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AMPLITUDE FOR TRANSITIONS BETWEEN MOLECULAR (TWO-CENTER) CHANNELS

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Abstract: We derive an exact expression for the transition amplitude between molecular (two-center) states, using an extension of the well known method of auxiliary Hamiltonians (two-potential formalism). A first order approximation, corresponding to DWBA, is also given.

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Since some time there has been considerable interest in describing quasi-elastic reactions induced by heavy ions in terms of a "molecular" picture, utilizing two-center states to describe internal motion.^{1) - 7)} Work along these lines has been inspired, in part, by the intuitive appeal of two-center single particle states, and in part by a failure of conventional reaction theories, based upon "atomic" channels, to account for experimental data.^{5), 7)}

An obstacle to the molecular approach has been the fact that no satisfactory method was known for computing cross sections for transitions between two-center states.^{7) - 9)} In this paper we derive an exact formula as well as a practically useful DWBA-type approximation.

The amplitude for a rearrangement reaction from some initial channel i into a final channel f' can be written

$$T_{f',i} = \langle \Phi_{f'} | V' | \Psi_i^{(+)} \rangle \quad (1)$$

where $\Psi_i^{(+)}$ is an eigenstate of the full many-body Hamiltonian H , with ingoing waves only in the entrance channel.¹⁰⁾ $\Phi_{f'}$ is an eigenstate of $H'_0 = h_{\beta'} + T_{\beta'}$, with $h_{\beta'}$ the internal motion Hamiltonian and $T_{\beta'}$ the kinetic energy operator appropriate for the exit channel. $V' = H - H'_0$ is the interaction causing the transition. Eq. (1) is not in general useful because $\Psi_i^{(+)}$ is not known.

Two-potential theory enables us to re-write eq. (1) in terms of distorted waves which can be easily calculated.¹⁰⁾ To this end auxiliary Hamiltonians are introduced:

$$H'_1 = H'_0 + V'_0 \quad (2)$$

and likewise for the entrance channel (unprimed quantities). V_0 and V'_0 are

chosen as optical potentials, depending upon relative distance only, which describe elastic scattering. Eq. (1) becomes¹⁰⁾

$$T_{f,i} = \langle \phi_\beta \chi_\beta^{(-)} | V_1' \frac{i\varepsilon}{E+i\varepsilon-H} | \phi_\alpha \chi_\alpha^{(+)} \rangle \quad (3)$$

Here $\phi_{\alpha,\beta}$ are the internal motions in entrance and exit channels, respectively, which are eigenstates of the free separated nuclei. For definiteness, consider a one-nucleon transfer reaction $A(a,b)B$, with $a = b+x$, $B = A+x$. In the entrance channel $\alpha = (a,A)$ the internal motion is an eigenstate of

$$h_\alpha = t_{xb} + v_{xb} \quad (4)$$

where we have introduced an obvious notation for the kinetic and potential energy of x with respect to b (similar expressions hold for the exit channel). The distorted waves in eq. (3) are eigenstates of $T_\alpha + V_0$ (entrance channel) and $T_\beta + V_0'$ (exit channel), respectively. The interaction causing the rearrangement is $V_1' = H - H_1'$.

The formal development leading to eq. (3) holds for any choice of the auxiliary Hamiltonians H_1, H_1' , provided that V_0 and V_0' be operators with a finite range. Of course, in order that eq. (3) be practically useful it is required that the eigenstates of H_1, H_1' can be easily calculated. This is the case for central potentials V_0, V_0' .

We want to generalize eq. (3) to the case where the internal motion is represented by two-center states, which parametrically depend upon the relative distance between the nuclei. We define a two-center Hamiltonian

appropriate for the entrance channel as

$$h_{\alpha}^E = t_{xb} + v_{xb} + v_{xA}(r_{xb} + r_{\alpha}) + V_{Ab}(r_{\alpha}) \quad (5)$$

where v_{xA} is the potential between x and A, and V_{Ab} is the core-core potential.

The two-center states and energies depend parametrically upon the relative motion vector $\underline{r}_{\alpha} = \underline{r}_{aA}$.^{4), 6)}

$$h_{\alpha}^E \phi_{\alpha j \Omega}^E(r_{xb}) = \varepsilon_{\alpha j \Omega}(r_{\alpha}) \phi_{\alpha j \Omega}^E(r_{xb}) \quad (6)$$

We restrict ourselves to spherically symmetric potentials v_{xb} and v_{xA} , in which case the projection Ω of angular momentum j on the internal symmetry axis is a good quantum number. If written in terms of intrinsic coordinates the states ϕ_{α}^E do not depend upon the angles of $\underline{r}_{\alpha}$.^{4), 6)}

Perhaps it would seem more natural to define the two-center Hamiltonian by including all potential terms of the true Hamiltonian, i.e.

$$h_{\alpha}^R = H - T_{\alpha} = t_{xb} + v_{xb} + v_{xA}(r_{xb} + R) + V_{Ab}(R) \quad (7)$$

Eigenstates and -energies of the Hamiltonian eq. (7) depend parametrically upon the core-core vector $\underline{R} = \underline{r}_{bA} = \underline{r}_{\alpha} - (m_x/m_a)\underline{r}_{xb}$. As $\underline{R}$ varies with $\underline{r}_{xb}$ if $\underline{r}_{\alpha}$ is held fixed evaluation of derivatives $\nabla_{\underline{r}_{\alpha}}$ and $\nabla_{\underline{r}_{xb}}$, which are needed in the transition amplitude (see below), is more difficult. Therefore we prefer to use eqs. (5) and (6).

The two-center states as given in eq. (6) are not convenient as basis states in an expansion for scattering states, because two-center states with different Ω are strongly coupled even asymptotically. This is because asymptotically the z-projection m of particle angular momentum j rather than the

projection Ω on the internal symmetry axis is conserved. We follow the treatment of ref. 1) and introduce states

$$|\phi_{\alpha jm}^{\mathbf{r}_\alpha}\rangle = \sum_{\Omega} D_{m\Omega}^j(\hat{\mathbf{r}}_\alpha) |\phi_{\alpha j\Omega}^{\mathbf{r}_\alpha}\rangle \quad (8)$$

which asymptotically have good m rather than good Ω . These modified two-center states are orthonormalized in the usual way, i.e.

$$(\phi_{\alpha' j' m'}^{\mathbf{r}_\alpha} | \phi_{\alpha j m}^{\mathbf{r}_\alpha}) = \delta_{\alpha'\alpha} \delta_{j'j} \delta_{m'm} \quad (9)$$

In order to express the transition amplitude eq. (1) in terms of molecular states as given by eq. (8) we must introduce an auxiliary Hamiltonian which does not couple different molecular channels. Transitions between molecular states are caused essentially only by the kinetic energy of relative motion, and we therefore need to modify the latter. This is in contrast to the usual asymptotic ("atomic") channels, which are coupled by the potential. We define an auxiliary Hamiltonian

$$H_1 = \sum_{\alpha jm} P_{\alpha jm}^{\mathbf{r}_\alpha} (h_{\alpha}^{\mathbf{r}_\alpha} + T_{\alpha}) P_{\alpha jm}^{\mathbf{r}_\alpha} \quad (10)$$

where

$$P_{\alpha jm}^{\mathbf{r}_\alpha} = |\phi_{\alpha jm}^{\mathbf{r}_\alpha}\rangle \langle \phi_{\alpha jm}^{\mathbf{r}_\alpha}| \quad (11)$$

projects onto a single molecular channel. The sum in eq. (10) extends over a number of channels in partition (a,A). H_1 does not cause transitions between molecular channels so that

$$(E - H_1) |\phi_{\alpha jm}^{\mathbf{r}_\alpha} \chi_{\alpha}^{(+)}\rangle = 0 \quad (12)$$

has one-channel solutions and defines distorted waves $\chi_{\alpha}^{(+)}$ which describe

elastic scattering for molecular channels. In eq. (10) h_{α}^r must be included in the projection, because it couples states with different m, m' . The auxiliary Hamiltonian eq. (10) differs from the free motion Hamiltonian by

$$V_0 = H_1 - H_0 = \sum_{\alpha jm} \left[p_{\alpha jm}^r (h_{\alpha}^r + T_{\alpha}) p_{\alpha jm}^r \right] - h_{\alpha} - T_{\alpha} \quad (13)$$

which certainly is an operator of finite range, as the difference

$$\phi_{\alpha jm}^r - \phi_{\alpha jm} \quad \xrightarrow{r_{\alpha} \rightarrow \infty} 0 \quad (14)$$

In fact, the difference in eq. (14) vanishes exponentially for large r_{α} .⁶⁾

Similar definitions and considerations apply for the exit channel.

Because of the finite range of V_0 as given by eq. (13) and the analogous operator for the exit channel the formal development of the "two-potential method" can be carried over unchanged from ref. 10). Instead of eq. (3) we obtain (see appendix)

$$T_{f'i} = \langle \phi_{\beta j'm'}^r \chi_{\beta}^{(-)} | V_1 \frac{i\varepsilon}{E+i\varepsilon-H} | \phi_{\alpha jm}^r \chi_{\alpha}^{(+)} \rangle \quad (15)$$

with

$$V_1 = H - H_1 = H - \sum_{\beta j'm'} p_{\beta j'm'}^r (h_{\beta}^r + T_{\beta}) p_{\beta j'm'}^r \quad (16)$$

The distorted waves are given by

$$\left[E - \sum_{\alpha} |D_{m\alpha}^j(\hat{r}_{\alpha})|^2 \varepsilon_{\alpha j\alpha}(r_{\alpha}) - (\phi_{\alpha jm}^r | T_{\alpha} | \phi_{\alpha jm}^r) \right] \chi_{\alpha}^{(+)} = 0 \quad (17)$$

and likewise for the exit channel. Further development of this equation, which we do not pursue here, requires T_{α} to be expressed in terms of internal coordinates in a rotating frame as was done in ref. 1). Note that the

potential in eq. (17) is a linear combination of the two-center eigenenergies. It is non-central except for $j = 1/2$ states. The angular terms in T_α also give non-central contributions.

Eq. (15) gives an exact expression for the transition amplitude between molecular states. Approximations can be obtained by expanding $i\varepsilon/(E+i\varepsilon-H)$ in powers of $V_1 = H - H_1$. The lowest order approximation, which is analogous to the usual DWBA, amounts to just dropping the inverse operator, i.e.

$$\begin{aligned} T_{f'i}^{(1)} &= \langle \phi_{\beta j' m'}^{r_\beta} \chi_\beta^{(-)} | V_1 | \phi_{\alpha j m}^{r_\alpha} \chi_\alpha^{(+)} \rangle \\ &\approx \langle \phi_{\beta j' m'}^{r_\beta} \chi_\beta^{(-)} | T_\beta | \phi_{\alpha j m}^{r_\alpha} \chi_\alpha^{(+)} \rangle \end{aligned} \quad (18)$$

To obtain the last line we have dropped terms involving the difference $h_\beta^R - h_\beta^r$. This represents a no-recoil approximation.

Equation (18) gives the amplitude for one-step transitions between molecular channels, the transition operator being the kinetic energy of relative motion. This equation, in conjunction with the equations defining molecular channels and distorted waves, appears to be well suited for computing heavy-ion induced one-nucleon transfer reactions at low relative motion energies.

Appendix: Derivation of Eq. (15).

The transition amplitude eq. (1) can be written as

$$T_{f'i} = \langle \Phi_{f'} | V'_0 | \Psi_i^{(+)} \rangle + \langle \Phi_{f'} | V'_1 | \Psi_i^{(+)} \rangle \quad (A1)$$

with V'_0 given by the exit-channel analog of eq. (13), and V'_1 given by eq. (16).

$\Phi_{f'}$ is an eigenstate of H'_0 with energy E so that

$$(E - H'_1) \Phi_{f'} = -V'_0 \Phi_{f'} \quad (A2)$$

which implies

$$\Phi_{f'} = \frac{-i\varepsilon}{E - i\varepsilon - H'_1} \Phi_{f'} - \frac{1}{E - i\varepsilon - H'_1} V'_0 \Phi_{f'} \quad (A3)$$

In the limit $\varepsilon \rightarrow +0$ the first term on the right hand side becomes an eigenstate of H'_1 with energy E . This state is a product of a molecular internal motion and a distorted wave, cf. eq. (12). Eq. (A3) shows that asymptotically it differs from the free motion state $\Phi_{f'}$ only in its ingoing wave part, whence we denote it as $\chi_{f'}^{(-)}$. Introducing this into the second term of eq. (A1) we obtain

$$T_{f'i} = \langle \chi_{f'}^{(-)} | V'_1 | \Psi_i^{(+)} \rangle + \langle \Phi_{f'} | V'_0 \left[1 - \frac{1}{E + i\varepsilon - H'_1} V'_1 \right] | \Psi_i^{(+)} \rangle \quad (A4)$$

The second term on the right hand side is

$$\langle \Phi_{f'} | V'_0 \frac{i\varepsilon}{E + i\varepsilon - H'_1} | \Psi_i^{(+)} \rangle$$

which vanishes in the limit $\varepsilon \rightarrow 0$, because $V'_0 | \Phi_{f'} \rangle$ is a state vector with finite norm.¹¹⁾

We wish to express $\Psi_i^{(+)}$ in terms of the eigenstate $\chi_i^{(+)}$ of the molecular distorted wave Hamiltonian H_1 (see eq. (12)). This is done in a way analogous to expressing $\chi_{f'}^{(-)}$ in terms of $\Phi_{f'}$. We have

$$(E - H) \chi_i^{(+)} = -V_1 \chi_i^{(+)} \quad (A5)$$

from which we deduce

$$\chi_i^{(+)} = \frac{i\varepsilon}{E+i\varepsilon-H} \chi_i^{(+)} - \frac{1}{E+i\varepsilon-H} V_1 \chi_i^{(+)} \quad (A6)$$

The first term on the right hand side becomes, in the limit $\varepsilon \rightarrow 0$, an eigenstate of H with energy E . The second term on the right hand side contains, for $\varepsilon \rightarrow +0$, asymptotically only outgoing waves. From this it follows that, for $\varepsilon \rightarrow +0$, the first term on the right hand side actually becomes $\Psi_i^{(+)}$, i.e.

$$\Psi_i^{(+)} = \left[1 + \frac{1}{E+i\varepsilon-H} V_1 \right] \chi_i^{(+)} = \frac{i\varepsilon}{E+i\varepsilon-H} \chi_i^{(+)} \quad (A7)$$

Inserting this into eq. (A4) then yields the final expression eq. (15) for the transition amplitude in terms of molecular channels.

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