Optical Potential for Closely Coupled States*

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The method of closely coupled states is shown to be the lowest order approximation to a suitably modified optical potential set of equations. These equations are then used with a variational expression for the scattering amplitude to give an estimate for the correction to the method of closely coupled states.

I. INTRODUCTION

THE problem of the scattering of a particle from a complex scatterer (atom, nucleus, etc.) is one of the basic problems in physics. There are many methods for attacking this problem, heuristic and formal. The more formal[1] methods usually start with an expansion of the total wave function Ψ, in terms of the complete set of scatterer wave functions Φ_n,

$$\Psi(x,z)=\sum_n \psi_n(x)\Phi_n(z), \tag{1}$$

where x is the coordinate of the scattered particle and z represents all the coordinates of the medium.[2] The sum in Eq. (1) is over all members of an infinity of states so that some approximation must be made. We shall discuss here two common approximations and show their connection.

For the method of closely coupled states[3] one truncates the sum in (1) at some finite number and then uses the resulting expression as a trial function in a variational expression for the elastic scattering amplitude. There results a set of coupled equations for these variationally determined ψ_n. We shall describe this calculation briefly in the next section.

Another approximation scheme for Ψ is the optical potential method. In this method one seeks to obtain an equation for the scattered wave function, $\psi_0(x)$ with a complicated but in principle exact potential. In practice, one is forced to make approximations for this potential. This method can be generalized to yield a set of "coupled optical potential equations." The set of equations obtained by the closely coupled state method will appear as the first approximation to these equations.[4] This will be described in Sec. (III).

Finally, we shall use this set to obtain corrections to the method of closely coupled states and show that the error in the scattering amplitude is *linear* in the error in the optical potential.

III. THE METHOD OF CLOSELY COUPLED STATES

We start with Eq. (1) with the sum truncated at $n=N$. In effect, this assumes that the first N states of the scatterer are important and that the others don't exist. The unknown functions $\psi_n(x)$ are to be determined variationally and must have the asymptotic behavior

$$\lim_{x\to\infty}\psi_n(x)\to\delta_{n0}e^{i\mathbf{p}\cdot\mathbf{x}}+f_n(\hat{x},\hat{p})e^{ip_nx}/x, \tag{2}$$

where p_n is the momentum available to the scattered particle after the state n has been excited. f_0 is the elastic scattering amplitude.

Kohn[5] has given a variational expression for f_0 which can be written

$$\delta\left[f_0(\hat{p}_2,\hat{p}_1)-\frac{m}{2\pi\hbar^2}I(-p_2,p_1)\right]=0, \tag{3}$$

where

$$I(-p_2,p_1)=\int dxdz\,\Psi_{-p_2}{}^{(-)*}(E-H)\Psi_{p_1}{}^{(+)}. \tag{4}$$

Here H is the total Hamiltonian

$$H=H_z+T_x+V(x,z), \tag{5}$$

where H_z is the Hamiltonian for the scatterer alone, T_x is the kinetic energy of the scattered particle and $V(x,z)$ is the interaction of the two. The exact wave functions $\Psi^{(\pm)}$ have the asymptotic conditions

$$\lim_{x\to\infty}\Psi_p{}^{(\pm)}(x,z)\to$$
$$\sum_n{}'\left[e^{\pm ipx}\delta_{n0}+f_n{}^{(\pm)}(\hat{x},\hat{p})\frac{e^{\pm ip_nx}}{x}\right]\Phi_n(z). \tag{6}$$

The prime on the sum limits the sum to energetically open channels. If we use the truncated sum in (1) as a trial function in (3) and allow the functions ψ_n to be

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[1] H. Feshbach, Ann. Phys. **5**, 357 (1958); M. H. Mittleman and K. M. Watson, Phys. Rev. **113**, 198 (1959).

[2] When the scattered particle is identical with some of the particles in the scatterer. There are symmetry requirements on Ψ. Equation (1) is then correct but not as useful. The complications introduced by the Pauli principle will not be treated here.

[3] N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions* (Oxford University Press, New York, 1949).

[4] M. H. Mittleman and R. Pu, University of California Radiation Laboratory Report, UCRL-6269, 1961 (unpublished).

[5] W. Kohn, Phys. Rev. **74**, 1763 (1948).

determined variationally, there results the set

$$[E_n-T_x]\psi_n^{(+)}(x)=\sum_{m=1}^{n} V_{nm}(x)\psi_m^{(+)}(x),$$
$$n=1,\cdots,N, \quad (7)$$

where E_n is the energy available to the scattered particle when the scatterer is in the nth state and

$$V_{nm}(x)=\int dz\,\Phi_n^*(z)V(x,z)\Phi_m(z). \quad (8)$$

As we allow N to become larger, the approximate result should approach the correct result. The difficulty is that continuum states of the scatter cannot be included. These are sometimes important.

III. THE OPTICAL POTENTIAL METHOD

The usual optical potential methods seek to obtain an equation for $\psi_0(x)$ or its equivalent Ψ_c where

$$\Psi_c=\psi_0\Phi_0=\pi_0\Psi, \quad (9)$$

where π_0 projects onto the ground state of the scatterer. This can be accomplished in many ways. We show only the simplest here. The starting point is the integral equation for the total wave function.

$$\Psi^{(+)}=\chi+(1/a_0)V\Psi^{(+)}. \quad (10)$$

Here

$$a_0=a+V, \quad (11)$$

where

$$a=E-H+i\eta. \quad (12)$$

The positive infinitesimal, η, is inserted to insure the proper boundary condition for $\Psi^{(+)}$. χ is the incident wave, the product of a plane wave for the scattered particle and the ground state of the medium. Combining (9) and (10) yields

$$\Psi_c^{(+)}=\chi+(1/a_0)\pi_0V\Psi^{(+)}, \quad (13)$$

since $[\pi_0,a_0]=0$. [See Appendix.] If we subtract (13) from (10) we get

$$\Psi^{(+)}=\Psi_c^{(+)}+(1/a_0)(1-\pi_0)V\Psi^{(+)}. \quad (14)$$

We define the operator F^+ by

$$\Psi^{(+)}=F^{(+)}\Psi_c^{(+)} \quad (15)$$

so that

$$F^{(+)}=\pi_0+(1/a_0)(1-\pi_0)VF^{(+)}. \quad (16)$$

If we demand that $\Psi_c^{(+)}$ satisfy an optical equation

$$\Psi_c^{(+)}=\chi+(1/a_0)U^{(+)}\Psi_c^{(+)}, \quad (17)$$

then $U^{(+)}$ is given by

$$U^{(+)}=\pi_0VF^{(+)} \quad (18)$$

and we obtain

$$[E_0-(T_x+U_{00}^{(+)})]\psi_0=0. \quad (19)$$

In practice one can only obtain U_{00} approximately[6]

$$U_{00}\simeq V_{00}+\sum_{n\neq 0} V_{0n}[E_0-E_n+\epsilon_0-T_x+i\eta]^{-1}V_{n0}. \quad (20)$$

It is usually difficult to obtain any but the adiabatic ($T_x=\epsilon_0$) part of the second term in (20). Therefore, in practice this method allows excited states to enter only adiabatically.

We can generalize the optical potential method to allow for the nonadiabatic appearance of some of the excited states. To do this, we re-define the projection operator, π_0, so that it now projects onto the first N of the scatterer states

$$\pi=\sum_{n=1}^{N}\pi_n, \quad (21)$$

π is, of course, still a projection operator. The formalism leading to (18) is now modified by the replacement $\pi_0\rightarrow\pi$. Ψ_c is now interpreted as a column matrix and the "optical potential" U^+ now has non-diagonal matrix elements among the first N states, but does not couple to the higher states. We, therefore, obtain the set of coupled equations

$$(E_n-T_x)\psi_n^{(+)}(x)=\sum_{m=1}^{N} U_{nm}^{(+)}(x)\psi_m^{(+)}(x),$$
$$n=1,\cdots,N. \quad (22)$$

Here again we must approximate for U_{nm}.

$$U_{nm}^{(+)}\simeq V_{nm}+\textstyle\sum_{j>N} V_{nj}[E_0-E_j+\epsilon_0-T_x+i\eta]^{-1}V_{jm},$$
$$n,m\leqslant N. \quad (23)$$

Thus, the equations of the method of closely coupled states appear as the lowest approximation in this method. The second term in (23) can be obtained in certain limits where it may actually dominate the first.[7]

As we allow N to become larger, the number of states which are loosely coupled becomes smaller, and this method becomes formally identical with that of Sec. II. However, in this method the remaining loosely coupled states are always included, at least adiabatically.

IV. VARIATIONAL CORRECTIONS

The results of the preceding section may now be corrected by use of the Kohn variational principle. We shall take two approaches to this problem.

First, we allow for an error in the optical potentials U_{nm}, so that the actual potentials used are U_{nm_t}. The uncoupled states are completely neglected, $F_t=\pi$. Thus,

[6] M. H. Mittleman, Ann. Phys. **10**, 268 (1960).

[7] This method has been expanded to allow for the identity of the scattered particle with the particles in the scatterer. It will be discussed in detail in a subsequent publication. In reference 4 it was pointed out that the inclusion of the second order part of U gives the correct polarizability and that these corrections actually dominate the first order terms in some cases.

our trial function is $\Psi_t^{(\pm)}=\Psi_{c_t}^{(\pm)}$, where $\Psi_{c_t}^{(\pm)}$ is determined from (22) with U replaced by U_t.

The variational expression (3) then yields

$$f_0(\hat{p}_2,\hat{p}_1)=f_{0_t}(\hat{p}_2,\hat{p}_1)+\frac{m}{2\pi h^2}\int dx \times\sum_{n,m=1}^{N}\Psi_{n_t}^{(-)*}(x)[V_{nm}-U_{nm_t}]\Psi_{m_t}^{(+)}(x), \quad (24)$$

so that the correction is proportional to the second order terms in the optical potential.

A second approach is to assume an error in the optical potential δU with a resultant error in Ψ_c but to use the exact F. This takes the, presumably small, errors in the lowest N coupled states and reflects them in the higher states. We shall see that it proves to be a better approximation than simply dropping the higher states. Consider the integral in the variational expression. Its variation is

$$\begin{aligned}\delta I&=(m/2\pi h^2)\langle\Psi^{(-)}a\delta\Psi^{(+)}\rangle\\&=(m/2\pi h^2)\langle\Psi_c^{(-)}Q\delta\Psi_c^{(+)}\rangle.\end{aligned} \quad (25)$$

We have set

$$Q=F^{(-)\dagger}aF^{(+)}. \quad (26)$$

We had

$$F^{(+)}=\pi+(1/a_0)(1-\pi)VF^{(+)} \quad (27a)$$

and

$$F^{(-)\dagger}=\pi+F^{(-)\dagger}V(1-\pi)(1/a_0). \quad (27b)$$

Then

$$\begin{aligned}Q&=F^{(-)\dagger}a_0F^{(+)}-F^{(-)\dagger}VF^{(+)}\\&=F^{(-)\dagger}[a_0\pi+(1-\pi)VF^{(+)}]-F^{(-)\dagger}VF^{(+)}.\end{aligned}$$

But

$$F^{(-)\dagger}\pi=\pi.$$

So

$$\begin{aligned}Q&=a_0\pi+F^{(-)\dagger}(1-\pi)VF^{(+)}-F^{(-)\dagger}VF^{(+)}\\&=a_0\pi-F^{(-)\dagger}\pi VF^{(+)}\\&=\pi[a_0-\pi VF^{(+)}]=\pi(a_0-U^{(+)}).\end{aligned} \quad (28)$$

The error in Ψ_c is due to an error in U and a possible error in the bound state wave function, so that

$$\delta\Psi_c^{(+)}=\frac{1}{a_0-U^{(+)}}[a_0\delta\pi\chi+\delta U^{+}\Psi_c^{(+)}]. \quad (29)$$

Here, $\delta\pi$ allows for an error in the bound-state wave functions.

If we preserve the normalization of the bound states, $\delta\pi$ is not completely arbitrary. The normalization condition

$$\pi\pi=\pi \quad (30)$$

leads to a constraint on $\delta\pi$ of the form

$$\delta\pi\pi=(1-\pi)\delta\pi \quad (31a)$$

or

$$\pi\delta\pi=\delta\pi(1-\pi). \quad (31b)$$

Thus,

$$\delta I=\frac{m}{2\pi h^2}\langle\Psi_c^{(-)}\pi\,|\,a_0\delta\pi\chi+\delta U^{(+)}\Psi_c^{(+)}\rangle. \quad (32)$$

The use of (31b) eliminates the χ term yielding the previously obtained result[5] that an error in the bound state does not give any contribution to the scattering amplitude in the variational expression. We are then left with

$$f_0=f_{0_t}-\frac{m}{2\pi h^2}\int dx\sum_{n,m=1}^{N}\psi_{n_t}^{(-)*}\delta U_{nm}^{(+)}\psi_{m_t}^{(+)}(x). \quad (33)$$

Thus the error in the scattering amplitude is linear in the error in the optical potential. However, the error in the optical potential must be at least bilinear in the potential if it is to be an improvement over the method of coupled states.

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APPENDIX

The proof of the relationship $[\pi_0,a_0]$ which we use in obtaining (13) involves the definition of the projection operator, π_0. In the notation of (1) it is defined as

$$\pi_0=\delta(x-x')\Phi_0(z)\Phi_0^*(z'). \quad (A.1)$$

That is, π_0 projects onto the ground state of the medium, and any state of the relative coordinate of the scattered particle. This may also be written

$$\pi_0=\int\frac{d^3k}{(2\pi)^3}\Phi_0(z)e^{i\mathbf{k}\cdot\mathbf{x}}[\Phi_0(z')e^{i\mathbf{k}\cdot\mathbf{x}'}]^*. \quad (A.2)$$

Now, since $\Phi_0e^{i\mathbf{k}\cdot\mathbf{x}}$ is an eigenfunction of a_0, π_0 must commute with a_0.

No assumption has been made about the ratio of projectile mass to the target mass. z is to be interpreted as the internal coordinates of the target and x as the coordinate of the projectile relative to the (moving) center of mass of the target. In Eq. (5), the total center of mass motion has already been removed.