g(\xi,\eta) = (\tfrac{1}{2}\Delta_n^2+k^{-1}V_0)(\xi-\eta), \qquad z_0 = z_1-\{a^2+(\boldsymbol{b}-\boldsymbol{b}_1)^2\}^{\frac{1}{2}}, \tag{24}$$

and

$$t(\boldsymbol{r},\boldsymbol{r}_1) = \frac{1}{\Delta_n^2+2V_0}\left\{\Delta_n^2+2V_0\exp\left(-\frac{\mathrm{i}}{2k}(\Delta_n^2+2V_0)(z-z_0)\right)\right\}. \tag{25}$$

The Glauber approximation is given if $\Delta_n^2 \ll 2V_0$, and the Born approximation if $\Delta_n^2 \ll 2V_0$ and $V_0 \ll k$.

If we consider positron scattering from hydrogen which does not necessitate exchange terms, then the interaction potential is given by the Coulomb expression

$$V_0(\boldsymbol{r}, \boldsymbol{r}_1) = |\boldsymbol{r}|^{-1} - |\boldsymbol{r}-\boldsymbol{r}_1|^{-1}.$$

In this case

$$g_c(\xi, \eta) = \tfrac{1}{2}k^{-1}\Delta_n^2(\xi-\eta) + k^{-1}\ln|h(\xi)/h(\eta)|, \tag{26}$$

where

$$h(\xi) = \frac{\xi+(\xi^2+\boldsymbol{b}^2)^{\frac{1}{2}}}{\xi-z_1+\{(\xi-z_1)^2+(\boldsymbol{b}-\boldsymbol{b}_1)^2\}^{\frac{1}{2}}}, \qquad \lim_{\xi\to\infty} h(\xi) = 1.$$

The normalized t-function becomes

$$t(\boldsymbol{r}, \boldsymbol{r}_1) = \exp\{-\mathrm{i}g_c(z, z_0)\} + \mathrm{i}\frac{\Delta_n^2}{2k}\int_{z_0}^{z} \mathrm{d}z' \exp\{\mathrm{i}g_c(z', z)\}, \tag{27}$$

which may be written as

$$t(\boldsymbol{r}, \boldsymbol{r}_1) = \left|\frac{h(z_0)}{h(z)}\right|^{\mathrm{i}/k} \exp\left(-\frac{\mathrm{i}\Delta_n^2}{2k}(z-z_0)\right) + \frac{\mathrm{i}\Delta_n^2}{2k}\int_{z_0}^{z} \mathrm{d}z' \left|\frac{h(z')}{h(z)}\right|^{\mathrm{i}/k} \exp\left(\frac{\mathrm{i}\Delta_n^2}{2k}(z'-z)\right). \tag{28}$$

If we take $k = k_n^2$, that is, $\Delta_n^2 = 0$, we have the Glauber approximation and if $\Delta_n^2 = 0$ and $k \to \infty$ we have the Born approximation.

As the Coulomb field has an infinite range, equation (28) should be considered in the limit of z_0 approaching minus infinity. This should not present any difficulties since equation (28) must be inserted in the transition matrix element and the limit of $h(\xi) = 1$ as $\xi \to \infty$.

IV. Conclusions

Although solutions of the normalized t-function, or optical potential, have been considered here only to order k^{-1}, one can in principle extend the approximation to any order providing q^2 is less than $2\boldsymbol{q}\,.\,\boldsymbol{k}_n$. The price paid is that the integral equation for $t(\boldsymbol{r}, \boldsymbol{r}_1)$ becomes more difficult to solve, and it is questionable whether the rewards are worth the effort. If exchange terms arise then these could become significant even to the order considered here. The coupling with intermediate states will also become important at lower energies and in this case the use of closure and an average energy for the intermediate states would not be valid. One would then have to use a technique similar to that of Byron (1971).

In order to calculate a differential cross section with the above approximation one must do a seven-fold integration unless the interaction potential is particularly simple. The alternative is to use an approximate expression for the t-function similar to the procedure of Joachain and Mittleman (1971). The parameter Δ_n^2 may be chosen in several different ways. The method used by Joachain and Mittleman is to choose Δ_n^2 so that the next highest term in the t-expansion vanishes. For elastic scattering of electrons from helium, they find that Δ_n^2 is approximately equal to the ionization energy. Their results are fairly insensitive to the exact value of Δ_n^2, except at small scattering angles, and this suggests that Δ_n^2 may be approximated by the ionization energy for other cases as well.

It should be pointed out that Byron (1971) has used the eikonal ansatz and therefore has not included the phase term which arises when $\Delta_n^2 \neq 0$.

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