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Theory of atom-diatom rearrangement collisions based on the coupled-channel Born approximation

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Based on the first Born approximation and coupled-channel wave functions, a full three-dimensional treatment of state-to-state reactive scattering (rearrangement collision) has been made to derive explicitly the transition amplitude, differential cross section, and total cross section for atom-diatomic molecule systems. The present coupled-channel Born-approximation method will serve as a generalization of the distorted-wave Born-approximation method that we discussed elsewhere.

I. INTRODUCTION

The three-dimensional treatment of elementary molecular rearrangement collisions has been of great interest. Two of the computationally used three-dimensional methods are the close-coupling[1,2] and DWBA (distorted-wave-Born-approximation)[3,4] methods. In the DWBA, the interaction potential in the Hamiltonian is divided into two potentials, the distorting and perturbation potentials. The former is used to obtain the distorted wave function by solving the resulting Schrödinger equation. The latter is the interaction potential responsible for opening a new arrangement channel. The first Born approximation and the distorted-wave functions are used to construct the transition amplitude from which the differential and total cross sections are obtained. In the close-coupling method, the total wave function is expanded in terms of rovibrational basis functions. Wave functions properly constructed from the solutions of the resulting coupled Schrödinger equations are then used to obtain the S matrix. The S matrix is required to satisfy asymptotic boundary conditions. The scattering amplitude constructed from the S matrix is used to derive the differential and total cross sections. Unfortunately, the exact close-coupling methods demand excessively large computation time.

In general, the effect of coupling is not ignorable in rearrangement collisions (reactive scattering). In the usual DWBA, the coupling effect is not taken into account. The distorted-wave function used in the DWBA transition amplitude is simply the solution of the Schrödinger equation which describes only elastic scattering in the entrance and exit channels, respectively. In this paper, by considering the first Born approximation and coupling between channels in each arrangement (that is, the initial and final arrangement, respectively), we derive a three-dimensional CCBA (coupled-channel Born-approximation) formalism that describes state-to-state reactive scattering processes involving atom-diatomic molecule systems. The present CCBA will serve as a generalization of the DWBA method that we presented elsewhere.[4] The theoretical development will be largely self-contained in nature, requiring only a small number of references.

II. FORMAL CCBA TRANSITION AMPLITUDE

Discussions which follow below are general for reactive scattering (particle transfer) processes that occur as a consequence of collision between two composite particles. The transferred particle can also be a composite system. We write the Schrödinger equation to describe the system of two interacting composite particles,

$$H\Psi=E\Psi\ . \tag{2.1}$$

Ψ is the total wave function and H the Hamiltonian. H can be viewed in terms of an arrangement channel α,

$$H=H_\alpha\ , \tag{2.2a}$$

with

$$H_\alpha=h_\alpha+T_\alpha+U_\alpha\ , \tag{2.2b}$$

where h is the intrinsic Hamiltonian which describes the internal motions, T the relative kinetic energy, and U_α the interaction energy between the two particles in the arrangement channel α.

We introduce the projection operators, P, Q, and R. P is to denote projection onto an entrance channel state (in the initial arrangement channel α), Q onto other states in the same initial arrangement channel α, and R onto states in the final arrangement channel β. These projection operators satisfy

$$P+Q+R=1\ , \tag{2.3}$$

$$P^2=P,\ \ Q^2=Q\ \ R^2=R\ , \tag{2.4}$$

and

$$PQ=QR=PR=0\ . \tag{2.5}$$

In addition, they are commutative. The interaction potential viewed in terms of the arrangement channel α is

$$U_\alpha=(P+Q+R)U_\alpha(P+Q+R)\ . \tag{2.6}$$

The two-potential Hamiltonian suitable for the description of the CCBA is written

$$H_\alpha=H_\alpha^0+(P+Q)U_\alpha(P+Q)+W_\alpha\ , \tag{2.7}$$

or

$$H_\alpha=\mathscr{H}_\alpha+W_\alpha$$

with

$$H_\alpha^0=h_\alpha+T_\alpha\ , \tag{2.8}$$

$$\mathscr{H}_\alpha=H_\alpha^0+(P+Q)U_\alpha(P+Q)$$

$$=H_\alpha^0+U_\alpha-W_\alpha\ , \tag{2.9}$$

and

$$W_\alpha=U_\alpha-(P+Q)U_\alpha(P+Q)\ . \tag{2.10}$$

Considering the Hamiltonian (2.7), we write the scattering integral equation that satisfies the boundary condition of an outgoing wave in the arrangement channel α,

$$\Psi_\alpha^{(+)}=X_\alpha^{(+)}+g_\alpha^+W_\alpha X_\alpha^{(+)}\ , \tag{2.11}$$

or

$$\Psi_\alpha^{(+)}=X_\alpha^{(+)}+g_\alpha^{(+)}[U_\alpha-(P+Q)U_\alpha(P+Q)]X_\alpha^{(+)}\ , \tag{2.12}$$

where the Green's function is

$$g_\alpha^+=g_{1\alpha}^+ +g_{1\alpha}^+W_\alpha g_\alpha^+ \tag{2.13}$$

with

$$g_{1\alpha}^+=1/[E-H_\alpha^0-(P+Q)U_\alpha(P+Q)+i\epsilon]\ . \tag{2.14}$$

$X_\alpha^{(+)}$ above is the solution of the scattering integral equation corresonding to the Hamiltonian $\mathscr{H}_\alpha$ which prohibits the opening of a new arrangement channel

$$X_\alpha^{(+)}=\Phi_\alpha+g_{1\alpha}^+(P+Q)U_\alpha(P+Q)\Phi_\alpha\ , \tag{2.15}$$

where Φ_α is the free state, that is, the solution of

$$H_\alpha^0\Phi_\alpha=E\Phi_\alpha\ . \tag{2.16}$$

Following the Gell-Mann–Goldberger transformation,[5] we find the T-matrix element for the state-to-state rearrangement collision between the two arrangement channels α and β,

$$T_{\beta\alpha}=\langle\Phi_\beta|(P+Q)U_\alpha(P+Q)-W_\beta|X_\alpha^{(+)}\rangle -\langle X_\beta^{(-)}|U_\alpha-(P+Q)U_\alpha(P+Q)|\Psi_\alpha^{(+)}\rangle\ . \tag{2.17}$$

The insertion of (2.12) and (2.15) into (2.17) yields

$$T_{\beta\alpha}=\langle\Phi_\beta|(P+Q)U_\alpha(P+Q)+(P+Q)U_\alpha(P+Q)g_{1\alpha}^+(P+Q)U_\alpha(P+Q)-W_\beta|\Phi_\alpha\rangle$$
$$+\langle X_\beta^{(-)}|U_\alpha-(P+Q)U_\alpha(P+Q)$$
$$+[U_\alpha-(P+Q)U_\alpha(P+Q)]g_\alpha^+[U_\alpha-(P+Q)U_\alpha(P+Q)]|X_\alpha^{(+)}\rangle\ , \tag{2.18}$$

where W_β is the expression (2.10) for the arrangement channel β. In the case of the same coordinate system, the first term of (2.18) vanishes due to the othogonality between the bound state and scattering state. This definitely occurs when a transferred particle forms a bound state with an in-

finitely massive core after the interaction between a projectile and an infinitely massive target particle. Otherwise, a recoil effect causes the bound and scattering states to be in different coordinate systems. In this case the first term will not vanish.

However, in the DWBA and CCBA expressions, the first term is usually neglected and the higher-order contribution in the second term of (2.18) is ignored. Thus the first Born approximation leads to the CCBA transition amplitude of the type.

$$T_{\beta\alpha}^{\mathrm{CCBA}}=\langle X_\beta^{(-)}\,|\,U_\alpha-(P+Q)U_\alpha(P+Q)\,|\,X_\alpha^{(+)}\rangle\ , \tag{2.19}$$

or using (2.10),

$$T_{\beta\alpha}^{\mathrm{CCBA}}=\langle X_\beta^{(-)}\,|\,W_\alpha\,|\,X_\alpha^{(+)}\rangle\ . \tag{2.20}$$

The use of (2.6) for (2.19) above yields

$$T_{\beta\alpha}^{\mathrm{CCBA}}=\langle X_\beta^{(-)}\,|\,RU_\alpha(P+Q)\,|\,X_\alpha^{(+)}\rangle\ , \tag{2.21}$$

since

$$R\,|\,X_\alpha^{(+)}\rangle=P\,|\,X_\beta^{(-)}\rangle=Q\,|\,X_\beta^{(-)}\rangle=0\ . \tag{2.22}$$

From the inspection of (2.20) and (2.21), above, we now see that the perturbation potential W_α defined in (2.10) takes the role of opening a new arrangement channel β. Explicit descriptions of the state-to-state CCBA transition amplitude, differential cross section, and total cross section follow in Sec. III.

III. EXPLICIT CCBA TRANSITION AMPLITUDE AND CROSS SECTIONS

In the previous section, the colliding and departing particles were considered to be the composite systems made of any number of "elementary particles." The elementary particle is to mean a particle with no internal degree of freedom. Here we limit our discussions only to the case of reactive atom-diatomic molecule systems of type $A+BC$. Such a study has the merit of simplicity. Besides, many of the important elementary molecular reactions fall into this category.

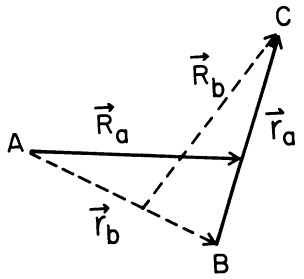

FIG. 1. Vector diagram of reactive scattering $A+BC\rightarrow AB+C$. The continuous line is for the initial arrangement channel while the dotted line is for the final arrangement channel.

Introducing the set of channel quantum numbers $\{n_a,j_a,L_a\}$ in an arrangement channel α, we rewrite the Schrödinger equation (2.1), given in the previous section, as

$$H\Psi_{n_aj_aL_a}^{JM}(\vec{\mathrm{R}}_a,\vec{\mathrm{r}}_a)=E\Psi_{n_aj_aL_a}^{JM}(\vec{\mathrm{R}}_a,\vec{\mathrm{r}}_a)\ . \tag{3.1}$$

Here n_a is the vibrational quantum number and j_a the rotational angular-momentum quantum number of a diatomic molecule. L_a is the relative orbital angular-momentum quantum number between the atom and diatomic molecule, J is the total angular-momentum quantum number, and M is its projection quantum number. $\vec{\mathrm{R}}_a$ is the channel coordinate vector connecting an atom and the c.m. (center of mass) of the diatomic molecule and $\vec{\mathrm{r}}_a$ the interatomic displacement vector of the diatomic molecule in an arrangement channel α (see Fig. 1 for details).

We introduce the partial-wave function which describes the relative motion between the atom and diatomic molecule with the relative angular momentum L_i and its projection M_i,

$$\chi_{L_iM_i}(\vec{\mathrm{R}})=[\chi_{L_i}(R)/R]Y_{L_i}^{M_i}(\hat{R})\ , \tag{3.2}$$

and the rovibrational wave function of the diatomic molecule

$$\phi_{njm}(\vec{\mathrm{r}})=[u_{nj}(r)/r]Y_j^m(\hat{r})\ . \tag{3.3}$$

The complete wave function is expanded in terms of the rovibrational basis functions

$$\Psi_{n_aj_aL_a}^{JM}(\vec{\mathrm{R}}_a,\vec{\mathrm{r}}_a)=\sum_{n_a'j_a'L_a'}[\chi_{n_a'j_a'L_a'\leftarrow n_aj_aL_a}^{J}(\vec{\mathrm{R}}_\alpha)\otimes\phi_{n_a'j_a'}(\vec{\mathrm{r}}_\alpha)]_{JM}\ , \tag{3.4}$$

where

$$[\chi_{n_a'j_a'L_a'\leftarrow n_aj_aL_a}^{J}(\vec{\mathrm{R}}_a)\otimes\phi_{n_a'j_a'}(\vec{\mathrm{r}}_a)]_{JM}=\mathscr{Y}_{j_a'L_a'}^{JM}(\hat{R}_a,\hat{r}_a)[\chi_{n_a'j_a'L_a'\leftarrow n_aj_aL_a}^{J}(R_a)/R_a][u_{n_a'j_a'}(r_a)/r_a] \tag{3.5}$$

with

$$\mathscr{Y}^{JM}_{j'_a L'_a}(\hat{R}_a,\hat{r}_a)=\sum_{m'_a M'_a}\langle j'_a L'_a m'_a M'_a \mid JM\rangle Y^{m'_a}_{j'_a}(\hat{r}_a)Y^{M'_a}_{L'_a}(\hat{R}_a)\,. \tag{3.6}$$

α in the expansion of (3.4) is an index to introduce all possible arrangement channels. The scalar product of (3.1) by the product of the radial molecular wave function $u_{n'_a j'_a}(r_a)/r_a$ and the bipolar spherical harmonics $\mathscr{Y}^{JM}_{j'_a L'_a}(\hat{R}_a,\hat{r}_a)$ leads to the set of the coupled differential equations

$$\begin{aligned}
&-\frac{\hbar^2}{2\mu_a}\left[\frac{d^2}{dR_a^2}-\frac{L'_a(L'_a+1)}{R_a^2}+K^2_{n'_a j'_a}\right]\chi^J_{n'_a j'_a L'_a\leftarrow n_a j_a L_a}(R_a)\\
&\quad=-\sum_{n''_a j''_a L''_a}\langle n'_a j'_a L'_a \mid U_\alpha \mid n''_a j''_a L''_a\rangle^J\chi^J_{n''_a j''_a L''_a\leftarrow n_a j_a L_a}(R_a)\\
&\qquad-\sum_{n_b j_b L_b}{}^{\beta}R_a\int d^3r_a d^2\hat{R}_a[u^*_{n'_a j'_a}(r_a)/r_a]\mathscr{Y}^{JM*}_{j'_a L'_a}(\hat{R}_a,\hat{r}_a)(H-E)[u_{n_b j_b}(r_b)/r_b]\\
&\qquad\qquad\times\mathscr{Y}^{JM}_{j_b L_b}(\hat{R}_b,\hat{r}_b)\chi^J_{n_b j_b L_b\leftarrow n_a j_a L_a}(R_b)/R_b\,,
\end{aligned} \tag{3.7}$$

where the wave number $K_{n'_a j'_a}$ is

$$K_{n'_a j'_a}\equiv K'_a=\left[\frac{2\mu_a}{\hbar^2}(E-\epsilon_{n'_a j'_a})\right]^{1/2}, \tag{3.8}$$

and the interaction matrix element is

$$\langle n'_a j'_a L'_a \mid U_\alpha \mid n_a j_a L_a\rangle^J=\int\int u^*_{n'_a j'_a}(r_a)\mathscr{Y}^{JM*}_{j'_a L'_a}(\hat{R}_a,\hat{r}_a)U_\alpha u_{n_a j_a}(r_a)\mathscr{Y}^{JM}_{j_a L_a}(\hat{R}_a,\hat{r}_a)d^2\hat{R}_a d^3r_a\,, \tag{3.9a}$$

or more explicitly[6]

$$\begin{aligned}
\langle n'_a j'_a L'_a \mid U_\alpha \mid n_a j_a L_a\rangle^J&=(-1)^{J_a+j'_a+J}[(2j_a+1)(2j'_a+1)(2L_a+1)(2L'_a+1)]^{1/2}\\
&\quad\times\sum_j U^j_{n'_a j'_a\leftarrow n_a j_a}(R_a)\langle j_a j'_a 00\mid j0\rangle\langle L_a L'_a 00\mid j0\rangle\\
&\quad\times W(j_a L_a j'_a L'_a;Jj)/(2j+1)\,.
\end{aligned} \tag{3.9b}$$

The undefined symbols above are as follows: μ_a is the reduced mass and $\epsilon_{n'_a j'_a}$ the internal (rovibrational) energy of the diatomic molecule. $U_{n'_a j'_a\leftarrow n_a j_a}(R_a)$ is given by

$$U^j_{n'_a j'_a\leftarrow n_a j_a}(R_a)=\int dr_a u^*_{n'_a j'_a}(r_a)U^j_\alpha(R_a,r_a)u_{n_a j_a}(r_a) \tag{3.10}$$

with

$$U^j_\alpha(R_a,r_a)=[(2j+1)/2]\int_{-1}^{1}U_\alpha(\vec{R}_a,\vec{r}_a)P_j(\hat{R}_a\cdot\hat{r}_a)d(\hat{R}_a\cdot\hat{r}_a)\,, \tag{3.11}$$

which results from

$$U_\alpha(\vec{R}_a,\vec{r}_a)=\sum_j U^j_\alpha(R_a,r_a)P_j(\hat{R}_a\cdot\hat{r}_a)\,. \tag{3.12}$$

$W(j_a L_a j'_a L'_a;Jj)$ in (3.9b) is the Racah coefficient. Finally, $\sum^\beta$ in the last term of Eq. (3.7) is to denote the summation over arrangement channels other than α. This last term represents coupling between arrangement channels.

However, in the CCBA[7] we use the Hamiltonian which describes only elastic and inelastic scattering processes in both the initial and final arrangement channels. Such Hamiltonian has the property of (2.9) shown in the previous section. Thus the Schrödinger equation is in the form of

$$\mathscr{H}_\alpha X^{JM}_{n_a j_a L_a}(\vec{\mathrm{R}}_a,\vec{\mathrm{r}}_a)=EX^{JM}_{n_a j_a L_a}(\vec{\mathrm{R}}_a,\vec{\mathrm{r}}_a)\ . \tag{3.13}$$

The resulting coupled Schrödinger equations from (3.13) exclude the arrangement coupling term and replaces U_α by $U_\alpha - W_\alpha$ in (3.7),

$$\begin{aligned}-\frac{\hbar^2}{2\mu_\alpha}\left[\frac{d^2}{dR_a^2}-\frac{L_a'(L_a'+1)}{R_a^2}+K^2_{n_a' j_a'}\right]&\chi^J_{n_a' j_a' L_a' \leftarrow n_a j_a L_a}(R_a)\\ =-\sum_{n_a'' j_a'' L_a''}&\langle n_a' j_a' L_a' \mid U_\alpha - W_\alpha \mid n_a'' j_a'' L_a''\rangle \chi^J_{n_a'' j_a'' L_a'' \leftarrow n_a j_a L_a}(R_a)\ .\end{aligned} \tag{3.14}$$

We write the total wave functions

$$X^{(+)}_{n_a j_a m_a}(\vec{\mathrm{K}}_a,\vec{\mathrm{R}}_a,\vec{\mathrm{r}}_a)=\frac{4\pi}{K_a}\sum i^{L_a}e^{i\sigma_{L_a}}\langle j_a L_a m_a M_a \mid JM\rangle[\chi_{n_a' j_a' L_a' \leftarrow n_a j_a L_a}(\vec{\mathrm{R}}_a)\otimes\phi_{n_a' j_a' m_a'}(\vec{\mathrm{r}}_a)]_{JM}Y^{M_a^*}_{L_a}(\hat{K}_a)\ , \tag{3.15}$$

for the initial arrangement channel, and

$$\begin{aligned}X^{(-)^*}_{n_b j_b m_b}(\vec{\mathrm{K}}_b,\vec{\mathrm{R}}_b,\vec{\mathrm{r}}_b)=\frac{4\pi}{K_b}\sum i^{-L_b}e^{i\sigma_{L_b}}&\langle j_b L_b m_b M_b \mid J'M'\rangle\\ \times[\chi^*_{n_b' j_b' L_b' \leftarrow n_b j_b L_b}(\vec{\mathrm{R}}_b)\otimes\phi^*_{n_b' j_b' m_b'}(\vec{\mathrm{r}}_b)]_{J'M'}&(-1)^{M_b}Y^{-M_b^*}_{L_b}(\hat{K}_b)\end{aligned} \tag{3.16}$$

for the final arrangement channel. In the case of negligible coupling in (3.15) and (3.16), the coupled-channel wave functions which describe relative motions are reduced to the usual distorted-wave functions,[4,8]

$$\chi^{(+)}_a(\vec{\mathrm{K}}_a,\vec{\mathrm{R}}_a)=\frac{4\pi}{K_a R_a}\sum_{L_a M_a} i^{L_a}e^{i\sigma_{L_a}}\chi_{L_a}(K_a,R_a)Y^{M_a}_{L_a}(\hat{R}_a)Y^{M_a^*}_{L_a}(\hat{K}_a) \tag{3.17}$$

and

$$\chi^{(-)*}_b(\vec{\mathrm{K}}_b,\vec{\mathrm{R}}_b)=\frac{4\pi}{K_b R_b}\sum_{L_b M_b} i^{-L_b}e^{i\sigma_{L_b}}\chi_{L_b}(K_b,R_b)Y^{-M_b}_{L_b}(\hat{R}_b)Y^{-M_b^*}_{L_b}(\hat{K}_b)\ . \tag{3.18}$$

Now we introduce (3.15) and (3.16) into the CCBA transition amplitude (2.20), in order to obtain $T^{\mathrm{CCBA}}_{\beta\alpha}\equiv T^{\mathrm{CCBA}}_{n_b j_b m_b \leftarrow n_a j_a m_a}$

$$\begin{aligned}=\frac{(4\pi)^2}{K_a K_b}\sum i^{L_a-L_b}e^{i(\sigma_{L_a}+\sigma_{L_b})}&(-1)^{M_b}\delta_{JJ'}\delta_{MM'}\langle j_a L_a m_a M_a \mid JM\rangle\langle j_b L_b m_b M_b \mid J'M'\rangle\langle j_a' L_a' m_a' M_a' \mid JM\rangle\\ \times\langle j_b' L_b' m_b' M_b' \mid J'M'\rangle Y^{M_a^*}_{L_a}(\hat{K}_a)Y^{-M_b^*}_{L_b}(\hat{K}_b)\mathscr{J}\int&\chi^{J^*}_{n_b' j_b' L_b' \leftarrow n_b j_b L_b}(\vec{\mathrm{R}}_b)\phi^*_{n_b' j_b' m_b'}(\vec{\mathrm{r}}_b)W_\alpha\phi_{n_a' j_a' m_a'}(\vec{\mathrm{r}}_a)\\ &\times\chi_{n_a' j_a' L_a' \leftarrow n_a j_a L_a}(\vec{\mathrm{R}}_a)d\vec{\mathrm{R}}_b d\vec{\mathrm{R}}_a\ .\end{aligned} \tag{3.19}$$

$\mathscr{J}$ is the Jacobian of transformation from $\vec{\mathrm{r}}_a$ and $\vec{\mathrm{r}}_b$ to $\vec{\mathrm{R}}_a$ and $\vec{\mathrm{R}}_b$. From the inspectation of (2.19) and

(2.20) along with (3.14), we write the perturbation potential (operator) in the form of

$$W_\alpha = U_\alpha - \Bigg\{ |n_a j_a L_a\rangle\langle n_a j_a L_a| U_\alpha |n_a j_a L_a\rangle\langle n_a j_a L_a| + \sum_{n'_a j'_a L'_a}{}' |n'_a j'_a L'_a\rangle\langle n'_a j'_a L'_a| U_\alpha |n_a j_a L_a\rangle\langle n_a j_a L_a|$$
$$+ \sum_{n'_a j'_a L'_a}{}' |n_a j_a L_a\rangle\langle n_a j_a L_a| U_\alpha |n'_a j'_a L'_a\rangle\langle n'_a j'_a L'_a|$$
$$+ \sum_{\substack{n'_a j'_a L'_a \\ n''_a j''_a L''_a}}{}' |n''_a j''_a L''_a\rangle\langle n''_a j''_a L''_a| U_\alpha |n'_a j'_a L'_a\rangle\langle n'_a j'_a L'_a| \Bigg\} . \tag{3.20}$$

$\sum'$ stands for the exclusion of summation over the state $|n_a j_a L_a\rangle$.

Consider now the expression

$$\phi^*_{n'_b j'_b m'_b}(\vec{r}_b)\phi_{n'_a j'_a m'_a}(\vec{r}_a) = \sum_{j'm'} (-1)^{m'_a} \langle j'_b j'_a m'_b - m'_a | j'm'\rangle [\phi^*_{n'_b j'_b m'_b}(\vec{r}_b) \otimes \phi_{n'_a j'_a m'_a}(\vec{r}_a)]_{j'm'} \tag{3.21}$$

with

$$[\phi_{n'_b j'_b m'_b}(\vec{r}_b) \otimes \phi_{n'_a j'_a m'_a}(\vec{r}_a)]_{j'm'} = \sum_{m'_b} (-1)^{m'_a} \langle j'_b j'_a m'_b - m'_a | j'm'\rangle \phi^*_{n'_b j'_b m'_b}(\vec{r}_b)\phi_{n'_a j'_a m'_a}(\vec{r}_a) . \tag{3.22}$$

Here j' is the transferred angular-momentum quantum number between the intermediate states in the two arrangement channels and is constrained by

$$\vec{j}' = \vec{j}'_b - \vec{j}'_a = \vec{L}'_a - \vec{L}'_b , \tag{3.23}$$

which assures the conservation of the total angular momentum

$$J = \vec{j}_a + \vec{L}_a = \vec{j}'_a + \vec{L}'_a = \vec{j}'_b + \vec{L}'_b = \vec{j}_b + \vec{L}_b . \tag{3.24}$$

The substitution of (3.21) into (3.19) yields

$$T^{\mathrm{CCBA}}_{n'_b j'_b m'_b \leftarrow n_a j_a m_a} = \frac{(4\pi)^2}{K_b K_a} \mathcal{J} \sum i^{L_a - L_b} e^{i(\sigma_{L_a} + \sigma_{L_b})} (-1)^{m'_a + M'_b + M_b} \delta_{JJ'} \delta_{MM'} \langle j_a L_a m_a M_a | JM\rangle \langle j_b L_b m_b M_b | J'M'\rangle$$
$$\times \langle j'_a L'_a m'_a M'_a | JM\rangle \langle j'_b L'_b m'_b M'_b | J'M'\rangle$$
$$\times \langle j'_b j'_a m'_b - m'_a | j'm'\rangle Y^{M^*_a}_{L_a}(\hat{K}_a) Y^{-M^*_b}_{L_b}(\hat{K}_b)$$
$$\times \int \chi^{J^*}_{n'_b j'_b L'_b \leftarrow n_b j_b L_b}(\vec{R}_b) W_\alpha(\vec{R}_a, \vec{r}_a) [\phi^*_{n'_b j'_b m'_b}(\vec{r}_b) \otimes \phi_{n'_a j'_a m'_a}(\vec{r}_a)]_{j'm'}$$
$$\times \chi^J_{n'_a j'_a L'_a \leftarrow n_a j_a L_a}(\vec{R}_a) d\vec{R}_b d\vec{R}_a . \tag{3.25}$$

Note that in the limiting case of zero coupling, the expression (3.25) here is reduced to the DWBA expression [Eq. (19) of Ref. 4]

$$T^{\mathrm{DWBA}}_{n_b j_b m_b \leftarrow n_a j_a m_a} = \sum_{jm} (-1)^{m_a} \langle j_b j_a m_b - m_a | jm\rangle$$
$$\times \int \chi^{(-)^*}_b(\vec{K}_b, \vec{R}_b) W(\vec{R}_a, \vec{r}_a) [\phi^*_{n_b j_b m_b}(\vec{r}_b) \otimes \phi_{n_a j_a m_a}(\vec{r}_a)]_{jm} \chi^{(+)}_a(\vec{K}_a, \vec{R}_a) d\vec{R}_b d\vec{R}_a , \tag{3.26}$$

where the perturbation potential W is of the form

$$W_\alpha(\vec{R}_a, \vec{r}_a) = U_\alpha - U^\alpha_{00} , \tag{3.27}$$

with U_{00}^{α} being a properly chosen spherically symmetric distorting potential.

We define

$$f_{j'm'}^{j'_b j'_a}(\vec{\mathrm{R}}_b,\vec{\mathrm{R}}_a)=i^{j'}W_{\alpha}(\vec{\mathrm{R}}_a,\vec{\mathrm{r}}_a)[\phi^*_{n'_b j'_b m'_b}(\vec{\mathrm{r}}_b)\otimes\phi_{n'_a j'_a m'_a}(\vec{\mathrm{r}}_a)]_{j'm'} \tag{3.28}$$

and

$$\phi_{n_k j_k m_k}(\vec{\mathrm{r}}_k)=i^{j_k}u_{n_k j_k}(r_k)Y_{j_k}^{m_k}(\hat{r}_k) \tag{3.29}$$

with $k=a$ or b. We note that the form factor f above transforms under rotations of the coordinate system like the complex conjugate of a tensor operator of rank j,

$$f_{j'm'}^{j'_b j'_a}(\vec{\mathrm{R}}_b,\vec{\mathrm{R}}_a)=\sum_{L_2 L_1}F_{L_2 L_1 j}^{j'_b j'_a}(R_b,R_a)\mathscr{Y}_{L_2 L_1}^{j'm'}(\hat{R}_b,\hat{R}_a) \tag{3.30}$$

with

$$\mathscr{Y}_{L_2 L_1}^{j'm'}(\hat{R}_b,R_a)=\sum_{M_2}\langle L_2 L_1 -M_2 M_1\,|\,j'm'\rangle Y_{L_2}^{-M_2^*}(\hat{R}_b)Y_{L_1}^{M_1^*}(\hat{R}_a)\,, \tag{3.31}$$

and

$$F_{L_2 L_1 j'}^{j'_b j'_a}(R_b,R_a)=\sum_{M_2}\langle L_2 L_1 -M_2 M_1\,|\,j'm'\rangle\int f_{j'm'}^{j'_b j'_a}(\vec{\mathrm{R}}_b,\vec{\mathrm{R}}_a)Y_{L_2}^{-M_2}(\hat{R}_b)Y_{L_1}^{M_1}(\hat{R}_a)d\hat{R}_b d\hat{R}_a\,. \tag{3.32}$$

The use of (3.28)–(3.32) for (3.25) leads to

$$\begin{aligned}T^{\mathrm{CCBA}}_{n_b j_b m_b\leftarrow n_a j_a m_a}=\frac{(4\pi)^2}{K_b K_a}\mathscr{F}\sum i^{L_a-L_b-j'}e^{i(\sigma_{L_a}+\sigma_{L_b})}(-1)^{m'_a+M'_b+M_b}\\ \times\langle j_a L_a m_a M_a\,|\,JM\rangle\langle j_b L_b m_b M_b\,|\,JM\rangle\langle j'_a L'_a m'_a M'_a\,|\,JM\rangle\\ \times\langle j'_b L'_b m'_b M'_b\,|\,JM\rangle\langle j'_b j'_a m'_b -m'_a\,|\,j'm'\rangle\langle L'_b L'_a -M'_b M'_a\,|\,j'm'\rangle\\ \times Y_{L_a}^{M_a^*}(\hat{K}_a)Y_{L_b}^{-M_b^*}(\hat{K}_b)\int\chi^J_{n'_b j'_b L'_b\leftarrow n_b j_b L_b}(R_b)F_{L'_b L'_a j'}^{j'_b j'_a}(R_b,R_a)\\ \times\chi^J_{n'_a j'_a L'_a\leftarrow n_a j_a L_a}(R_a)R_b dR_b R_a dR_a\,.\end{aligned} \tag{3.33}$$

We choose the z axis along the incident wave vector $\vec{\mathrm{K}}_a$ and the y axis along $\vec{\mathrm{K}}_a\times\vec{\mathrm{K}}_b$, by requiring the wave vector $\vec{\mathrm{K}}_b$ of the scattered particle to be in the x-z plane. Thus the polar angles $\hat{K}=(\theta,\phi)$ become $\hat{K}_a=(0,0)$ and $\hat{K}_b=(\theta,0)$, θ being the scattering angle. This yields

$$Y_{L_a}^{M_a}(\hat{K}_a)=[(2L_a+1)/4\pi]^{1/2}\delta_{M_a,0}\,. \tag{3.34}$$

and

$$Y_{L_b}^{M_b}(\hat{K}_b)=(-1)^{(|M_b|+M_b)/2}\left[\frac{(2L_b+1)(L_b-|M_b|)!}{4\pi(L_b+|M_b|)!}\right]^{1/2}P_{L_b}^{|M_b|}(\theta)\,. \tag{3.35}$$

In view of the angular-momentum vector coupling $\langle L_b L_a -M_b M_a\,|\,jm\rangle$ due to

$$\vec{\mathrm{j}}=\vec{\mathrm{L}}_a-\vec{\mathrm{L}}_b=\vec{\mathrm{j}}_b-\vec{\mathrm{j}}_a\,, \tag{3.36}$$

which obeys the conservation of the total angular momentum J, we write[4]

$$\delta_{M_a,0}=\delta_{m+M_b,0} \tag{3.37}$$

and, therefore,

$$Y_{L_b}^{M_b}(\hat{K}_b)=(-1)^{(|m|-m)/2}\left[\frac{(2L_b+1)}{4\pi}\frac{(L_b-|m|)!}{(L_b+|m|)!}\right]^{1/2}P_{L_b}^{|m|}(\theta)\ . \tag{3.38}$$

The introduction of (3.34) and (3.38) into (3.33) yields

$$\begin{aligned}T^{\mathrm{CCBA}}_{n_bj_bm_b\leftarrow n_aj_am_a}=&\frac{4\pi}{K_bK_a}\mathcal{J}\sum i^{L_a-L_b-j'}e^{i(\sigma_{L_a}+\sigma_{L_b})}(-1)^{m_a'+M_b'}(-1)^{(|m|-m)/2}[(2L_a+1)(2L_b+1)]^{1/2}\\
&\times\left[\frac{(L_b-|m|)!}{(L_b+|m|)!}\right]^{1/2}P_{L_b}^{|m|}(\theta)\langle j_aL_am_a0\,|\,Jm_a\rangle\langle j_bL_bm_b-m\,|\,Jm_a\rangle\langle j_a'L_a'm_a'M_a'\,|\,JM\rangle\\
&\times\langle j_b'L_b'm_b'M_b'\,|\,JM\rangle\langle j_b'j_a'm_b'-m_a'\,|\,j'm'\rangle\langle L_b'L_a'-M_b'M_a'\,|\,j'm'\rangle\\
&\times\int\chi^J_{n_b'j_b'L_b'\leftarrow n_bj_bL_b}(R_b)F^{j_b'j_a'}_{L_b'L_a'j'}(R_b,R_a)\\
&\times\chi^J_{n_a'j_a'L_a'\leftarrow n_aj_aL_a}(R_a)R_bdR_bR_adR_a\ ,\end{aligned} \tag{3.39}$$

where the form-factor coefficient is given by[4]

$$\begin{aligned}F^{j_bj_a}_{L_bL_aj}=&\tfrac{1}{2}i^{j+j_a-j_b}(-1)^{L_a-j_a}(2j_a+1)(2j_b+1)\\
&\times\sum_k\sum_{\lambda_b\lambda_a}(-1)^{\lambda_b-\lambda_a}(2k+1)\begin{bmatrix}2j_a\\2\lambda_a\end{bmatrix}^{1/2}\begin{bmatrix}2j_b\\2\lambda_b\end{bmatrix}^{1/2}(s_bR_a)^{\lambda_b}(t_bR_b)^{j_b-\lambda_b}(s_aR_a)^{j_a-\lambda_a}\\
&\times(t_aR_b)^{\lambda_a}G_k^{n_bj_bn_aj_a}(R_b,R_a)Z^{j_bj_a\lambda_b\lambda_ak}_{L_bL_aj}\ ,\end{aligned} \tag{3.40}$$

where

$$G_k^{n_bj_bn_aj_a}(R_b,R_a)=\int_{-1}^{1}[u_{n_bj_b}(r_b)/r_b^{j_b}]W_\alpha(\vec{R}_a,\vec{r}_a)[u_{n_aj_a}(r_a)/r_a^{j_a}]P_k(\hat{R}_a\cdot\hat{r}_a)d(\hat{R}_a\cdot\hat{r}_a) \tag{3.41}$$

and

$$Z^{j_bj_a\lambda_b\lambda_ak}_{L_bL_aj}=\sum_{d_bd_a}M^{d_bd_ak}_{L_bL_aj}N^{j_bj_aj}_{\lambda_b\lambda_ad_bd_a} \tag{3.42}$$

with

$$M^{d_bd_ak}_{L_bL_aj}=\langle d_bk00\,|\,L_b0\rangle\langle d_ak00\,|\,L_a0\rangle W(d_bL_bd_aL_a;kj) \tag{3.43}$$

and

$$\begin{aligned}N^{j_bj_aj}_{\lambda_b\lambda_ad_bd_a}=&[(2d_a+1)(2d_b+1)]^{1/2}\langle j_b-\lambda_b\lambda_a00\,|\,d_b0\rangle\\
&\times\langle j_a-\lambda_a\lambda_b00\,|\,d_a0\rangle\begin{Bmatrix}\lambda_b & j_a-\lambda_a & d_a\\ j_b-\lambda_b & \lambda_a & d_b\\ j_b & j_a & j\end{Bmatrix},\end{aligned} \tag{3.44}$$

where

$$\begin{Bmatrix}j_1 & j_2 & J_{12}\\ j_3 & j_4 & J_{34}\\ j_{13} & j_{24} & J\end{Bmatrix}$$

above is the 9-j symbol.[9] The mass factors are given by[4]

$$s_a=-M_A(M_B+M_C)/[M_B(M_A+M_B+M_C)]\ , \tag{3.45a}$$

$$t_a=(M_A+M_B)(M_B+M_C)/[M_B(M_A+M_B+M_C)]\ , \tag{3.45b}$$

$$s_b=t_a\ , \tag{3.45c}$$

and

$$t_b=-(M_A+M_B)M_C/[M_B(M_A+M_B+M_C)]\ . \tag{3.45d}$$

The summing indices are constrained by the following triangular inequalities:

$$0\le\lambda_a\le j_a\ , \tag{3.46a}$$

$$0\le\lambda_b\le j_b\ , \tag{3.46b}$$

$$|j_a-\lambda_a-\lambda_b|\le d_a\le j_a-\lambda_a+\lambda_b\ , \tag{3.46c}$$

$$|j_b-\lambda_b-\lambda_a|\le d_b\le j_b-\lambda_b+\lambda_a\ , \tag{3.46d}$$

$$|d_a-j|\le d_b\le d_a+j\ , \tag{3.46e}$$

$$|L_a-d_a|\le k\le L_a+d_a\ , \tag{3.46f}$$

and

$$|L_b-d_b|\le k\le L_b+d_b\ . \tag{3.46g}$$

The insertion of (3.40) into (3.39) and further reduction leads to

$$\begin{aligned}T^{\mathrm{CCBA}}_{n_bj_bm_b\leftarrow n_aj_am_a}=\frac{2\pi}{k_bk_a}\mathscr{J}\sum i^{L_a-L_b}e^{i(\sigma_{L_a}+\sigma_{L_b})}(-1)^{(|m|-m)/2}i^{-j'_a-j'_b}\\ \times(-1)^{j'_a+j'_b+L'_b+j'+J}(2j'_a+1)(2j'_b+1)[(2L_a+1)(2L_b+1)]^{1/2}\\ \times\left[\frac{(L_b-|m|)!}{(L_b+|m|)!}\right]^{1/2}P_{L_b}^{|m|}(\theta)\langle j_aL_am_a0\,|\,Jm_a\rangle\langle j_bL_bm_b-m\,|\,Jm_a\rangle\\ \times W(j'_aj'_bL'_aL'_b;j'J)\Lambda^{j'_bj'_a;J}_{L'_bL'_aj'}\ ,\end{aligned} \tag{3.47}$$

where

$$\Lambda^{j'_bj'_a;J}_{L'_bL'_aj'}=\sum_{k'}\sum_{\lambda'_b\lambda'_a}(-1)^{\lambda'_b-\lambda'_a}(2k'+1)\begin{bmatrix}2j'_b\\2\lambda'_b\end{bmatrix}^{1/2}\begin{bmatrix}2j'_a\\2\lambda'_a\end{bmatrix}^{1/2}Z^{j'_bj'_a\lambda'_b\lambda'_ak'}_{L'_bL'_aj'}S^{j'_bj'_a\lambda'_b\lambda'_ak'}_{L'_bL'_a;J}\ , \tag{3.48}$$

with the overlap integral S given by[4]

$$\begin{aligned}S^{j'_bj'_a\lambda'_b\lambda'_ak'}_{L'_bL'_a;J}=s_b^{\lambda'_b}t_b^{j'_b-\lambda'_b}s_a^{j'_a-\lambda'_a}t_a^{\lambda'_a}\int\chi^J_{n'_bj'_bL'_b\leftarrow n_bj_bL_b}(K'_b,R_b)G_{k'}^{n'_bj'_bn'_aj'_a}(R_b,R_a)\chi^J_{n'_aj'_aL'_a\leftarrow n_aj_aL_a}(K'_a,R_a)\\ \times R_b^{j'_b-\lambda'_b+\lambda'_a+1}R_a^{j'_a-\lambda'_a+\lambda'_b+1}dR_bdR_a\ .\end{aligned} \tag{3.49}$$

Thus, the CCBA differential cross section for unpolarized diatomic molecules in the initial state is given by

$$\frac{d\sigma^{\mathrm{CCBA}}}{d\Omega}(n_bj_b\leftarrow n_aj_a)=\frac{\mu_a\mu_b}{(2\pi\hbar^2)^2}\frac{K_b}{K_a}\frac{1}{2j_a+1}\sum_{m_bm_a}|T^{\mathrm{CCBA}}_{n_bj_bm_b\leftarrow n_aj_am_a}|^2\ . \tag{3.50}$$

Now for the case of negligibly small (zero) coupling, we find from (3.47) that

$$T^{\mathrm{CCBA}}_{n_b j_b m_b \leftarrow n_a j_a m_a} = \frac{2\pi}{K_b K_a}(2j_a+1)(2j_b+1)\not{i}^{-j_a-j_b}$$
$$\times \sum i^{-L_a-L_b} e^{i(\sigma_{L_a}+\sigma_{L_b})}(-1)^{(|m|-m)/2}(-1)^{m_a}[(2L_a+1)(2L_b+1)]^{1/2}$$
$$\times \left[\frac{(L_b-|m|)!}{(L_b+|m|)!}\right]^{1/2} P_{L_b}^{|m|}(\theta)\langle L_b L_a m 0 \,|\, jm\rangle\langle j_b j_a m_b - m_a \,|\, jm\rangle$$
$$\times \sum_k \sum_{\lambda_b \lambda_a} (-1)^{\lambda_b-\lambda_a}(2k+1)\begin{bmatrix}2j_b\\2\lambda_b\end{bmatrix}^{1/2}\begin{bmatrix}2j_a\\2\lambda_a\end{bmatrix}^{1/2} Z^{j_b j_a \lambda_b \lambda_a k}_{L_b L_a j} S^{j_b j_a \lambda_b \lambda_a k}_{L_b L_a} \tag{3.51}$$

and

$$\sum_{m_b m_a} |T^{\mathrm{CCBA}}_{n_b j_b m_b \leftarrow n_a j_a L_a}|^2 = \sum_{jm} |T^{\mathrm{DWBA}}_{n_b j_b \leftarrow n_a j_a; jm}|^2 , \tag{3.52}$$

where the DWBA transition amplitude is given by

$$T^{\mathrm{DWBA}}_{n_b j_b \leftarrow n_a j_a; jm} = 2\pi/(K_b K_a)(2j_a+1)(2j_b+1)\not{i}^{j-j_a-j_b}(-1)^{(|m|+m)/2}$$
$$\times \sum_{L_b L_a} i^{-L_a-L_b} e^{i(\sigma_{L_a}+\sigma_{L_b})}[(2L_a+1)(2L_b+1)^{1/2}$$
$$\times \left[\frac{(L_b-|m|)!}{(L_b+|m|)!}\right]^{1/2} P_{L_b}^{|m|}(\theta)\langle L_b L_a m 0 \,|\, jm\rangle \Lambda^{j_b j_a}_{L_b L_a j} . \tag{3.53}$$

where [4]

$$\Lambda^{j_b j_a}_{L_b L_a j} = \sum_k \sum_{\lambda_b \lambda_a} (-1)^{\lambda_b-\lambda_a}(2k+1)\begin{bmatrix}2j_b\\2\lambda_b\end{bmatrix}^{1/2}\begin{bmatrix}2j_a\\2\lambda_a\end{bmatrix}^{1/2} Z^{j_b j_a \lambda_b \lambda_a k}_{L_b L_a j} S^{j_b j_a \lambda_b \lambda_a k}_{L_b L_a} . \tag{3.54}$$

The phase factor $i^{j-j_a-j_b}$ in (3.53) does not affect the DWBA cross sections.

Thus the DWBA differential cross section is

$$\frac{d\sigma^{\mathrm{DWBA}}}{d\Omega}(n_b j_b \leftarrow n_a j_a) = \frac{\mu_a \mu_b}{(2\pi\hbar^2)^2}\frac{K_b}{K_a}\frac{1}{(2j_a+1)}\sum_{jm} |T^{\mathrm{DWBA}}_{n_b j_b \leftarrow n_a j_a; jm}|^2 . \tag{3.55}$$

We now note that this is the same as the DWBA expression derived elsewhere [examine Eq. (3.48) and its related equations of Ref. 4 for verification]. Using the symmetry relation[4]

$$T^{\mathrm{DWBA}}_{n_b j_b \leftarrow n_a j_a; jm} = (-1)^{j_a+j_b+j+m} T^{\mathrm{DWBA}}_{n_b j_b \leftarrow n_a j_a; j-m} , \tag{3.56}$$

we obtain

$$\frac{d\sigma^{\mathrm{DWBA}}}{d\Omega}(n_b j_b \leftarrow n_a j_a) = \frac{\mu_a \mu_b}{(2\pi\hbar^2)^2}\frac{K_b}{K_a}\frac{1}{(2j_a+1)}\sum_{jm\geq}[1+\gamma(m)]\,|T^{\mathrm{DWBA}}_{n_b j_b \leftarrow n_a j_a; jm}|^2 \tag{3.57}$$

with

$$\gamma(m)=0 \quad \text{for} \quad m=0 \tag{3.58a}$$

and

$$\gamma(m)=1 \quad \text{for} \quad m>0 ; \tag{3.58b}$$

$m \geq$ stands for m greater than or equal to 0.

Finally, we use

$$\sigma = \int_{-1}^{1} d(\cos\theta) \int_{0}^{2\pi} d\phi \, \frac{d\sigma}{d\Omega} , \tag{3.59}$$

in order to obtain the CCBA total cross section

$$\sigma^{\mathrm{CCBA}}(n_b j_b \leftarrow n_a j_a) = \frac{\mu_a \mu_b}{\pi \hbar^4} \frac{K_b}{K_a} \frac{1}{(2j_a+1)} \sum_{L_b} | T^{\mathrm{CCBA}}_{n_b j_b \leftarrow n_a j_a; L_b} |^2 , \tag{3.60}$$

where

$$\begin{aligned} T^{\mathrm{CCBA}}_{n_b j_a \leftarrow n_a j_a; L_b} = \frac{2\pi}{K_b K_a} \mathcal{J} \sum i^{-L_a} e^{i\sigma_{L_a}} (-1)^{(|m|-m)/2} i^{-j'_a - j'_b} (-1)^{m'_a + M'_b} (2j'_a+1)(2j'_b+1)(2L_a+1)^{1/2} \\ \times \langle j_a L_a m_a 0 \,|\, J m_a \rangle \langle j_b L_b m_b - m \,|\, J m_a \rangle \langle j'_a L'_a m'_a M'_a \,|\, JM \rangle \langle j'_b L'_b m'_b M'_b \,|\, JM \rangle \\ \times \langle j'_b j'_a m'_b - m'_a \,|\, j' m' \rangle \langle L'_b L'_a - M'_b M'_a \,|\, j' m' \rangle \Lambda^{j'_b j'_a; J}_{L'_b L'_a j'} , \end{aligned} \tag{3.61}$$

or briefly,

$$\begin{aligned} T^{\mathrm{CCBA}}_{n_b j_b \leftarrow n_a j_a; L_b} = \frac{2\pi}{K_b K_a} \mathcal{J} \sum i^{-L_a + j'_a + j'_b} e^{i\sigma_{L_a}} (-1)^{L'_b + j' + J} (-1)^{(|m|-m)/2} (2j'_a+1)(2j'_b+1)(2L_a+1)^{1/2} \\ \times \langle j_a L_a m_a 0 \,|\, J m_a \rangle \langle j_b L_b m_b - m \,|\, J m_a \rangle W(j'_a j'_b L'_a L'_b; j' J) \Lambda^{j'_b j'_a; J}_{L'_b L'_a j'} . \end{aligned} \tag{3.62}$$

In the limiting case of zero coupling, the expression (3.60) is reduced to the DWBA total cross section,

$$\sigma^{\mathrm{DWBA}}(n_b j_b \leftarrow n_a j_a) = \frac{\mu_a \mu_b}{\pi \hbar^4} \frac{K_b}{K_a} \frac{1}{(2j_a+1)} \sum_{jm} \sum_{L_b} | T^{\mathrm{DWBA}}_{n_b j_b \leftarrow n_a j_a; L_b jm} |^2 , \tag{3.63}$$

where

$$T^{\mathrm{DWBA}}_{n_b j_b \leftarrow n_a j_a; L_b} = \frac{2\pi}{K_b K_a} \mathcal{J} (2j_a+1)(2j_b+1) \sum_{L_a} i^{-L_a} e^{i\sigma_{L_a}} (2L_a+1)^{1/2} \langle L_b L_a m 0 \,|\, jm \rangle \Lambda^{j_b j_a}_{L_b L_a j} . \tag{3.64}$$

Using the symmetry relation similar to (3.56),

$$T^{\mathrm{DWBA}}_{n_b j_b \leftarrow n_a j_a; L_b jm} = (-1)^{j_a + j_b + j + m} T^{\mathrm{DWBA}}_{n_b j_b \leftarrow n_a j_a; L_b j - m} , \tag{3.65}$$

we obtain

$$\sigma^{\mathrm{DWBA}}(n_b j_b \leftarrow n_a j_a) = \frac{\mu_a \mu_b}{\pi \hbar^4} \frac{K_b}{K_a} \frac{1}{2j_a+1} \sum_{jm \geq} \sum_{L_b} [1 + \gamma(m)] \, | T^{\mathrm{DWBA}}_{n_b j_b \leftarrow n_a j_a; L_b jm} |^2 . \tag{3.66}$$

IV. DISCUSSION AND CONCLUSION

Based on the first Born approximation and coupled-channel wave functions in the initial and final arrangement channels, we have presented the systematic derivations of the state-to-state transition amplitude, differential cross section, and integral (total) cross section in order to describe the rearrangement collision processes of atom-diatomic molecule systems. We have also deduced the DWBA expressions from the present CCBA as a limiting case of zero coupling between channels in each arrangement.

Coupling effects are expected to be more significant at larger collision energies. For this reason, the DWBA should selectively be used. The DWBA here refers to the "conventional" treatment, that is, the distorted-wave functions describing the relative motion between the colliding or departing pair are elastic waves and the diatomic

molecules remain free (unperturbed) during collision. Such treatment is easily transferable to our DWBA formalism, also. However, in a qualitative sense, the "free molecule" treatment in the DWBA is found to be good in describing the physics of molecular reactions despite its inherent failure of unitarity and quantitative accuracy. In the future, it will be of great interest to see how well the present CCBA method will improve over the DWBA.[4] Also, it will be of great interest to study the variation of coupling effects with the scattering angle based on the CCBA.

The direct solution of the coupled Schrödinger equation (2.7) for rearrangement collisions requires excessive computation time. An excessively large number of terms which take into account the highly excited state (bound states) and unbound states of the diatomic molecule would be required in order to represent a new arrangement. In the CCBA, we truncate the infinite set of equations to a relatively small number of channels. This includes the neglect of coupling between arrangement channels. Such a strong coupling approximation with the first Born approximation has been termed coupled-channel Born approximation in nuclear reaction. It is expected that our present molecular version of the CCBA will be economically feasible.

Finally, we find from the present study that (1) the transferred angular momenta incoherently add to both differential and integral (total) cross sections only in the case of ignorable coupling as can be seen from Eqs. (3.55), (3.57), (3.63), and (3.66). (2) The incoherent contribution of product partial waves to the integral cross section is predicted to be universal for both cases of the zero coupling and nonzero coupling, an (3) the difference between the CCBA and DWBA differential cross section defines the variation of coupling effects (excluding coupling between arrangement channels) as a function of the center-of-mass scattering angle. The last study will be of great value for further understanding of microphysical reaction mechanisms. In view of various qualitative successes with the DWBA, the present CCBA method is highly promising for better quantitative results.

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[1]G. C. Schatz and A. Kuppermann, J. Chem. Phys. 65, 4642 (1976).

[2](a) A. B. Elkowitz and R. E. Wyatt, J. Chem. Phys. 62, 2504 (1975); (b) 62, 3683 (1975).

[3]B. H. Choi and K. T. Tang, J. Chem. Phys. 61, 5147 (1974).

[4](a) S. H. Suck, Phys. Rev. A 15, 1893 (1977); (b) *ibid.* 25, 2865 (1981); (c) S. H. Suck and R. W. Emmons, *ibid.* 24, 129 (1981).

[5]M. Gell-Mann and M. L. Goldberger, Phys. Rev. 91, 398 (1953); A. Messiah, *Quantum Mechanics* (Wiley, New York, 1966), Vol. V.II, pp. 839–841.

[6]A. M. Arthurs and A. Dalgarno, Proc. R. Soc. London, Ser. A. 256, 540 (1960).

[7]T. Tamura, Phys. Rep. 14, 59 (1974).

[8]A. Messiah, *Quantum Mechanics* (Wiley, New York, 1966), Vol. V.II, p. 824.

[9]A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957).