# $R$-matrix method for nuclear reaction theory

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The $R$-matrix method has been used by Tobocman as a basis for deriving the equations of $N$-body scattering theory. It is claimed that this method avoids some of the ambiguities inherent in the more conventional approaches. We point out and correct some errors in Tobocman's treatment. We also give arguments to support the contention that our correction terms make a negligible contribution to the final equations.

[NUCLEAR REACTIONS Errors in Tobocman's $R$-matrix method formulation of $N$-body scattering theory are pointed out and corrected; correction terms appear to be negligible.]

## I. INTRODUCTION

Several years ago Tobocman proposed a $K$-matrix theory of nuclear form factors.[1] The formalism developed in that paper constitutes a derivation of the dynamical equations for many-body scattering on the basis of the Wigner-Peierls $R$-matrix method.[2] The results are a generalization and refinement of those of Brown and deDominicis[3] and of Garside and Tobocman.[4] This method is a completely time-independent alternative to the usual time-dependent derivation of the many-body scattering equations.[5] The equations given by the new method are very similar to the standard ones. The difference consists in the presence of certain projection operator factors and in a somewhat different definition of the Green's function operators used. The limiting process implicit in the scattering formalism is one of allowing the normalization volume to become arbitrarily large rather than one of allowing wave packets to become arbitrarily large.

The purpose of this paper is to point out two flaws in Tobocman's treatment and to analyze their consequences. The first flaw results from the fact that the lack of self-adjointness of the kinetic energy operator was not fully taken into account. The second flaw is the result of omitting a projection operator factor from the integral equations for the reaction operators.

Correcting these flaws introduces additional terms into the scattering equations which appear to destroy the similarity with the standard equations. However, we are able to present arguments to support the contention that these additional terms in fact make no contribution in the scattering equations. Thus the similarity between the equations of the time-independent formulation of many-body theory and the standard ones is preserved.

The errors in the original treatment are outlined in Sec. II, and the corrected formulas are supplied. Reasons why the correction terms are not expected to be important are given in Sec. III. As the ideas of Sec. III are presented in a rather general form, we provide in Secs. IV, V, and VI an illustration of these ideas in terms of a simple three-body model.

## II. EQUATIONS FOR THE WAVE FUNCTIONS

As in all $R$-matrix formalisms, the system point in $3N$-dimensional configuration space is confined to a finite volume $\mathcal{V}$. This point represents the simultaneous position of the $N$ particles making up the system. The boundary of $\mathcal{V}$ is a $3N$-1 dimensional polyhedron; its faces, the channel entrances, are regions of fixed channel radius $r_\alpha = a_\alpha$. There is one channel entrance $\Sigma_\alpha$ for each partition $\alpha$ of the system into two groups or clusters of particles. $\vec{r}_\alpha$ is the relative displacement of the centers of mass of the two clusters of partition $\alpha$.

Within the volume $\mathcal{V}$ we define for each partition $\alpha$ the region $\mathcal{V}_\alpha$ which is the $3N$-dimensional cylinder having channel entrance $\Sigma_\alpha$ as a cross section. The partition regions $\mathcal{V}_\alpha$ partially overlap each other, and the union of the $\mathcal{V}_\alpha$ equals the volume $\mathcal{V}$. Let $P$ be the projection onto the volume $\mathcal{V}$, and let $P_\alpha$ be the projection onto the volume $\mathcal{V}_\alpha$.

Associated with each partition $\alpha$ of the system is a representation of the Hamiltonian $H$ of the system as the sum of a partition Hamiltonian $H_\alpha$ and a partition residual interaction $V^\alpha$,

$$H = H_\alpha + V^\alpha = H_\beta + V^\beta = \cdots . \tag{1}$$

The partition $\alpha$ channels are the eigenstates of

$H_\alpha$ with eigenvalue equal to the system energy $E$. This set of channels consists of a discrete set corresponding to the two-body asymptotic states and a continuum associated with the three-or-more-body breakup configurations.[6] The Green's function operator $G$ and partition $\alpha$ Green's function operator $G_\alpha$ are defined by

$$(E-H)G=G(E-H^\dagger)=P \tag{2}$$

and

$$(E-H_\alpha)G_\alpha=G_\alpha(E-H_\alpha^\dagger)=P_\alpha. \tag{3}$$

The Green's function operator $G$ is set equal to zero outside the volume $\mathcal{V}$ as is $G_\alpha$ outside the volume $\mathcal{V}_\alpha$. Thus

$$PG=GP=G, \tag{4}$$

$$P_\alpha G_\alpha=G_\alpha P_\alpha=G_\alpha. \tag{5}$$

Equations (2) and (3) are our corrected versions of Eqs. (13a) and (14b) of Ref. 1, in which the operator

$$\Delta=H-H^\dagger=H_\alpha-H_\alpha^\dagger=T-T^\dagger \tag{6}$$

was tacitly, and erroneously, assumed to be zero. $T$ represents the operator for the total kinetic energy.

By operating on Eq. (3) from the right with $G$ and making use of Eqs. (1) and (2) one finds

$$P_\alpha G=G_\alpha+G_\alpha V_\alpha^{(+)}G, \tag{7a}$$

$$V_\alpha^{(+)}=V^\alpha+\Delta. \tag{7b}$$

A similar procedure starting with Eq. (3) again and operating from the left with $G$ gives

$$GP_\alpha=G_\alpha+GV_\alpha^{(-)}G_\alpha, \tag{8a}$$

$$V_\alpha^{(-)}=V^\alpha-\Delta. \tag{8b}$$

Equations (7) and (8) replace the basic Eq. (15) of Ref. 1. They represent the $R$-matrix theory version of the resolvent equation.

The remainder of the development of Ref. 1 is correct provided that the following replacements are made: The reaction operators $X_{\alpha\beta}$ and $X'_{\alpha\beta}$, defined by Eqs. (17b) and (17c) of Ref. 1, are to be replaced by

$$X_{\alpha\beta}=(1+V_\alpha^{(+)}G)\,V_\beta^{(-)} \tag{9a}$$

and

$$X'_{\alpha\beta}=V_\alpha^{(+)}(1+GV_\beta^{(-)}). \tag{9b}$$

The modified Lippmann-Schwinger equations, Eqs. (28a) and (29b) of Ref. 1, are to be replaced by

$$P_\alpha\Psi_{\beta j}=G_\alpha(E-H_\beta)\phi_{\beta j}+G_\alpha V_\alpha^{(+)}\Psi_{\beta j} \tag{10a}$$

for scattering states and

$$P_\beta\Psi_b=G_\beta V_\beta^{(+)}\Psi_b \tag{10b}$$

for bound states. For the case where $\alpha\neq\beta$ Eq. (10a) becomes

$$P_\alpha\Psi_{\beta j}=G_\alpha V_\alpha\Psi_{\beta j}+G_\alpha(T-T^\dagger)\Psi_{\beta j} \tag{10c}$$

since

$$(E-H_\beta)\phi_{\beta j}=0. \tag{10d}$$

For the case where $\alpha=\beta$, Eq. (10a) becomes

$$P_\beta\Psi_{\beta j}=\phi_{\beta j}+G_\beta V_\beta\Psi_{\beta j}+G_\beta(T-T^\dagger)(\Psi_{\beta j}-\phi_{\beta j}) \tag{10e}$$

since

$$P_\beta\phi_{\beta j}=\phi_{\beta j}. \tag{10f}$$

These expressions are identical to the usual forms given for the Lippmann-Schwinger equation except for the projection operator factor on the left and the last term on the right. The last term on the right vanishes by virtue of the fact that the partition Green's function operators fulfill outgoing wave boundary conditions and therefore have the same asymptotic behavior as the outgoing part of $\Psi_{\beta j}$.

## III. EQUATIONS FOR THE REACTION OPERATORS

In Ref. 4 dynamical equations for the reaction operators $X_{\alpha\beta}$ have been derived, again tacitly assuming that $\Delta$ vanishes. The corrected dynamical equations are found as follows. Let $\gamma$ be any partition and write the identity

$$X_{\alpha\beta}=V_\beta^{(-)}+V_\alpha^{(+)}(1-P_\gamma)GV_\beta^{(-)}+V_\alpha^{(+)}P_\gamma GV_\beta^{(-)}. \tag{11}$$

Note from Eqs. (7a) and (9a) that

$$P_\gamma GV_\beta^{(-)}=G_\gamma X_{\gamma\beta}. \tag{12}$$

Substitute this result into Eq. (11) to obtain the corrected dynamical equation

$$X_{\alpha\beta}=V_\beta^{(-)}+V_\alpha^{(+)}(1-P_\gamma)GV_\beta^{(-)}+V_\alpha^{(+)}G_\gamma X_{\gamma\beta}. \tag{13}$$

This would replace an equation which has the form

$$\hat{X}_{\alpha\beta}=V_\beta+V_\alpha G_\gamma\hat{X}_{\gamma\beta}. \tag{14}$$

We use the circumflex to distinguish the solution of Eq. (14) from that of Eq. (13).

If the quantities $\Delta$ and $1-P_\gamma$ in Eq. (13) are set equal to zero then Eq. (13) becomes identical to Eq. (14). One can show that it is reasonable to expect that these quantities can be neglected in the limit as the channel radii $a_\alpha$ and consequently the volume $\mathcal{V}$ becomes infinite. It is only in this limit that the channel states become representative of physical configurations.

The $\Delta$ terms convert to surface contributions

with the use of Green's theorem. This results in expressions involving the values and derivatives of continuum channel radial wave functions evaluated at large $r_\alpha$, say $r_\alpha = b_\alpha$. The $b_\alpha$ will increase along with the channel radii $a_\alpha$ as we go to the infinite volume limit $\mathcal{V} \to \infty$. These expressions will therefore be oscillatory functions of the energy. As the $b_\alpha$ get larger, these expressions become more rapidly oscillating. It thus seems reasonable that averaging the equations over a small energy interval will cause the $\Delta$-term contributions to vanish in the infinite volume limit.

To discuss the contributions of $1 - P_\gamma$ we note that the term in which it appears may be written

$$P_\alpha V_\alpha (1 - P_\gamma) G V_\beta P_\beta . \tag{15}$$

The $\Delta$ terms have been dropped by virtue of the previous argument. The factors $P_\alpha$ and $P_\beta$ have been introduced in recognition of the fact that the reaction operators $X_{\alpha\beta}$ are to be evaluated between channel states in which such projection operators are implicit.

There is a volume $\mathcal{V}_0$ at the center of $\mathcal{V}$ formed by the intersection of all the partition volumes $\mathcal{V}_\alpha$. Each quantity $P_\alpha V_\alpha$ is contained almost entirely in $\mathcal{V}_0$. The small portion of $P_\alpha V_\alpha$ that lies outside of $\mathcal{V}_0$ becomes relatively negligible as $\mathcal{V}_0$ and all the $\mathcal{V}_\alpha$ become infinitely large. Clearly, if the limit is taken in a manner such that the ratios of all the channel radii to one another remain fixed, then the portion of $P_\alpha V_\alpha$ that is exterior to $\mathcal{V}_0$ remains fixed while the interior part becomes infinite in extent. It is then plausible that in this limit we can set

$$P_\alpha V_\alpha P_\gamma = P_\alpha V_\alpha \quad (\mathcal{V} \to \infty) . \tag{16}$$

Thus the $(1 - P_\gamma)$ term may be reasonably neglected.

## IV. SIMPLE ILLUSTRATIVE EXAMPLE

We consider a simple example to illustrate the concepts and arguments given above. The system consists of three particles labeled $N$, $P$, and $C$ in one dimension. Particle $C$ is infinitely massive and inpenetrable for the other two particles. The interaction between the particles is described in terms of finite range two-body potentials. The Hamiltonian for this system is

$$H = T + V , \tag{17a}$$

$$T = -\frac{\hbar^2}{2M_N}\frac{\partial^2}{\partial R_N^2} - \frac{\hbar^2}{2M_P}\frac{\partial^2}{\partial R_P^2} , \tag{17b}$$

$$V = V_N(R_N) + V_P(R_P) + V_{NP}(|R_N - R_P|) . \tag{17c}$$

To discuss the asymptotic behavior of the system we need to introduce the relative motion and internal motion coordinates for each partition. There are three partitions:

$$\alpha = P: \ (P)(NC) , \tag{18a}$$

$$\alpha = N: \ (N)(PC) , \tag{18b}$$

$$\alpha = D: \ (NP)(C) . \tag{18c}$$

The relative ($r_\alpha$) and internal ($\rho_\alpha$) coordinates for each partition are

$$r_P = R_P , \quad \rho_P = R_N , \tag{19a}$$

$$r_N = R_N , \quad \rho_N = R_P , \tag{19b}$$

$$r_D = \frac{M_N R_N + M_P R_P}{M_N + M_P} , \quad \rho_D = R_N - R_P . \tag{19c}$$

In terms of these coordinates the kinetic energy operator is

$$T = T_\alpha + \tau_\alpha , \tag{20}$$

$$T_\alpha = -\frac{\hbar^2}{2m_\alpha}\frac{\partial^2}{\partial r_\alpha^2} , \tag{20b}$$

$$\tau_\alpha = -\frac{\hbar^2}{2\mu_\alpha}\frac{\partial^2}{\partial \rho_\alpha^2} , \tag{20c}$$

where

$$m_P = M_P , \quad \mu_P = M_N , \tag{21a}$$

$$m_N = M_N , \quad \mu_N = M_P , \tag{21b}$$

$$m_D = M_N + M_P , \quad \mu_D = \frac{M_N M_P}{M_N + M_P} . \tag{21c}$$

Next we introduce the partition Hamiltonians $H_\alpha$, the partition internal motion Hamiltonians $\mathcal{H}_\alpha$, and the partition residual interactions $V^\alpha$:

$$H = H_\alpha + V^\alpha , \tag{22a}$$

$$H_\alpha = T_\alpha + \mathcal{H}_\alpha , \tag{22b}$$

where

$$\mathcal{H}_P = \tau_P + V_N , \quad V^P = V_P + V_{NP} , \tag{23a}$$

$$\mathcal{H}_N = \tau_N + V_P , \quad V^N = V_N + V_{NP} , \tag{23b}$$

$$\mathcal{H}_D = \tau_D + V_{NP} , \quad V^D = V_N + V_P . \tag{23c}$$

Now the asymptotic behavior of the system can be discussed in terms of the channel states $\phi_{\alpha j}(\rho_\alpha)$, which are eigenfunctions of the partition internal motion Hamiltonians:

$$(\mathcal{E}_{\alpha j} - \mathcal{H}_\alpha)\phi_{\alpha j}(\rho_\alpha) = 0 . \tag{24}$$

Let $E$ be the energy of the system, and let $\Psi$ be its wave function:

$$(E - H)\Psi_{\alpha i}(r_\alpha, \rho_\alpha) = 0 . \tag{25}$$

Associated with each partition $\alpha$ is an asymptotic region of configuration space corresponding to large values of $r_\alpha$ where the partition residual interaction vanishes. In that region a channel state expansion

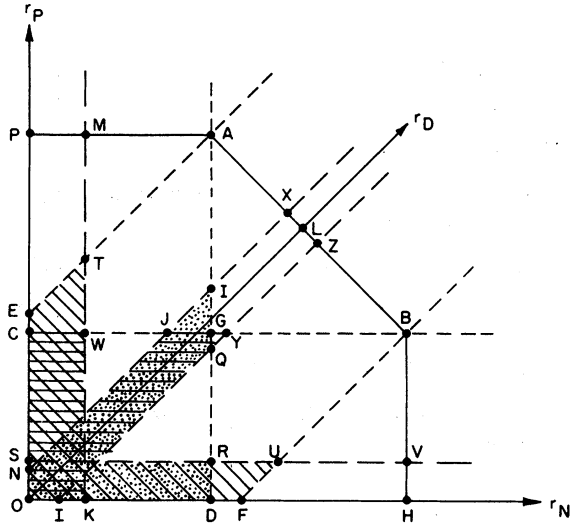


FIG. 1. Configuration space diagram for the one dimensional three-body system. $r_N$ and $r_P$ are the displacements of particles $N$ and $P$ respectively from the infinite mass, impenetrable particle $C$: $r_D = (m_N r_N + m_P r_P)/(m_N + m_P)$.

$$\Psi_{\alpha i} = \sum_j \phi_{\beta j}(\rho_\beta) u_{\beta j,\alpha i}(r_\beta) \quad (r_\beta \text{ large}) \tag{26}$$

defines the channel radial wave functions $u_{\beta j,\alpha i}$ which are solutions of

$$\left(\frac{\hbar^2 k_{\beta i}^2}{2m_\beta} - T_\beta\right) u_{\beta j,\alpha i}(r_\beta) = 0\,, \tag{27a}$$

$$\frac{\hbar^2 k_{\beta j}^2}{2m_\beta} = E - \mathcal{E}_{\beta j}\,. \tag{27b}$$

Then the asymptotic behavior of the system is described in terms of the amplitudes of the ingoing and outgoing wave parts of the radial wave functions $u_{\beta j,\alpha i}$:

$$u_{\beta j,\alpha i} = \left(\frac{m_\beta}{\hbar k_{\beta j}}\right)^{1/2} (e^{-ik_{\beta j} r_\beta} \delta_{\alpha\beta}\delta_{ij} - e^{ik_{\beta j} r_\beta} U_{\beta j,\alpha i})\,. \tag{28}$$

$U$ is the collision matrix.

Having described our system and introduced some of the relevant concepts and quantities, let us now diagram configuration space and the channel entrance surface. This is shown in Fig. 1. For our simple system configuration space is two-dimensional. The channel entrance surface is made up of the segments $PA$, $AB$, and $BH$. These segments are the channel entrances for partitions $P$, $D$, and $N$, respectively.

The projector $P$ of Eq. (2) is 1 inside the polygon $OPABH$ and vanishes elsewhere. The partition projectors of Eq. (3) are defined as follows:

$$P_P = 1 \text{ inside } OPAD\,, \quad = 0 \text{ elsewhere}\,, \tag{29a}$$

$$P_N = 1 \text{ inside } OCBH\,, \quad = 0 \text{ elsewhere}\,, \tag{29b}$$

$$P_D = 1 \text{ inside } OEABF\,, \quad = 0 \text{ elsewhere}\,. \tag{29c}$$

The channel radii are

$$a_P = OP\,, \tag{30a}$$

$$a_N = OH\,, \tag{30b}$$

$$a_D = OL\,. \tag{30c}$$

In the $R$-matrix formalism the channel states $\phi_{\alpha j}$ are required to vanish at the channel entrance edges. Thus,

$$\phi_{Pi} = 0 \text{ for } \rho_P = 0, OD\,, \tag{31a}$$

$$\phi_{Nj} = 0 \text{ for } \rho_N = 0, OC\,, \tag{31b}$$

$$\phi_{Dk} = 0 \text{ for } \rho_D = -LA, LB\,. \tag{31c}$$

For this reason the formalism provides a description of physical reality only in the limit as the channel radii $a_P$, $a_N$, and $a_D$ all approach infinity.

The dashed lines in Fig. 1 have been used to delimit the ranges of interaction of the two-body potentials. The potential $V_P$ is different from zero only between the lines $SV$ and $OH$, the potential $V_N$ vanishes everywhere except between the lines $PO$ and $MK$, and the potential $V_D$ is nonzero only between the lines $NX$ and $IZ$.

## V. ANALYSIS OF THE Δ CONTRIBUTIONS

To discuss the contributions of the operators Δ defined by Eq. (6) we introduce the asymptotic states

$$\Phi_{\alpha j} = \phi_{\alpha j}(\rho_\alpha) f_{\alpha j}(r_\alpha) \tag{32}$$

and the partition Green's function operators

$$G_\alpha = \sum_j \int_0^{a_\alpha} dr \int_0^{a_\alpha} dr' \, |\phi_{\alpha j}\delta(r_\alpha - r)\rangle (-2/\hbar) f_{\alpha j}(r_<) \times g_{\alpha j}(r_>) \langle \phi_{\alpha j}\delta(r_\alpha - r')| \,, \tag{33}$$

where

$$f_{\alpha j}(r) = \left(\frac{m_\alpha}{\hbar k_{\alpha j}}\right)^{1/2} \sin k_{\alpha j} r\,, \tag{34a}$$

$$g_{\alpha j}(r) = \left(\frac{m_\alpha}{\hbar k_{\alpha j}}\right)^{1/2} (\cos k_{\alpha j} r - s_{\alpha j} \sin k_{\alpha j} r)\,. \tag{34b}$$

The parameters $s_{\alpha j}$ can be assigned any finite

value; they control the asymptotic boundary conditions fulfilled by $G_\alpha$. The reaction amplitudes $\mathfrak{X}_{\alpha i,\beta j}$ are then defined as the matrix elements with respect to the asymptotic states of the reaction operators defined by Eq. (9):

$$\mathfrak{X}_{\alpha i,\beta j} = \langle \Phi_{\alpha i} | X_{\alpha\beta} | \Phi_{\beta j} \rangle . \tag{35}$$

The integrations required to evaluate this matrix element are understood to be confined to the inside region volume $\mathcal{V}$ which for our system is the area enclosed by the polygon *OPABH*.

From Eq. (13) we see that the evaluation of the reaction amplitudes requires the solution of the coupled integral equations

$$\langle \alpha i; r | X_{\alpha\beta} | \Phi_{\beta j} \rangle = \langle \alpha i; r | V_\beta^{(-)} + V_\alpha^{(+)}(1 - P_\gamma) G V_\beta^{(-)} | \Phi_{\beta j} \rangle + \sum_k \int dr' \langle \alpha i; r | V_\alpha^{(+)} G_\gamma | \gamma k; r' \rangle \langle \gamma k; r' | X_{\gamma\beta} | \Phi_{\beta j} \rangle \tag{36a}$$

and the subsequent evaluation of

$$\mathfrak{X}_{\alpha i,\beta j} = \int_0^{a_\alpha} dr\, f_{\alpha i}(r) \langle \alpha i; r | X_{\alpha\beta} | \Phi_{\beta j} \rangle , \tag{36b}$$

where

$$\langle r_\gamma, \rho_\gamma | \gamma k; r \rangle = \phi_{\gamma k}(\rho_\gamma) \delta(r_\gamma - r) . \tag{36c}$$

The first $\Delta$ contribution on the right of Eq. (36a) is

$$\delta_{\alpha i,\beta j}(r) = -\langle \alpha i; r | \Delta | \Phi_{\beta j} \rangle . \tag{37}$$

Consider the case where $\alpha = N$ and $\beta = P$ and use the Green's theorem to transform the volume integral to a surface integral. The volume in this case is the intersection of projectors $P_N$ and $P_P$, the rectangle *OCGD*, and the surface is line segments *CG* and *GD*. The result is

$$\delta_{Ni,Pj}(r) = \frac{\hbar^2}{2m_N} (\phi_{Ni} | f_{Pj}) \delta(b_N - r) \left( \frac{\overrightarrow{\partial}}{\partial b_N} - \frac{\overleftarrow{\partial}}{\partial b_N} \right) \phi_{Pj}(b_N) + \frac{\hbar^2}{2m_P} \phi_{Pj}(r) \phi_{Ni}(b_P) \left( \frac{\overrightarrow{\partial}}{\partial b_P} - \frac{\overleftarrow{\partial}}{\partial b_P} \right) f_{Pj}(b_P) , \tag{38}$$

where

$$b_N = OD, \quad b_P = OC . \tag{39}$$

In accordance with Eq. (36b) this $\Delta$ contribution to the reaction amplitude is

$$\Delta_{Ni,Pj} = \frac{\hbar^2}{2m_N} (\phi_{Ni} | f_{Pj}) f_{Ni}(b_N) \left( \frac{\overrightarrow{\partial}}{\partial b_N} - \frac{\overleftarrow{\partial}}{\partial b_N} \right) \phi_{Pj}(b_N) + \frac{\hbar^2}{2m_P} (f_{Ni} | \phi_{Pj}) \phi_{NI}(b_P) \left( \frac{\overrightarrow{\partial}}{\partial b_P} - \frac{\overleftarrow{\partial}}{\partial b_P} \right) f_{Pj}(b_P) . \tag{40}$$

The question is: How does $\Delta_{Ni,Pj}$ behave in the limit as $b_N$ and $b_P$ approach infinity? The channel states $\phi_{\alpha i}(\rho)$ decay exponentially with $\rho$ for channels $\alpha i$ that are two-body channels. Thus $\Delta_{Ni,Pj}$ vanishes in the infinite $b$ limit if both $Ni$ and $Pj$ are two-body channels. In any case, $f_{Ni}(b_N)$ and $f_{Pj}(b_P)$ for large $b_N$ and $b_P$ will be strongly oscillatory functions of the energy provided $Ni$ and $Pj$ are open channels. By choosing the parameters $s_{\alpha i}$ of Eq. (34b) appropriately[7] we can restrict ourselves to the evaluation of reaction amplitudes involving only open channels. We conclude that $\Delta_{Ni,Pj}$ becomes an increasingly strongly oscillatory function of energy as $b_N$ and $b_P$ increase and therefore can be eliminated by averaging over a small energy interval.

Let us consider $\delta_{\alpha i,\beta j}(r)$ of Eq. (37) for another choice of $\alpha$ and $\beta$. Let us set $\alpha = D$ and $\beta = N$. Then the volume of integration is the intersection of $P_D$ and $P_N$, polygon *OCBF*. By use of the Green's theorem the volume integral is converted to a surface integral which in this case is a line integral along *CB* and *BF*. The result is

$$\Delta_{Di,Nj} = \int_0^{a_D} dr\, f_{Di}(r) \delta_{Di,Nj}(r) = \frac{\hbar^2}{2m_P} \left[ \phi_{Di}(r) f_{Di}\left( \frac{m_N}{m_D} r + b_P \right) | f_{Nj}(r + b_P) \right] \times \left( \frac{\overrightarrow{\partial}}{b_P} - \frac{\overleftarrow{\partial}}{b_P} \right) \phi_{Nj}(b_P) + \frac{\hbar^2}{2\mu_D} \phi_{Di}(b_D) \left( \frac{\overrightarrow{\partial}}{\partial b_D} - \frac{\overleftarrow{\partial}}{\partial b_D} \right) \times \left[ f_{Di}\left( r + \frac{m_N}{m_D} b_D \right) | \phi_{Nj}(r) f_{Nj}(r + b_D) \right] , \tag{41}$$

where

$$b_D = DB . \tag{42}$$

The behavior of $\Delta_{Di,nj}$ for large values of $b_P$ and $b_D$ is similar to that of $\Delta_{Ni,Pj}$. If $Di$ and $Nj$ are two-body channels, $\Delta_{Di,Nj}$ will tend to vanish because $\phi_{Nj}(b_P)$ and $\phi_{Di}(b_D)$ will decay exponentially with increasing $b$. In any case, the matrix elements, involving $f_{Di}$ and $f_{Nj}$ the way they do, will become increasingly strong oscillatory functions of the energy with increasingly large values of $b_P$ and $b_D$.

This completes our discussion of the $\Delta$ contribution to the first term on the right of Eq. (36a). In the other terms, the operator $\Delta$ is always multiplied by a Green's function operator. Let us next direct our attention to the third term and analyze the $\Delta$ contribution to the kernel of the integral

equation:

$$\eta_{\alpha i,\gamma k}(r,r') = \langle \alpha i; r | T - T^\dagger) G_\gamma | \gamma k; r' \rangle$$
$$= -\frac{2}{\hbar} \langle \phi_{\alpha i} \delta(r_\alpha - r) | T - T^\dagger$$
$$\times | \phi_{\gamma k} g_{\gamma k}(r_>) f_{\gamma k}(r_<) \rangle , \quad (43)$$

where $r_>, r_< = r'$, $r_\alpha$ for $r' > r_\alpha$ and $r_\alpha$, $r'$ for $r_\alpha > r'$. The resultant contribution to the right side of Eq. (36a) is

$$\sum \int dr' \left(-\frac{2}{\hbar}\right) \langle \phi_{\alpha i} \delta(r_\alpha - r) | T - T^\dagger | \phi_{\gamma k} g_{\gamma k} \rangle$$
$$\times \langle \phi_{\gamma k} f_k | X_{\gamma\beta} | \Phi_{\beta j} \rangle , \quad (44)$$

where the assignments of $g$ and $f$ have been made in anticipation of the fact that the matrix element of $T - T^\dagger$ is to be transformed into a surface integral. The matrix element of $T - T^\dagger$ is seen to be identical to the definition of $\delta_{\alpha i,\gamma k}(r)$ as given in Eq. (37) except that $f_{\gamma k}$ has been replaced by $-g_{\gamma k}$. The energy dependence of $g$ is similar to that of $f$ so the arguments given above showing that $\delta_{\alpha i,\gamma k}(r)$ makes no contribution also apply to the $\Delta$ contribution of the third term on the right side of Eq. (36a).

The $\Delta$ contributions to the first and third terms on the right of Eq. (36a) have been shown to be negligible. The second term is similar to the third term except that $G$ appears in place of a partition Green's function operator $G_\alpha$. However, the Green's function operator $G$ is required to have the same behavior as the partition Green's function operator $G_\alpha$ in the $\alpha$ partition asymptotic region. Thus the $\Delta$ contributions of the second term will be of the same kind as those of the other two terms, so they can also be eliminated by averaging over a small energy interval.

## VI. ANALYSIS OF THE $(1 - P_\gamma)$ CONTRIBUTION

We now analyze the second term of Eq. (36a) disregarding the $\Delta$ contributions. In particular, we consider the operator

$$\Theta_{\alpha\gamma\beta} = P_\alpha V_\alpha (1 - P_\gamma) G V_\beta P_\beta . \quad (45)$$

We argue that the operator $P_\alpha V_\alpha = V_\alpha P'_\alpha$ is contained almost entirely in the volume $\mathfrak{V}_0$, the intersection of all partition projection operators. The operator $1 - P_\gamma$ vanishes within $\mathfrak{V}_0$, so the operator $P_\alpha V_\alpha (1 - P_\gamma)$ would also vanish if all the $P_\alpha V_\alpha$'s were contained entirely in $\mathfrak{V}_0$.

The volume $\mathfrak{V}_0$ for our example is the rectangle $OCGD$. The area in which $P_N V_N$ does not vanish in Fig. 1 has horizontal stripes, the area in which $P_D V_D$ does not vanish has diagonal stripes, and the area in which $P_P V_P$ does not vanish is speckled. We see that these areas are contained almost entirely in $\mathfrak{V}_0$. $P_D V_D$ is nonvanishing outside of $\mathfrak{V}_0$ only in the quadrangles $CETW$ and $RUFD$. $P_N V_N$ is nonvanishing outside of $\mathfrak{V}_0$ only in the triangle $QGY$. $P_P V_P$ is nonvanishing outside of $\mathfrak{V}_0$ only in the triangle $JIG$.

Now consider what happens when the channel radii $a_N$, $a_P$, and $a_D$ all become very large maintaining fixed ratios to each other. The striped and speckled areas where $P_N V_N$, $P_P V_P$, and $P_D V_D$ do not vanish all become very large, but the areas of the quadrangles $CETW$ and $RUFD$ and the areas of the triangle $QGY$ and $JIG$ remain fixed. Thus the relative contributions of these areas become negligible in the inifinite channel radius limit, provided they do not occur in the regions corresponding to the central parts of the bound state channel state wave functions. Just the opposite is true.

For the operator $P_D V_D$, we must consider the overlap of partition $D$ channel states with the quadrangles $CETW$ and $RUFD$. For the operator $P_N V_N$ we must consider the overlap of partition $N$ channel states with the triangle $QGY$. For the operator $P_P V_P$ we must consider the overlap of partition $P$ channel states with the triangle $JIG$. In every case the area in question is located at the edge of the channel entrance as far away as possible from the place where the bound state channel states, the ones associated with two-body channels, would be localized. So it is clear that as the channel radii increase in magnitude the extent of the channel entrances increases, and since the quadrangles $CETW$ and $RUFD$ and the triangles $QGY$ and $JIG$ remain fixed in size their contributions to matrix elements involving the channel state wave functions must become relatively less and less important.

We conclude that the operator $P_\alpha V_\alpha (1 - P_\gamma)$, which is the left-hand factor of $\Theta_{\alpha\gamma\beta}$ of Eq. (45), will cause the vanishing of the large channel radius limit of matrix elements of $\Theta_{\alpha\gamma\beta}$ which have partition channel states on the left. Therefore, the second term on the right side of Eq. (36a) may be ignored. Having thus justified the neglect of the $\Delta$ contributions and the $(1 - P_\gamma)$ contribution to Eq. (36a), we conclude that Eq. (36a) may be replaced by

$$\langle \alpha i; r | X_{\alpha\beta} | \Phi_{\beta j} \rangle$$
$$= \langle \alpha i; r | V_\beta | \Phi_{\beta j} \rangle + \sum_k \int dr' \langle \alpha i; r | V_\alpha G_\gamma | \gamma k; r' \rangle$$
$$\times \langle \gamma k; r' | X_{\alpha\beta} | \Phi_{\beta j} \rangle . \quad (46)$$

*Note added in proof.* The surface contributions

resulting from the kinetic energy operator not being self-adjoint has been discussed previously by E. Gerjuoy in Phys. Rev. 109, 1806 (1958). His analysis is based on the Lippmann-Schwinger integral equations. His conclusion that the surface contributions vanish if the energy is given a small positive imaginary part is very similar to our use of an average over a small energy interval to eliminate the surface contributions in the context of the $R$-matrix formalism.

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