# Formal Theory of Multichannel Rearrangement Collisions*

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A general formulation for rearrangement collisions using projection-operator techniques is presented. This formulation is suitable both for multichannel direct and for multichannel resonant reactions in which intermediate compound states are formed. A method for the construction of projection operators is discussed, and explicit expressions of the projection operators are derived for general three-body rearrangement collisions.

## I. INTRODUCTION

THE general theory for rearrangement collisions (symbolically denoted by $a+b\rightarrow c+d$) was first formulated by Lippmann in 1956.[1] The basic concepts used in the formulation are that the Hamiltonian $H$ for the reaction system may be decomposed into the unperturbed and the interaction parts in two different ways, and that the total-reaction wave function may be transformed from one basis to the other by manipulating between the two different ways of decomposing of the Hamiltonian. Hence

$$H=H_i+V_i=H_f+V_f, \tag{1.1}$$

where $H_i$ is the Hamiltonian of the noninteracting reactants $a$ and $b$ in their initial states, and $V_i$ is the interaction between $a$ and $b$. Similarly, $H_f$ and $V_f$ are defined for the final-state products $c$ and $d$. The total wave function $\Psi$ of the reaction system is given by the integral equation

$$\Psi^{(+)}=\chi_i+(1/a_i^{(+)})V_i\Psi^{(+)} \tag{1.2}$$

with

$$(E-H_i)\chi_i=0, \tag{1.3}$$

$$a_i^{(+)}=E-H_i+i\eta. \tag{1.4}$$

This equation is of course not in a form convenient for obtaining the rearrangement amplitude, since the propagator $(a_i^{(+)})^{-1}$ is not diagonal in the final set of unperturbed states $\chi_f$ which are solutions of

$$(E-H_f)\chi_f=0. \tag{1.5}$$

Lippmann has shown how the state vector $\Psi^{(+)}$ may be transformed from the original basis to the basis of the rearranged system[1]:

$$\Psi^{(+)}=(1/a_f^{(+)})a_i^{(+)}\chi_i+(1/a_f^{(+)})V_f\Psi^{(+)} \tag{1.6}$$

with

$$a_f^{(\pm)}=E-H_f\pm i\eta. \tag{1.7}$$

Since $(a_f^{(+)})^{-1}a_i^{(+)}\chi_i$ contains no amplitude for outgoing waves in the final states,[2] the transition matrix is then given by the asymptotic behavior of the second term

$$\mathcal{T}=\langle\chi_f|V_f|\Psi^{(+)}\rangle=\langle\Psi^{(-)}|V_i|\chi_i\rangle \tag{1.8}$$

with

$$\Psi^{(-)}=\chi_f+(1/a_f^{(-)})V_f\Psi^{(-)}, \tag{1.9}$$

where $\Psi^{(-)}$ is the time-reversed state vector.

One of the difficulties associated with this general formulation is the lack of orthogonality between the initial and final states of the system. This results in a situation where approximations which are in fact always necessary may yield nonsensical results. This difficulty was later removed by Mittleman[3] who used optical potentials $\mathcal{U}_i$ and $\mathcal{U}_f$ which are chosen so that they give the exact elastic scattering

$$\psi_i^{(+)}=\chi_i+(1/a_i^{(+)})\mathcal{U}_i\psi_i^{(+)}, \tag{1.10}$$

$$\psi_f^{(-)}=\chi_f+(1/a_f^{(-)})\mathcal{U}_f\psi_f^{(-)}. \tag{1.11}$$

When Eqs. (1.10) and (1.11) are utilized, the transition matrix may be rewritten as

$$\mathcal{T}=\langle\Psi^{(-)}|V_i-\mathcal{U}_i|\psi_i^{(+)}\rangle=\langle\psi_f^{(-)}|V_f-\mathcal{U}_f|\Psi^{(+)}\rangle. \tag{1.12}$$

Now if we construct an operator $\Pi$ so that it projects onto the perturbed states of the system, we then have

$$\Pi_i\chi_i=\chi_i, \quad \Pi_i\Psi^{(+)}=\psi_i^{(+)}, \tag{1.13}$$

$$\Pi_f\chi_f=\chi_f, \quad \Pi_f\Psi^{(-)}=\psi_f^{(-)}. \tag{1.14}$$

Operating on $\Psi^{(+)}$ [Eq. (1.2)] by $\Pi_i$ from the left, we obtain

$$\psi_i^{(+)}=\chi_i+(1/a_i^{(+)})\Pi_iV_i\Psi^{(+)}, \tag{1.15}$$

where we have used the commutator property $[\Pi_i,a_i^{(+)}]=0$. Comparison of Eq. (1.15) with Eq. (1.10) reveals

$$\Pi_iV_i\Psi^{(+)}=\mathcal{U}_i\psi_i^{(+)}. \tag{1.16}$$

Utilizing relations given by Eqs. (1.13) and (1.16) in Eq. (1.12), we obtain

$$\mathcal{T}=\langle\Psi^{(-)}|[V_i,\Pi_i]|\Psi^{(+)}\rangle, \tag{1.17}$$

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[1] B. A. Lippmann, Phys. Rev. **102**, 264 (1956).

[2] For a careful discussion of the outgoing boundary conditions see E. Gerjuoy, Phys. Rev. **109**, 1806 (1958); Ann. Phys. (N. Y.) **5**, 58 (1958).

[3] M. H. Mittleman, Phys. Rev. **122**, 1930 (1961); **126**, 373 (1962).

and similarly

$$\mathcal{T}=\langle\Psi^{(-)}|[\Pi_f,V_f]|\Psi^{(+)}\rangle. \tag{1.18}$$

Thus, we obtain a transition matrix with transitions only between mutually orthogonal states.

The Lippmann-Mittleman theory, though exact in its general form, does not give a clear picture of resonant phenomena[4] which are characteristic of a large class of rearrangement collisions. In addition this theory, as do the usual theories for scattering collisions, utilizes the concept of decomposition of the total Hamiltonian into the unperturbed and perturbation parts. Such a concept is not always useful for rearrangement collisions, since there is no unique way of decomposing the Hamiltonian. The interaction which may act as a perturbation in the initial state becomes binding in the final state, and hence, in principle, there is no interaction which may be treated as a unique perturbation. It is therefore desirable to have a theory which requires no decomposition of the Hamiltonian and which gives a clear picture of the resonant phenomena. For this reason we adopt the projection-operator techniques suggested by Feshbach[5,6] to formulate the problem of rearrangement collisions. This is presented in Sec. II. In Sec. III, a method for construction of the projection operator is given in great detail for rearrangement collisions.

## II. REARRANGEMENT-COLLISION FORMALISM

Consider a reaction system in which $j_0$ different reaction paths are energetically accessible. We have

$$a+b\rightarrow a+b \tag{2.1a}$$

$$\rightarrow c+d \tag{2.1b}$$

$$\rightarrow e+f \tag{2.1c}$$

$$\rightarrow \text{etc.}, \tag{2.1d}$$

where each of the possible reaction paths may be represented by a set of open channels. Hence, Eq. (2.1a) corresponds to a set of scattering channels in which the elastic-scattering channel will always take place, and Eqs. (2.1b) to (2.1d) correspond to different sets of rearrangement channels in which various transmutations may take place.

Let $p_j$ denote the projector which projects onto the $j$th set of open channels and which satisfies the idempotent and orthogonal relations

$$p_jp_{j'}=p_j\delta_{jj'}, \tag{2.2}$$

where $\delta_{jj'}$ is the delta function. Then it is obvious that $p_j$ is capable of projecting out the $j$th set of open channels from the total-reaction wave function of the system $\Psi$. Asymptotically, we have

$$p_1\Psi\underset{r_1\rightarrow\infty}{\longrightarrow}\sum_\nu \chi_{\nu 1}\{[\exp(i\mathbf{k}_i\cdot\mathbf{r}_1)]\delta_{1\nu}+f_{\nu 1}(\hat{k}_i,\hat{r}_1)[\exp(ik_{i\nu}r_1)]/r_1\}, \tag{2.3}$$

$$p_j\Psi\underset{r_j\rightarrow\infty}{\longrightarrow}\sum_\lambda \phi_{\lambda j}g_{\lambda j}(\hat{k}_i,\hat{r}_j)[\exp(ik_{f\lambda}r_j)/r_j], \tag{2.4}$$

where the $\chi_{\nu i}$'s and the $\phi_{\lambda j}$'s are the appropriate wave functions for the noninteracting reactants and products with $\nu$ and $\lambda$ labeling the intrinsic states, respectively, where the $f_{\nu 1}$'s and the $g_{\lambda j}$'s are the scattering and rearrangement amplitudes and where the $r_j$'s are the channel coordinates. We have chosen $j=1$ to represent the scattering set of open channels. Note that in general the projectors are not projection operators, since they are not necessarily Hermitian. The sum of all the projectors is however Hermitian.[7] The lack of Hermiticity in the inidividual projector arises from the possibilities of interchange of flux between different sets of open channels. The projectors nevertheless become Hermitian at large channel coordinates, so that asymptotically as expected there is no removal of flux in various channels. The asymptotic Hermiticity of projectors will be shown in Sec. III where a method for the construction of the projection operators which are expressed in terms of projectors is given. It should be noted that our discussion in this section requires only the existence of the projectors.

The projection operator for the open and closed channels denoted by $P$ and $Q$, respectively, can now be constructed in terms of the projectors:

$$P=\sum_{j=1}^{j_0}p_j,\quad Q=1-P=1-\sum_{j=1}^{j_0}p_j. \tag{2.5}$$

We note that sometimes it may be convenient to include some open channels in the $Q$ subspace. Clearly if all the rearrangement channels are closed, the projector for scattering channels becomes the projection operator $P$. In this case $p_1$ should of course possess the Hermitian property $p_1=p_1^\dagger$. From Eq. (2.2) it is clear that

$$p_jP=p_j,\quad p_jQ=0. \tag{2.6}$$

When the projection operators $P$ and $Q$ are utilized, the Schrödinger equations

$$(H-E)\Psi=0 \tag{2.7}$$

for the reaction system $(a,b)$ may be rewritten as[5]

$$(\mathcal{H}_P-E)P\Psi=0 \tag{2.8}$$

with

$$\mathcal{H}_P=P\left\{H+HQ\frac{1}{E-QHQ}QH\right\}P. \tag{2.9}$$

If $P$ does not include all the open channels, the $E$ in

[4] See however, the formalism of Faddeev and Weinberg: L. D. Faddeev, Zh. Eksperim. i Teor. Fiz. **39**, 1459 (1960) [English transl.: Soviet Phys.—JETP **12**, 1014 (1961)]; Dokl. Akad. Nauk. SSR **138**, 565 (1961); **145**, 301 (1962) [English transls.: Soviet Phys.—Doklady **6**, 384 (1961); **7**, 600 (1963)]; S. Weinberg, Phys. Rev. **130**, 776 (1963); **131**, 440 (1963); **133**, B232 (1964); C. Lovelace, *ibid.* **135**, B1225 (1964).

[5] H. Feshbach, Ann. Phys. (N. Y.) **5**, 357 (1958); **19**, 287 (1962).

[6] L. Fonda and R. G. Newton, Ann. Phys. (N. Y.) **10**, 490 (1960).

[7] Such an operator was first discussed by M. Coz. [See Ref. 10.]

Eq. (2.9) should be replaced by $E+i\eta$ with $\eta \to 0^+$. The effective Schrödinger equation (2.8) is an exact representation of Eq. (2.7) with the $Q$ subspace transformed into a nonlocal optical potential which corresponds physically to potentials arising from virtual excitation of the system. It has been shown by Feshbach[5] that resonances come from bound-state solutions of $QHQ$ in the effective Hamiltonian [Eq. (2.9)].

Operating on Eq. (2.8) from the left by the projector $p_j$, we obtain the set of coupled equations for rearrangement collisions:

$$\{E-\mathcal{H}_{p_j}\}p_j\Psi=\sum_{j'\neq j}^{j_0}\mathcal{H}_{p_jp_{j'}}p_{j'}\Psi\,,\quad j=1,2,\cdots j_0 \tag{2.10}$$

with

$$\mathcal{H}_{p_j}=p_j\left\{H+HQ\frac{1}{E-QHQ}QH\right\}p_j\,, \tag{2.11}$$

$$\mathcal{H}_{p_jp_{j'}}=p_j\left\{H+HQ\frac{1}{E-QHQ}QH\right\}p_{j'}\,, \tag{2.12}$$

where we have used the idempotent and orthogonal properties of the projectors. If there are $\alpha_0$ bound-state solutions of $QHQ$,

$$(QHQ-\mathcal{E}_\alpha)Q\Phi_\alpha=0\,, \tag{2.13}$$

lying within the energy regions of concern, the coupled equations may be rewritten as

$$\{E-\mathcal{H}_{p_j}{}^{(\alpha_0)}\}p_j\Psi=\sum_{\alpha=1}^{\alpha_0}\Lambda_\alpha p_jHQ\Phi_\alpha+\sum_{j'\neq j}^{j_0}\mathcal{H}_{p_jp_{j'}}{}^{(\alpha_0)}p_{j'}\Psi\,,$$
$$j=1,2,\cdots j_0 \tag{2.14}$$

with

$$\Lambda_\alpha=\sum_{j=1}^{j_0}\Lambda_{\alpha j}=\sum_{j=1}^{j_0}\langle Q\Phi_\alpha|QHp_j|p_j\Psi\rangle/(E-\mathcal{E}_\alpha)\,, \tag{2.15}$$

$$\mathcal{H}_{p_j}{}^{(\alpha_0)}=\mathcal{H}_{p_j}-\sum_{\alpha=1}^{\alpha_0}\left\{p_jHQ\frac{|Q\Phi_\alpha\rangle\langle Q\Phi_\alpha|}{E-\mathcal{E}_\alpha}QHp_j\right\}\,, \tag{2.16}$$

$$\mathcal{H}_{p_jp_{j'}}{}^{(\alpha_0)}=\mathcal{H}_{p_jp_{j'}}-\sum_{\alpha=1}^{\alpha_0}\left\{p_jHQ\frac{|Q\Phi_\alpha\rangle\langle Q\Phi_\alpha|}{E-\mathcal{E}_\alpha}QHp_{j'}\right\}\,, \tag{2.17}$$

where the $\Lambda_{\alpha j}$'s are the resonance channel-structure functions.

Solving Eq. (2.14) formally, we obtain

$$p_j\Psi=p_jv^{(+)}\delta_{1j}+\frac{1}{a_j{}^{(\alpha_0)}}\{\sum_{\alpha=1}^{\alpha_0}\Lambda_\alpha p_jHQ\Phi_\alpha+\sum_{j'\neq j}^{j_0}\mathcal{H}_{p_jp_{j'}}{}^{(\alpha_0)}p_{j'}\Psi\}\,,$$
$$j=1,2,\cdots j_0 \tag{2.18}$$

with

$$a_j{}^{(\alpha_0)}=E-\mathcal{H}_{p_j}{}^{(\alpha_0)}+i\eta\,, \tag{2.19}$$

where $p_jv^{(+)}$ is the appropriate solution of

$$\{E-\mathcal{H}_{p_j}{}^{(\alpha_0)}\}p_jv^{(+)}=0\,. \tag{2.20}$$

In order to have a clear picture of the resonant and direct contributions to the transition amplitude, it is desirable to decouple the reaction wave functions into resonant and direct parts. By defining the following wave functions,

$$p_j\psi=p_jv^{(+)}\delta_{1j}+\frac{1}{a_j{}^{(\alpha_0)}}\sum_{j'\neq j}^{j_0}\mathcal{H}_{p_jp_{j'}}{}^{(\alpha_0)}p_{j'}\psi\,,$$
$$j=1,2,\cdots j_0, \tag{2.21}$$

the reaction wave function for the $j$th set of channels may be rearranged as

$$p_j\Psi=p_jv^{(+)}\delta_{1j}+\frac{1}{a_j{}^{(\alpha_0)}}\{\sum_{\alpha=1}^{\alpha_0}\Lambda_\alpha\tilde{p}_jHQ\Phi_\alpha+\sum_{j'\neq j}^{j_0}\mathcal{H}_{p_jp_{j'}}{}^{(\alpha_0)}p_{j'}\psi\}\,,$$
$$j=1,2,\cdots j_0 \tag{2.22}$$

with

$$\tilde{p}_j=p_j+\sum_{j'\neq j}^{j_0}\mathcal{H}_{p_jp_{j'}}\frac{1}{a_{j'}{}^{(\alpha_0)}}\tilde{p}_{j'}\,, \tag{2.23}$$

where $\tilde{p}_j$ defined by Eq. (2.23) represents an operator series. To see that the decoupled expression for $p_j\Psi$ given by Eq. (2.22) is equivalent to Eq. (2.18), it is sufficient to substitute Eqs. (2.21) and (2.23) into Eq. (2.22) and to compare their expanded series.

Substitution of $p_j\Psi$ from Eq. (2.22) back into the definition of $\Lambda_{\alpha j}$ given by Eq. (2.15) yields the set of coupled equations for the resonance structure functions:

$$\sum_{\alpha'=1}^{\alpha_0}\{(E-\mathcal{E}_\alpha)\delta_{\alpha\alpha'}-\Delta_{\alpha'}-W_{\alpha'}+\tfrac{1}{2}i\Gamma_{\alpha'}\}\Lambda_{\alpha'}$$
$$=\langle Q\Phi_\alpha|QHp_1|p_1v^{(+)}\rangle+\sum_{j=1}^{j_0}\sum_{j'\neq j}^{j_0}\langle Q\Phi_\alpha|QHp_j\frac{1}{a_j{}^{(\alpha_0)}}\mathcal{H}_{p_jp_{j'}}|p_{j'}\psi\rangle \tag{2.24}$$

with

$$\Delta_{\alpha'}=\sum_{j=1}^{j_0}\Delta_{\alpha'j}=\sum_{j=1}^{j_0}\mathrm{Re}\langle Q\Phi_\alpha|QHp_j\frac{1}{a_j{}^{(\alpha_0)}}p_jHQ|Q\Phi_{\alpha'}\rangle\,, \tag{2.25}$$

$$\Gamma_{\alpha'}=\sum_{j=1}^{j_0}\Gamma_{\alpha'j}=-2\sum_{j=1}^{j_0}\mathrm{Im}\langle Q\Phi_\alpha|QHp_j\frac{1}{a_j{}^{(\alpha_0)}}p_jHQ|Q\Phi_{\alpha'}\rangle\,, \tag{2.26}$$

$$W_{\alpha'}=\sum_{j=1}^{j_0}\sum_{j'\neq j}^{j_0}\langle Q\Phi_\alpha|QHp_j\frac{1}{a_{j'}{}^{(\alpha_0)}}\mathcal{H}p_jp_{j'}\times\frac{1}{a_{j'}{}^{(\alpha_0)}}p_{j'}HQ|Q\Phi_{\alpha'}\rangle\,, \tag{2.27}$$

where $\Delta_{\alpha j}$ is the shift from the quasistationary energy arising from the coupling with the $j$th set of open channels, $\Gamma_{\alpha j}$ is the decaying width of the compound states $Q\Phi_\alpha$ into the $j$th set of open channels, and finally $W_\alpha$ is the complex shift arising from multiple back-forth coupling between channels. The complex shift is usually very small. We note that it is sometimes convenient to introduce the concept of averaged width

$$\langle\Gamma_j\rangle=\alpha_0^{-1}\sum_{\alpha=1}^{\alpha_0}\Gamma_{\alpha j}.$$

The transition matrix $\mathcal{T}_j$ for both scattering and rearrangement collisions can now be obtained from the asymptotic behavior of $P\Psi$ given by Eq. (2.22):

$$\mathcal{T}_j=\mathcal{T}_j^{(p)}\delta_{1j}+\mathcal{T}_j^{(r)}+\mathcal{T}_j^{(d)},\quad j=1,2,\cdots j_0 \tag{2.28}$$

with

$$\mathcal{T}_j^{(r)}=\sum_{\alpha=1}^{\alpha_0}\langle p_j v^{(-)}|\tilde{p}_j HQ|Q\Phi_\alpha\rangle\Lambda_\alpha, \tag{2.29}$$

$$\mathcal{T}_j^{(d)}=\sum_{j'\neq j}^{j_0}\langle p_j v^{(-)}|\mathcal{K}_{p_j p_{j'}}{}^{(\alpha_0)}|p_{j'}\psi\rangle, \tag{2.30}$$

where $\mathcal{T}_1^{(p)}$ is the transition amplitude arising from potential scattering in Eq. (2.20), where the second term is the transition amplitude for resonant scattering and reactions arising from various compound-state formations and where finally the last term is the transition amplitude for direct scattering and reactions.

For isolated resonance (i.e., taking $\alpha_0=1$), the resonance structure function can be readily solved from Eq. (2.24):

$$\Lambda_\alpha=\left\{\langle Q\Phi_\alpha|QHp_1|p_1v^{(+)}\rangle+\sum_{j=1}^{j_0}\sum_{j'\neq j}^{j_0}\langle Q\Phi_\alpha|QHp_j\frac{1}{a_j^{(1)}}\mathcal{K}_{p_j p_{j'}}|p_{j'}\psi\rangle\right\}\Big/(E-\mathcal{E}_\alpha'+\tfrac{1}{2}i\Gamma_\alpha'), \tag{2.31}$$

where

$$\mathcal{E}_\alpha'=\mathcal{E}_\alpha+\Delta_\alpha+\mathrm{Re}(W_\alpha), \tag{2.32}$$

$$\Gamma_\alpha'=\Gamma_\alpha-2\,\mathrm{Im}(W_\alpha). \tag{2.33}$$

It is now apparent that $\mathcal{E}_\alpha'$ and $\Gamma_\alpha'$ are, respectively, the resonance energy and total width. Substitution of $\Lambda_\alpha$ from Eq. (2.31) back into Eq. (2.29) yields the expression for the resonant transition matrix:

$$\begin{aligned}\mathcal{T}_j^{(r)}&=\frac{\langle p_j v^{(-)}|\tilde{p}_j HQ|Q\Phi_\alpha\rangle}{E-\mathcal{E}_\alpha'+\frac{1}{2}i\Gamma_\alpha'}\left\{\langle Q\Phi_\alpha|QHp_1|p_1v^{(+)}\rangle+\sum_{j=1}^{j_0}\sum_{j'\neq j}^{j_0}\langle Q\Phi_\alpha|QHp_j\frac{1}{a_j^{(1)}}\mathcal{K}_{p_j p_{j'}}|p_{j'}\psi\rangle\right\}\\&=\frac{\langle p_j v^{(-)}|p_j HQ|Q\Phi_\alpha\rangle\langle Q\Phi_\alpha|QHp_1|p_1v^{(+)}\rangle}{E-\mathcal{E}_\alpha'+\frac{1}{2}i\Gamma_\alpha'}+\sum_{j'\neq j}^{j_0}\frac{\langle p_j v^{(-)}|\mathcal{K}_{p_j p_{j'}}{}^{(1)}[a_{j'}{}^{(1)}]^{-1}p_{j'}HQ|Q\Phi_\alpha\rangle\langle Q\Phi_\alpha|QHp_1|p_1v^{(+)}\rangle}{E-\mathcal{E}_\alpha'+\frac{1}{2}i\Gamma_\alpha'}\\&\quad+\sum_{j'\neq 1}^{j_0}\frac{\langle p_j v^{(-)}|p_j HQ'|Q\Phi_\alpha\rangle\langle Q\Phi_\alpha|QHp_{j'}[a_{j'}{}^{(1)}]^{-1}\mathcal{K}_{p_{j'}p_1}|p_1v^{(+)}\rangle}{E-\mathcal{E}_\alpha'+\frac{1}{2}i\Gamma_\alpha'}+\cdots,\end{aligned} \tag{2.34}$$

where we have used Eqs. (2.21) and (2.23) to carry out the expansion for the resonant transition matrix. In most practical cases, the transition matrix for resonant scattering, or reaction, may, to a good approximation, be represented by the first term. Clearly, if all the rearrangement channels are closed, then $P=p_1$, and the scattering transition matrix takes the familiar expression[5]

$$\mathcal{T}_1=\mathcal{T}^{(p)}+\frac{\langle Pv^{(-)}|PHQ|Q\Phi_\alpha\rangle\langle Q\Phi_\alpha|QHP|Pv^{(+)}\rangle}{E-\mathcal{E}_\alpha-\Delta_\alpha+\frac{1}{2}i\Gamma_\alpha}, \tag{2.35}$$

where $W_\alpha$ in this case is identically zero.

A similar expansion for the direct transition matrix can be readily obtained from Eq. (2.30) using Eq. (2.21). The expansion so obtained is nothing but the Born series for rearrangement collisions (for $j\neq 1$) with resonances which are associated with bound states in the $Q$ subspace being projected out. This modified Born series is suspected to be convergent and has been proven recently for some special cases.[8]

[8] A. Chen, S. Tani, and S. Borowitz, Phys. Rev. **137**, B236 (1965).

## III. REARRANGEMENT PROJECTION OPERATORS

The formal theory presented in Sec. II provides a convenient basis for interpreting experimental data on resonant reactions by using the concept of resonance energy and width. In order to carry out an explicit calculation of these quantities or of the cross section, the appropriate projection operators must be constructed. A projection operator for rearrangement collision was first derived by Mittleman,[9] but the result was so discouragingly complicated that arbitrary functional forms for the reaction wave function were later assumed by Coz[10] in order to obtain a simpler expression for the projection operator. Recently, a new method which resulted in much simpler expressions for projection operators was proposed by Chen and Mittleman.[11] The method, however, was limited in that the recoil of the target must be neglected except for very special cases.[12]

[9] M. H. Mittleman, Ann. Phys. (N. Y.) **28**, 430 (1964).
[10] M. Coz, Ann. Phys. (N. Y.) **35**, 53 (1965); **36**, 217 (1966).
[11] J. C. Y. Chen and M. H. Mittleman, Ann. Phys. (N. Y.) **37**, 264 (1966).
[12] J. C. Y. Chen, Phys. Rev. **148**, 66 (1966).

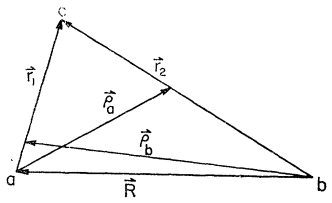


FIG. 1. Coordinates for a three-body collision system.

Here we show how the recoil of the target may be accounted for in a three-body reaction system.

We consider a three-body rearrangement collision of the type

$$ac+b\rightarrow a+bc, \tag{3.1}$$

where $a$, $b$, and $c$ are distinguishable. Let $\{\chi_\nu(\mathbf{r}_1)\}$ and $\{\phi_\lambda(\mathbf{r}_2)\}$ denote, respectively, the sets of wave functions of $ac$ and $bc$ with their coordinate defined as in Fig. 1. The total reaction wave function must satisfy the asymptotic boundary conditions

$$\lim_{\rho_b\rightarrow\infty,\, r_1 \text{ finite}} \Psi\rightarrow\sum_{\nu=1}^{\nu_0}\chi_\nu(\mathbf{r}_1)\{[\exp(i\mathbf{k}_i\cdot\boldsymbol{\varrho}_b)]\delta_{\nu 1} + f_\nu(\hat{k}_i,\hat{\rho}_b)[\exp(ik_{i\nu}\rho_b)]/\rho_b\}, \tag{3.2}$$

$$\lim_{\rho_a\rightarrow\infty,\, r_2 \text{ finite}} \Psi\rightarrow\sum_{\lambda=1}^{\lambda_0}\phi_\lambda(\mathbf{r}_2)g_\lambda(\hat{k}_i,\hat{\rho}_a)[\exp(ik_{f\lambda}\rho_a)]/\rho_a, \tag{3.3}$$

where we have assumed that there are $\nu_0$ scattering and $\lambda_0$ rearrangement open channels.

Following Chen and Mittleman[11] we make use of the geometric relations provided by Fig. 1:

$$\boldsymbol{\varrho}_a=\mathbf{R}-\mu_b\mathbf{r}_2, \quad \mu_b=M_c/(M_b+M_c), \tag{3.4}$$

$$\boldsymbol{\varrho}_b=\mathbf{R}+\mu_a\mathbf{r}_1, \quad \mu_a=M_c/(M_a+M_c), \tag{3.5}$$

where $M_a$, $M_b$, and $M_c$ are the masses of $a$, $b$, and $c$ particles, respectively. In view of the fact that the $\chi_\nu$'s and the $\phi_\lambda$'s vanish exponentially as their respective arguments $r_1$ and $r_2$ become large, we may write from Eqs. (3.4) and (3.5):

$$\rho_a=|\boldsymbol{\varrho}_a|\rightarrow R-\mu_b\hat{R}\cdot\mathbf{r}_2+O(1/R), \tag{3.6}$$

$$\rho_b=|\boldsymbol{\varrho}_b|\rightarrow R+\mu_a\hat{R}\cdot\mathbf{r}_1+O(1/R). \tag{3.7}$$

Substitution of Eqs. (3.4), (3.6), and (3.7) into Eqs. (3.2) and (3.3) yields

$$\lim_{R\rightarrow\infty,\, r_1 \text{ finite}} \Psi\rightarrow|i,1'\rangle\exp(i\mathbf{k}_i\cdot\mathbf{R})+\sum_{\nu=1}^{\nu_0}|i,\nu\rangle f_\nu(\hat{k}_i,\hat{R}) \times[\exp(ik_{i\nu}R)]/R, \tag{3.8}$$

$$\lim_{R\rightarrow\infty,\, r_2 \text{ finite}} \Psi\rightarrow\sum_{\lambda=1}^{\lambda_0}|f,\lambda\rangle g_\lambda(\hat{k}_i,\hat{R})[\exp(ik_{f\lambda}R)]/R \tag{3.9}$$

with

$$|i,1'\rangle\equiv\chi_1(\mathbf{r}_1)\exp(i\mu_a\mathbf{k}_i\cdot\mathbf{r}_1), \tag{3.10}$$

$$|i,\nu\rangle\equiv\chi_\nu(\mathbf{r}_1)\exp(i\mu_a k_{i\nu}\hat{R}\cdot\mathbf{r}_1), \tag{3.11}$$

$$|f,\lambda\rangle\equiv\phi_\lambda(\mathbf{r}_2)\exp(-i\mu_b k_{f\lambda}\hat{R}\cdot\mathbf{r}_2), \tag{3.12}$$

where $|i,1'\rangle$, $|i,\nu\rangle$, and $|f,\lambda\rangle$ are the recoil states.

The desired projectors which project onto the set of scattering and rearrangement channels can be defined, respectively, as

$$p_1\Psi=|i,1'\rangle F_{1'}(\mathbf{R})+\sum_{\nu=1}^{\nu_0}|i,\nu\rangle F_\nu(\mathbf{R}), \tag{3.13}$$

$$p_2\Psi=\sum_{\lambda=0}^{\lambda_0}|f,\lambda\rangle G_\lambda(\mathbf{R}), \tag{3.14}$$

where the unknown scattering and rearrangement functions satisfy the asymptotic expressions inferred from Eqs. (3.8) and (3.9):

$$F_{1'}(\mathbf{R})\xrightarrow[R\rightarrow\infty]{}\exp(i\mathbf{k}_i\cdot\mathbf{R}), \tag{3.15}$$

$$F_\nu(\mathbf{R})\xrightarrow[R\rightarrow\infty]{} f_\nu(\hat{k}_i,\hat{R})[\exp(ik_{i\nu}R)]/R, \tag{3.16}$$

$$G_\lambda(\mathbf{R})\xrightarrow[R\rightarrow\infty]{} g_\lambda(\hat{k}_i,\hat{R})[\exp(ik_{f\lambda}R)]/R. \tag{3.17}$$

These asymptotic expressions ensure that $p_1\Psi$ and $p_2\Psi$ satisfy the appropriate asymptotic boundary conditions.

The above conditions for the projectors are mathematically equivalent to the following equations:

$$\begin{aligned}&\langle i,1'|1-p_1-p_2|\Psi\rangle=0\\ &\langle i,\nu|1-p_1-p_2|\Psi\rangle=0, \quad \nu=1,2,\cdots,\nu_0\\ &\langle f,\lambda|1-p_1-p_2|\Psi\rangle=0, \quad \lambda=1,2,\cdots,\lambda_0.\end{aligned} \tag{3.18}$$

Since we have constrained the scattering and rearrangement channel coordinate to be $\mathbf{R}$ by introducing the recoil states [Eqs. (3.10) to (3.12)], the unknown functions $F_{1'}$, $F_\nu$, and $G_\lambda$ can easily be expressed in terms of $\Psi$ by solving the above set of linear equations. Substitution of the solutions so obtained for the unknown function back into Eqs. (3.13) and (3.14) yields immediately the explicit expressions for the projection operators. Such an algebraic manipulation can in general be carried out in terms of matrix notations. For the sake of clarity we consider here a simple case in which only the elastic and the lowest rearrangement channels are open (i.e., taking $\nu_0=\lambda_0=1$). When utilizing the definitions for the projectors given by Eqs. (3.13) and (3.14), the set of linear equations reduces for this case to the following:

$$\begin{aligned}&F_{1'}(\mathbf{R})+\eta_{1'1}(\mathbf{R})F_1(\mathbf{R})+\Delta_{1'1}(\mathbf{R})G_1(\mathbf{R})=U_{1'}(\mathbf{R}),\\ &\eta_{1'1}^*(\mathbf{R})F_{1'}(\mathbf{R})+F_1(\mathbf{R})+\Delta_{11}(\mathbf{R})G_1(\mathbf{R})=U_1(\mathbf{R}),\\ &\Delta_{1'1}^*(\mathbf{R})F_{1'}(\mathbf{R})+\Delta_{11}^*(\mathbf{R})F_1(\mathbf{R})+G_1(\mathbf{R})=V_1(\mathbf{R}),\end{aligned} \tag{3.19}$$

with

$$\eta_{1'1}(\mathbf{R})=\langle i,1'|i,1\rangle, \quad \Delta_{1'1}(\mathbf{R})=\langle i,1'|f,1\rangle, \quad \Delta_{11}(\mathbf{R})=\langle i,1|f,1\rangle, \quad \Delta_{11}^*(\mathbf{R})=\langle f,1|i,1\rangle, \tag{3.20}$$

$$U_{1'}(\mathbf{R})=\langle i,1'|\Psi\rangle, \quad U_1(\mathbf{R})=\langle i,1|\Psi\rangle, \quad V_1(\mathbf{R})=\langle f,1|\Psi\rangle, \tag{3.21}$$

where the integrals indicated by brackets in Eqs. (3.20) and (3.21) are over coordinates that are common on both sides in the brackets.

Solving Eqs. (3.19), we obtain

$$F_{1'}(\mathbf{R})=\beta(\mathbf{R})\{[1-|\Delta_{11}|^2]U_{1'}+[\Delta_{1'1}\Delta_{11}^*-\eta_{1'1}]U_1+[\eta_{1'1}\Delta_{11}-\Delta_{1'1}]V_1\}, \tag{3.22}$$

$$F_1(\mathbf{R})=\beta(\mathbf{R})\{[1-|\Delta_{1'1}|^2]U_1+[\Delta_{1'1}^*\Delta_{11}-\eta_{1'1}^*]U_{1'}+[\eta_{1'1}^*\Delta_{1'1}-\Delta_{11}]V_1\}, \tag{3.23}$$

$$G_1(\mathbf{R})=\beta(\mathbf{R})\{[1-|\eta_{1'1}|^2]V_1+[\eta_{1'1}^*\Delta_{11}^*-\Delta_{1'1}^*]U_{1'}+[\eta_{1'1}\Delta_{1'1}^*-\Delta_{11}^*]U_1\}, \tag{3.24}$$

with

$$\beta(\mathbf{R})^{-1}=[1-|\Delta_{1'1}|^2][1-|\Delta_{11}|^2]-[\Delta_{1'1}^*\Delta_{11}-\eta_{1'1}^*]\times[\Delta_{1'1}\Delta_{11}^*-\eta_{1'1}], \tag{3.25}$$

where the overlapping integrals, the $\Delta$'s, approach zero exponentially as $R$ becomes large. By substituting the asymptotic expressions for $\Psi$ into $U_{1'}$, $U_1$, and $V_1$ [see Eq. (2.21)], it can be easily seen that the unknown functions given by Eqs. (3.22) to (3.24) satisfy the asymptotic expressions required by Eqs. (3.15) to (3.17), respectively.

Substitution of $F_{1'}$ and $F_1$ back into Eq. (3.13) and $G_1$ into Eq. (3.14) yields, respectively, the projector for the elastic-scattering channel

$$\begin{aligned}p_1=\beta(\mathbf{R})\{&|i,1'\rangle[1-|\Delta_{11}|^2]\langle i,1'|\\&+|i,1\rangle[1-|\Delta_{1'1}|^2]\langle i,1|\\&+|i,1'\rangle[\Delta_{1'1}\Delta_{11}^*-\eta_{1'1}]\langle i,1|\\&+|i,1'\rangle[\eta_{1'1}\Delta_{11}-\Delta_{1'1}]\langle f,1|\\&+|i,1\rangle[\Delta_{1'1}^*\Delta_{11}-\eta_{1'1}^*]\langle i,1'|\\&+|i,1\rangle[\eta_{1'1}^*\Delta_{1'1}-\Delta_{11}]\langle f,1|\}\end{aligned} \tag{3.26}$$

and the projector for the rearrangement channel

$$\begin{aligned}p_2=\beta(\mathbf{R})\{&|f,1\rangle[1-|\eta_{1'1}|^2]\langle f,1|\\&+|f,1\rangle[\eta_{1'1}^*\Delta_{11}^*-\Delta_{1'1}^*]\langle i,1'|\\&+|f,1\rangle[\eta_{1'1}\Delta_{1'1}^*-\Delta_{11}^*]\langle i,1|\}.\end{aligned} \tag{3.27}$$

It is a straightforward to show that the projectors given above the idempotent and mutually orthogonal

$$p_1=p_1^2, \quad p_2=p_2^2, \quad p_1p_2=0. \tag{3.28}$$

It can be easily shown that the projectors are Hermitian asymptotically, since the overlapping integral approaches zero exponentially as $R$ becomes large. From Eqs. (3.26) and (3.27) we then have

$$p_1 \xrightarrow[R\to\infty]{} [1-|\eta_{1'1}|^2]^{-1}\{|i,1'\rangle\langle i,1'|+|i,1\rangle\langle i,1|-|i,1'\rangle\eta_{1'1}\langle i,1|-|i,1\rangle\eta_{1'1}^*\langle i,1'|\}, \tag{3.29}$$

$$p_2 \xrightarrow[R\to\infty]{} |f,1\rangle\langle f,1| \tag{3.30}$$

which are clearly Hermitian.

The projection operator $P$ for the open channels is then obtained by summing over the projectors; we have $P=p_1+p_2$. Clearly $P$ is idempotent from Eq. (3.28). From inspection of Eqs. (3.26) and (3.27), it is apparent that $P$ is also Hermitian even though the projectors themselves are not Hermitian. This then demonstrates that $P$ so constructed is a projection operator.

Since the exchange scattering arising from the Pauli principle can be considered as a special case of rearrangement collision in which identical particles are involved, the application of the derived projection operator to the exchange scattering is straightforward. As an example we consider the problem of elastic electron-hydrogen or neutron-deuteron exchange scattering. This corresponds to the case of taking $a$ and $b$ in Eq. (3.1) to be the same. The appropriate projection operator then takes the form

$$P=\mathfrak{A}\{p_1+p_2\}\mathfrak{A}, \tag{3.31}$$

where $\mathfrak{A}$ is the antisymmetrization operator in the case of fermions. It can be easily shown that $P\Psi$ with $P$ given by Eq. (3.31) satisfies the boundary condition

$$\lim_{\rho_j\to\infty} P\Psi \to \chi_1(r)\{\exp(i\mathbf{k}_i\cdot\boldsymbol{\rho}_j)+[f_1+g_1][\exp(ik_i\rho_j)]/\rho_j\}, \quad j=a,b \tag{3.32}$$

where $f$ and $g$ are now the direct and exchange scattering amplitudes.

Generalization of the method presented in this section to systems involving more than three particles is not at all trivial. At the present, we have not yet been able to construct, except for some special cases, a general rearrangement projection operator for more-than-three-particle systems without the recourse to infinite series.

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