

## Nonorthogonality, resonating group method, and multiparticle collision theory

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In this paper, the problems of nonorthogonality and possible overcompleteness in the resonating group method equations are treated by explicitly symmetrizing previously developed distinguishable-particle methods. It is shown that the orthogonalized resonating group method equations are equivalent to the two-cluster-subspace projections of a symmetrized set of multiparticle scattering equations with distortion operators. The result of the analysis is the conversion of the resonating group method to an in-principle, convergeable approximation scheme. Corrections to the resonating group method from three-cluster contributions are briefly discussed.

### I. INTRODUCTION

In going beyond semiphenomenological methods, such as the optical model or distorted-wave Born approximation (DWBA), standard reaction theories<sup>1</sup> work with a variational ansatz for the wave function. This wave function is constructed as a sum of terms, each of which is the product of the bound states of the clusters in some two-cluster channel and an arbitrary relative-motion wave function.

The variational principle which determines these arbitrary wave functions leads to a set of coupled equations. As applied to rearrangement reactions, these equations are known as coupled reaction channel (CRC) equations.<sup>2-6</sup> When a completely antisymmetrized trial wave function is used they are known as resonating group method (RGM) equations.<sup>7-9</sup>

Both rearrangement and antisymmetry mean that the asymptotic regions of interest cannot be described by a single asymptotic Hamiltonian for the free motion of the two clusters. Hence, the natural basis states for the problem are not orthogonal. As a result, the dynamical equations contain nonorthogonality (NO) terms. These terms are proportional to the overlaps of the bound cluster states in different arrangements. It is essential to retain these terms in the CRC or RGM equations if one wishes to treat the nonorthogonality of the basis correctly.

The CRC and RGM formalisms are designed to treat two-cluster final states. Many-cluster final states are most easily described by the equations of multiparticle scattering theories, which incorporate both the complete set of asymptotic boundary conditions and a mathematical formalism that yields, in principle, unique solutions.

If one wishes to extend the CRC or RGM to include, e.g., three-cluster final states, such theories provide a natural means for doing so.

In a previous paper it has been shown through an orthogonalizing procedure how to embed the CRC equations into a multiparticle scattering formalism.<sup>10</sup> In a separate work it has also been shown how to antisymmetrize wave function descriptions of multiparticle scattering.<sup>11</sup> Our purpose in the present article is to combine these two procedures and show how to embed the RGM equations into an antisymmetrized multiparticle collision theory. This establishes an expected connection and provides a framework for exploring, in a convergeable formalism, breakup corrections to the RGM.

This paper is organized as follows. In Sec. II, we review the orthogonalizing procedure for the case of distinguishable particles, while in Sec. III we extend this procedure to include the effects of particle identity. We apply these latter results, yielding the orthogonalized RGM equations, in Sec. IV. In Sec. V the symmetrization procedure<sup>11</sup> is reviewed and applied to the  $N$  particle, distorted wave function component equations developed by Levin;<sup>12</sup> these are the same equations used in Ref. 10. In Sec. VI we show how to choose the distortion operators introduced in Sec. V so that the two-cluster projection of the symmetrized multiparticle equations yield the RGM equations. The embedding of the RGM equations is accomplished in Sec. VII by means of a two-potential relation. Corrections due to three-cluster contributions are discussed in Sec. VIII, where it is shown that Faddeev-type techniques must be introduced in order to solve the resulting three-cluster equations. Our results are briefly summarized in Sec. IX, and the paper concludes with a technical appendix.

## II. REVIEW OF THE UNSYMMETRIZED ORTHOGONALIZING PROCEDURE

In this section we review those portions of Ref. 10 necessary for the later development of this paper and introduce relevant notation.

We wish to solve the Schrödinger equation

$$(E - H)\Psi = 0 \quad (2.1)$$

in a subspace consisting of a chosen set of two-cluster channels. By a channel we shall mean a product of given bound states, denoted  $\phi_{\beta m}$ . We use  $\beta$  to signify a specific two-cluster partition and  $m$  as the set of relevant quantum numbers. Corresponding to each is a decomposition of  $H$  into an asymptotic channel Hamiltonian  $H_\beta$  and a channel interaction  $V^\beta$ :

$$H = H_\beta + V^\beta, \quad \text{all } \beta. \quad (2.2)$$

$V^\beta$  contains all intercluster interactions and  $H_\beta$  governs the motion of the system when  $V^\beta = 0$ .

From the  $\phi_{\beta m}$  one can construct two-cluster projection operators  $P_\beta$  in the usual manner. The standard CRC equations approximating (2.1) then take the general form<sup>2-6,10</sup>

$$P_\beta(E - H) \sum_\gamma P_\gamma \psi_\gamma^{\text{CRC}} = 0, \quad (2.3)$$

which leads to

$$(E - H_\beta)P_\beta \psi_\beta^{\text{CRC}} = P_\beta \sum_\gamma V^\beta P_\gamma \psi_\gamma^{\text{CRC}} - \sum_\gamma (E - H_\beta) \bar{\delta}_{\beta\gamma} P_\beta P_\gamma \psi_\gamma^{\text{CRC}}. \quad (2.4)$$

The factor  $\bar{\delta}_{\beta\gamma} P_\beta P_\gamma$  is the nonorthogonality (NO) overlap, where  $\bar{\delta}_{\beta\gamma} = 1 - \delta_{\beta\gamma}$ . Applications of these equations to nuclear reactions can be found in Refs. 2-6.

By Eq. (2.3), the CRC ansatz

$$\psi^{\text{CRC}} = \sum_\gamma P_\gamma \psi_\gamma^{\text{CRC}}$$

is an approximate means of restricting the Schrödinger solution  $\Psi$  to the subspace spanned by the chosen two-cluster channels. We shall refer to this subspace as the model space. As in Refs. 10 and 13, we define  $P_\pi$  to be the projector onto the model space. We introduce

$$\mathcal{P} = \sum_\beta P_\beta \quad (2.5)$$

and its generalized inverse<sup>13</sup>  $\mathcal{P}^{-1}$  which satisfies

$$\mathcal{P} \mathcal{P}^{-1} = \mathcal{P}^{-1} \mathcal{P} = P_\pi. \quad (2.6)$$

Since

$$P_\beta P_\pi = P_\pi P_\beta = P_\beta \quad (2.7)$$

and any model space wave function  $P_\pi \psi$  can be expanded as

$$P_\pi \psi = \sum_\beta P_\beta \psi_\beta, \quad (2.8)$$

the CRC equations follow from

$$(E - P_\pi H P_\pi) P_\pi \psi = 0. \quad (2.9)$$

The quantities  $\psi_\beta$  are not always uniquely defined. As discussed in Ref. 10, a set of unique components can be defined using  $\mathcal{P}^{-1}$ :

$$P_\beta \psi_\beta = P_\beta \mathcal{P}^{-1} \psi. \quad (2.10)$$

An alternate set of unique quantities, the projections, are defined by

$$\bar{\psi}_\beta = P_\beta \psi, \quad (2.11)$$

and are related to  $P_\pi \psi$  by

$$P_\pi \psi = \mathcal{P}^{-1} \sum_\beta P_\beta \bar{\psi}_\beta. \quad (2.12)$$

The components  $\psi_\beta$  and the projections  $\bar{\psi}_\beta$  are, respectively, right- and left-hand dual eigenvectors of the non-Hermitian operator  $P_\beta \mathcal{P}^{-1} H P_\gamma$ . They are related by

$$\psi_\beta = \sum_\gamma \Lambda_{\beta\gamma} \bar{\psi}_\gamma, \quad (2.13)$$

where

$$\Lambda_{\beta\gamma} = P_\beta \mathcal{P}^{-2} P_\gamma. \quad (2.14)$$

The  $\Lambda_{\beta\gamma}$  are the generalized inverses of the NO kernel and obey

$$\Lambda_{\beta\gamma} = P_{\beta\gamma} - \sum_\epsilon \bar{\delta}_{\beta\epsilon} P_\beta P_\epsilon \Lambda_{\epsilon\gamma}, \quad (2.15)$$

where

$$P_{\beta\gamma} = P_\beta \mathcal{P}^{-1} P_\gamma. \quad (2.16)$$

If there is no overcompleteness among the states  $\phi_{\beta m}$ ,

$$P_{\beta\gamma} = \delta_{\beta\gamma} P_\beta. \quad (2.17)$$

In the case of overcompleteness,  $P_{\beta\gamma}$  is given by

$$P_{\beta\gamma} = \delta_{\beta\gamma} P_\gamma - Q_{\beta\gamma}, \quad (2.18)$$

where  $Q_{\beta\gamma}$  projects onto the space of spurious components. A vector of spurious components  $\xi_\gamma$  is one which obeys

$$P_\gamma \xi_\gamma = \xi_\gamma, \quad (2.19)$$

$$\sum_\gamma \xi_\gamma = 0.$$

These equations apply even if the particles are identical, although they are awkward to use because all the exchange equivalent partitions are included explicitly, resulting in an unnecessary duplication of equations. In Sec. III we show how to reduce the number of equations for the identical particle case.

## III. NONORTHOGONALITY AND PARTICLE IDENTITY

In this section we will discuss the identical particle case using the techniques of Bencze and Redish<sup>14</sup> applied to the previous analysis. These techniques apply to both fermions and bosons; the term symmetrization will be used to cover both cases.

We begin by replacing the partition labels  $\beta$  by equivalence class labels  $b(j)$ , where  $b$  refers to a generic  $m$ -cluster partition, and  $0 \leq j \leq N_b$  labels the members of the class. The set  $\{b(0)\}$  is the set of canonical labels.<sup>14</sup> The permutation operator which converts a state of partition  $b(j)$  to one of  $b(k)$  is denoted  $\hat{P}_{b(k)b(j)}$ , where the caret signifies the presence of the relevant fermion phase factors. The projector onto internally symmetrized states in partition  $b(j)$  is denoted  $R_{b(j)}$ . Finally, the full normalized symmetrizer is  $R$ , given by<sup>14</sup>

$$R = \frac{1}{\hat{N}_b} \sum_{j=0}^{N_b} \hat{P}_{b(j)b(k)} R_{b(k)}, \quad (3.1)$$

where  $\hat{N}_b = N_b + 1$ .

The internal states  $\phi_{b(j)m}$  projected onto by  $P_{b(j)}$  are assumed to be symmetrized, so that

$$R_{b(j)} P_{b(j)} = P_{b(j)} R_{b(j)} = P_{b(j)}. \quad (3.2)$$

As before, we define

$$\mathcal{P} = \sum_{b,j} P_{b(j)}, \quad (3.3)$$

its generalized inverse to be  $\mathcal{P}^{-1}$ , and  $P_\pi$  by

$$\mathcal{P} \mathcal{P}^{-1} = \mathcal{P}^{-1} \mathcal{P} = P_\pi. \quad (3.4)$$

$P_\pi$  is the projector onto the unsymmetrized model space.

Since  $P_\pi$  and  $\mathcal{P}$  contain internally symmetrized states from all members of all equivalence classes, the relations

$$\hat{P} P_\pi = P_\pi \hat{P}, \quad (3.5)$$

$$\hat{P} \mathcal{P} = \mathcal{P} \hat{P}, \quad (3.6)$$

$$\hat{P} \mathcal{P}^{-1} = \mathcal{P}^{-1} \hat{P}, \quad (3.7)$$

where  $\hat{P}$  is any permutation operator, are intuitively obvious. Detailed proofs are given in the Appendix.

Let us now introduce the projector  $P_A$  onto the fully symmetrized model space:

$$P_A = R P_\pi. \quad (3.8)$$

The analog of Eq. (2.8) is

$$P_A \psi = \sum_b \sqrt{\hat{N}_b} R P_{b(0)} \psi_{b(0)}. \quad (3.9)$$

By definition, the components in noncanonical partitions are

$$\psi_{b(j)} = \hat{P}_{b(j)b(0)} \psi_{b(0)}, \quad (3.10)$$

so that use of (3.10) in (3.9) yields

$$P_A \psi = \sum_{b,j} \sqrt{1/\hat{N}_b} \hat{P}_{b(j)} \psi_{b(j)}. \quad (3.11)$$

As in the unsymmetrized case, we may introduce unique components *via*

$$P_{b(j)} \psi_{b(j)} = \sqrt{\hat{N}_b} P_{b(j)} \mathcal{P}^{-1} P_A \psi. \quad (3.12)$$

Similarly, the projections  $\bar{\psi}_{b(j)}$  are given by

$$P_{b(j)} \bar{\psi}_{b(j)} = \sqrt{\hat{N}_b} P_{b(j)} P_A \psi. \quad (3.13)$$

The antisymmetrized wave function  $P_A \psi$  is expressed in terms of the  $\bar{\psi}_{b(j)}$  by

$$P_A \psi = \sum_{b,j} \hat{N}_b^{-1/2} \mathcal{P}^{-1} P_{b(j)} \bar{\psi}_{b(j)}, \quad (3.14a)$$

$$= \sum_b \hat{N}_b^{1/2} \mathcal{P}^{-1} R P_{b(0)} \bar{\psi}_{b(0)}. \quad (3.14b)$$

The projections are related to the components by

$$P_{b(0)} \bar{\psi}_{b(0)} = \sum_d (\hat{N}_b \hat{N}_d)^{1/2} P_{b(0)} R P_{d(0)} \psi_{d(0)}, \quad (3.15)$$

while the inverse relation can be written

$$P_{b(0)} \psi_{b(0)} = \sum_d \tilde{\Lambda}_{bd} P_{d(0)} \bar{\psi}_{d(0)}, \quad (3.16)$$

where

$$\tilde{\Lambda}_{bd} = (\hat{N}_b \hat{N}_d)^{1/2} P_{b(0)} \mathcal{P}^{-2} R P_{d(0)}. \quad (3.17)$$

The generalized inverse  $\tilde{\Lambda}_{bd}$  can be determined from

$$\sum_a (\hat{N}_b \hat{N}_d)^{1/2} P_{b(0)} R P_{a(0)} \tilde{\Lambda}_{ad} = \tilde{P}_{bd}, \quad (3.18)$$

where

$$\tilde{P}_{bd} = (\hat{N}_b \hat{N}_d)^{1/2} P_{b(0)} \mathcal{P}^{-1} R P_{d(0)}. \quad (3.19)$$

The matrix of  $\tilde{P}_{bd}$ 's is a projector, i.e., it is Hermitian and satisfies

$$\sum_d \tilde{P}_{bd} \tilde{P}_{da} = \tilde{P}_{ba}, \quad (3.20)$$

an equation easily proved on use of (3.19).

The operator  $\tilde{P}_{bd}$  can be written as

$$\tilde{P}_{bd} = \delta_{bd} P_{d(0)} - \tilde{Q}_{bd}, \quad (3.21)$$

where  $\tilde{Q}_{bd}$  projects onto the space of spurious states. These consist of Pauli forbidden states as well as overcomplete states. Such projectors have previously been discussed by Saito.<sup>15</sup> Note that Pauli-forbidden states only occur when Slater determinants are used to represent an antisymmetric wave function.<sup>16</sup>

#### IV. ORTHOGONALIZED RGM EQUATIONS

The standard form of the RGM equations<sup>8,9</sup> follows from

$$(E - P_A H P_A) P_A \psi^{\text{RGM}} = 0 \quad (4.1)$$

by expanding as in Eq. (3.9) and projecting with  $\hat{N}_b^{1/2} P_{b(0)}$ . This leads to a set of equations involving only canonical labels:

$$\sum_d [E (\hat{N}_b \hat{N}_d)^{1/2} P_{b(0)} R P_{d(0)} - (\hat{N}_b \hat{N}_d)^{1/2} P_{b(0)} H R P_{d(0)}] P_{d(0)} \psi_{d(0)}^{\text{RGM}} = 0. \quad (4.2)$$

Applications of these equations are discussed by Tang, LeMere, and Thompson.<sup>9</sup>

As in Sec. II, equations for unique components and projections can be derived. The equations for the components can be obtained by operating on (4.1) with  $\hat{N}_b^{1/2}P_{b(0)}\mathcal{P}^{-1}$  and using Eq. (3.12):

$$\sum_d [E\delta_{bd} - (\hat{N}_b\hat{N}_d)^{1/2}P_{b(0)}\mathcal{P}^{-1}RHP_{d(0)}]P_{d(0)}\psi_{d(0)} = 0, \quad (4.3)$$

which is the form of (4.2) obtained by inverting the NO terms and requiring that  $P_{d(0)}\psi_{d(0)}$  be nonspurious.

Similarly, the equations for the projections are obtained by using Eq. (3.13) and acting on (4.1) with  $\hat{N}_b^{1/2}P_{b(0)}$ :

$$\sum_d [E\delta_{bd} - (\hat{N}_b\hat{N}_d)^{1/2}P_{b(0)}HR\mathcal{P}^{-1}P_{d(0)}]P_{d(0)}\bar{\psi}_{d(0)} = 0. \quad (4.4)$$

The components and projections are easily seen to be right- and left-hand dual eigenstates of  $P_{b(0)}\mathcal{P}^{-1}RHP_{d(0)}$ , in strict analogy to the CRC case. Similar equations have also been derived by various authors using other techniques.

The detailed structure of (4.3) can be made more explicit by writing  $H$  as  $H = H_{d(0)} + V^{d(0)}$  and using Eqs. (3.19) and (3.21):

$$\sum_d [\delta_{bd}(E - H_{d(0)}) + Q_{bd}H_{d(0)} - (\hat{N}_b\hat{N}_d)^{1/2}P_{b(0)}\mathcal{P}^{-1}RV^{d(0)}P_{d(0)}]P_{d(0)}\psi_{d(0)} = 0. \quad (4.5)$$

We will show in Sec. V that (4.5) is the form taken by the distorted version of the projected, symmetrized multiparticle scattering equations.

Yet another representation of the RGM equations can be obtained by using (3.14b) and projecting (4.1) onto  $\hat{N}_b^{1/2}P_{b(0)}\mathcal{P}^{-1}$ :

$$\sum_d [E\tilde{\Lambda}_{bd} - (\hat{N}_b\hat{N}_d)^{1/2}P_{b(0)}\mathcal{P}^{-1}RH\mathcal{P}^{-1}P_{d(0)}]P_{d(0)}\bar{\psi}_{d(0)} = 0, \quad (4.6)$$

where we have employed Eq. (3.17). By generalizing the methods of Ref. 18, this result can be shown to be an approximate form of the symmetrized equations developed by Goldflam, Kowalski, and Picklesimer.<sup>19</sup>

## V. SYMMETRIZATION OF MULTIPARTICLE SCATTERING EQUATIONS

In order to establish that the symmetrized version of a multiparticle collision formalism can be reduced to Eq. (4.5), we must first show how to symmetrize the equations for the distinguishable-particle case. This procedure has recently been described in Ref. 11, and we briefly review it below. Although the procedure is general, we only consider its application to the wave function component equations introduced by Levin,<sup>12</sup> since these are the ones used in the unsymmetrized case of Ref. 10. These wave

function component equations have been variously referred to as extended Faddeev and as LBRS equations.

As in Ref. 12, the unsymmetrized solution of the full Schrödinger equation, with incident waves in the two-cluster partition  $\alpha(i)$ , is expressed as a sum of components:

$$\Psi^U[\alpha(i)] = \sum_{b,j} \psi_{b(j)}^U[\alpha(i)], \quad (5.1)$$

where  $b(j)$  is a general  $m$ -cluster partition label. These components satisfy the following set of coupled, distorted integral equations:<sup>12</sup>

$$\psi_{b(j)}^U[\alpha(i)] = \delta_{b(j)\alpha(i)}\Phi_{\alpha(i)} + G_{b(j)}(E) \sum_{d,k} [C_b V_{b(j)}^{d(k)} - C_b U_{b(j)}^{d(k)} + \delta_{b(j)d(k)} U^{d(k)}] \psi_{d(k)}^U[\alpha(i)]. \quad (5.2)$$

In this equation,  $\Phi_{\alpha(i)}$  is an incident plane wave in the partition  $\alpha(i)$ ;  $G_{b(j)}(E)$  is the usual outgoing-wave Green's function  $(E^+ - H_{b(j)})^{-1}$ ,  $C_b = (-1)^{n_b}(n_b - 1)!$ , where  $n_b$  is the number of clusters in partition  $b(j)$ ; and  $V_{b(j)}^{d(k)}$  is the set of interactions both external to  $d(k)$  and internal to  $b(j)$ .

The external interaction  $V^{d(k)}$  and the distortion potential  $U^{d(k)}$  are related to  $V_{b(j)}^{d(k)}$  and  $U_{b(j)}^{d(k)}$ , respectively, by the combinatorial distribution rules<sup>20</sup>

$$V^{d(k)} = \sum_{b,j} C_b V_{b(j)}^{d(k)} \quad (5.3)$$

and

$$U^{d(k)} = \sum_{b,j} C_b U_{b(j)}^{d(k)}. \quad (5.4)$$

In addition to satisfying (5.4), the distorting potentials must be compact so that they do not interfere with the treatment of the many-body boundary conditions. Apart from these two requirements they are completely arbitrary.

A symmetrized solution to the full Schrödinger equation can be expressed in terms of the unsymmetrized solutions by

$$\Psi^S(\alpha) = \frac{1}{\sqrt{\hat{N}_\alpha}} \sum_{i=0}^{N_\alpha} (-1)^{\sigma_{\alpha(i)}} \Psi^U[\alpha(i)], \quad (5.5)$$

where  $\sigma_{\alpha(i)}$  is the number of fermion exchanges needed in the permutation of  $\alpha(0)$  into  $\alpha(i)$ .

Using (5.1) and (5.5) we find that  $\Psi^S(\alpha)$  can be written in terms of unsymmetrized components as

$$\Psi^S(\alpha) = \frac{1}{\sqrt{\hat{N}_\alpha}} \sum_{i,b,j} (-1)^{\sigma_{\alpha(i)}} \psi_{b(j)}^U[\alpha(i)]. \quad (5.6)$$

This can be simplified if we introduce  $\alpha$ -symmetrized components defined by

$$\psi_{b(j)}^S(\alpha) \equiv \sqrt{\hat{N}_b / \hat{N}_\alpha} \sum_i (-1)^{\sigma_{\alpha(i)}} \psi_{b(j)}^U[\alpha(i)]. \quad (5.7)$$

The normalization has been chosen to agree with that used in Secs. III and IV. It differs from that of Ref. 11 by the factor  $(\hat{N}_b / \hat{N}_\alpha)^{1/2}$ . The symmetrized solution can now be written

$$\Psi^S(\alpha) = \sum_{b,j} \frac{1}{\sqrt{\hat{N}_b}} \psi_{b(j)}^S(\alpha). \quad (5.8)$$

$$\psi_{b(0)}(\alpha) = \delta_{b\alpha} \Phi_{\alpha(0)} + G_{b(0)} \sum_d \left( \frac{\hat{N}_b}{\hat{N}_d} \right)^{1/2} (\hat{V}_b^d - \hat{U}_b^d + \delta_{bd} \hat{U}^d) \psi_{d(0)}(\alpha), \quad (5.11)$$

where we have defined

$$\hat{V}_b^d = C_b \sum_k V_{b(0)}^{d(k)} \hat{P}_{d(k)d(0)}. \quad (5.12)$$

This is essentially the exchange interaction introduced in Ref. 11. Similar definitions hold for the distorting interactions  $\hat{U}_b^d$  and  $\hat{U}^d$ .

The symmetrization procedure outlined here has been used as a basis for generating a new class of symmetrized two-fragment, elastic scattering optical potentials. These differ significantly from those defined by Goldflam, Kowalski, and Picklesimer.<sup>19</sup> A full discussion is given in Ref. 11.

$$(E - H_{b(0)}) \psi_{b(0)}(\alpha) = \sum_d (\hat{N}_b / \hat{N}_d)^{1/2} (\hat{V}_b^d - \hat{U}_b^d + \delta_{bd} \hat{U}^d) \psi_{d(0)}(\alpha). \quad (6.1)$$

To obtain the bound state approximation to these equations we replace  $\psi_{b(0)}(\alpha)$  by  $P_{b(0)} \psi_{b(0)}^P(\alpha)$  and project each equation from the left with  $P_{b(0)}$ . As in Sec. II, we keep only two-cluster channels:  $P_{b(0)} = 0$  if  $n_b > 2$ . This yields

$$(E - H_{b(0)}) P_{b(0)} \psi_{b(0)}^P(\alpha) = \sum_d (\hat{N}_b / \hat{N}_d)^{1/2} P_{b(0)} \hat{W}_{bd} P_{d(0)} \psi_{d(0)}^P(\alpha), \quad (6.2)$$

where we have introduced [using (2.7)]

$$\hat{W}_{bd} = P_\pi \hat{V}_b^d P_{d(0)} - \hat{U}_b^d + \delta_{bd} \hat{U}^d. \quad (6.3)$$

Ideally we would like to choose the distorting potentials so as to make the solution of (6.2) a good approximation to the solution of (6.1), and hence to minimize the corrections to (6.2) from excluded channels. Since at present there is no procedure available for making this choice, we follow the approach of Ref. 10 and require that (6.2) yield the same solution as (6.1) when it is projected onto the full (unsymmetrized) model space. This projected form of (6.1) is<sup>10</sup>

$$(E - H_{b(0)}) P_{b(0)} \psi_{b(0)}^P(\alpha) = \sum_d (\hat{N}_b / \hat{N}_d)^{1/2} P_\pi \hat{W}_{bd} P_{d(0)} \psi_{d(0)}^P(\alpha). \quad (6.4)$$

If we require that the  $U_{b(j)}^{d(k)}$ , like the  $V_{b(j)}^{d(k)}$ , are label transforming,<sup>14</sup> then as shown in Ref. 11,  $\psi_{b(j)}^S(\alpha)$  and  $\psi_{b(0)}^S(\alpha)$  are related by

$$\psi_{b(j)}^S(\alpha) = \hat{P}_{b(j)b(0)} \psi_{b(0)}^S(\alpha). \quad (5.9)$$

It can also be shown<sup>11</sup> that  $\psi_{b(j)}^S(\alpha)$  is internally symmetrized, i.e., it contains a factor  $R_{b(j)}$ . Using this fact and (5.9) it is easily seen that (5.8) is equivalent to

$$\Psi^S(\alpha) = \sum_b \sqrt{\hat{N}_b} R \psi_{b(0)}^S(\alpha). \quad (5.10)$$

Henceforth we will be working only with symmetrized wave functions and will drop the superscript  $S$ .

From (5.2), (5.7), and (5.9), we can obtain the following equations for the symmetrized components:

## VI. THE RGM CHOICE OF DISTORTION OPERATORS

In this section we will show that by a proper choice of the distortion operators, the orthogonalized RGM equations (4.5) can be obtained by a straightforward projection of (5.11). The procedure followed is analogous to that of Ref. 10. As will be shown in Sec. VII, this provides a way to embed the orthogonalized RGM equations into the exact  $N$ -particle formalism just discussed.

It is convenient to work with the differential equations obtained by acting on both sides of (5.11) with  $G_{b(0)}^{-1}$ :

By restricting our attention to  $U$ 's which satisfy

$$P_\pi \hat{U}_b^d P_{d(0)} = \hat{U}_b^d$$

and

$$P_\pi \hat{U}^d P_{d(0)} = \hat{U}^d, \quad (6.5)$$

the requirement that (6.2) and (6.4) be equivalent leads to the condition that

$$\hat{W}_{bd} = P_{b(0)} \hat{W}_{bd}. \quad (6.6)$$

From (5.3) and (5.4), the  $\hat{W}$ 's must also satisfy a distribution rule. To obtain this rule we extend the definition (6.3) to include noncanonical partitions,

$$\begin{aligned} \hat{W}_{b(j)d} \equiv & P_\pi \sum_k (C_b V_{b(j)}^{d(k)} - C_b U_{b(j)}^{d(k)} + \delta_{b(j)d(k)} U^{d(k)}) \\ & \times \hat{P}_{d(k)d(0)} P_{d(0)}, \end{aligned} \quad (6.7)$$

so that  $\hat{W}_{bd} = \hat{W}_{b(0)d}$ . Using (5.3) and (5.4) we find

$$\sum_{b,j} \hat{W}_{b(j)d} = P_\pi \hat{V}^d P_{d(0)}, \quad (6.8)$$

where

$$\hat{V}^d \equiv \sum_k V^{d(k)} \hat{P}_{d(k)d(0)}. \quad (6.9)$$

From the equations obtained from (6.2) and (6.4) by permuting with  $\hat{P}_{b(j)b(0)}$ , we can extend (6.6) to

$$\hat{W}_{b(j)d} = P_{b(j)} \hat{W}_{b(j)d}. \quad (6.10)$$

The solution of (6.8) and (6.10) now proceeds exactly as in Ref. 10.

$$\sum_d \left[ \delta_{bd} (E - H_{d(0)}) + \tilde{Q}_{bd} H_{d(0)} - \left[ \frac{\hat{N}_b}{\hat{N}_d} \right]^{1/2} P_{b(0)} \mathcal{P}^{-1} \hat{V}^d P_{d(0)} \right] P_{d(0)} \psi_{d(0)}^P(\alpha) = 0. \quad (6.17)$$

Using (3.1), (6.9), and the label-transforming property of  $V^{d(k)}$ , we find that

$$\hat{V}^d P_{d(0)} = \hat{N}_d R V^{d(0)} P_{d(0)}. \quad (6.18)$$

Hence, (6.17) can be written

$$\sum_d [\delta_{bd} (E - H_{d(0)}) + \tilde{Q}_{bd} H_{d(0)} - (N_b N_d)^{1/2} P_{b(0)} \mathcal{P}^{-1} R V^{d(0)} P_{d(0)}] P_{d(0)} \psi_{d(0)}^P = 0. \quad (6.19)$$

The sets of equations (4.5) and (6.19) are identical in form. Since the solutions of (4.5) with specified boundary conditions are the unique nonspurious components (3.12), the solutions of (4.5) and (6.19) must be identical. This completes our demonstration of how the RGM is obtained as an approximation to (5.11). It is now straightforward to embed the orthogonalized RGM equations into the full theory, a task we will carry out in Sec. VII.

## VII. EMBEDDING OF THE RGM

In this section we carry out the embedding of the RGM into the exact scattering equations. We use a matrix notation, as this will also prove useful in Sec. VIII.

The general solution can be written in the form

$$\hat{W}_{b(j)d} = P_{b(j)} \mathcal{P}^{-1} \hat{V}^d P_{d(0)} + \hat{A}_{b(j)d}, \quad (6.11)$$

where the  $\hat{A}$ 's satisfy

$$\hat{A}_{b(j)d} = P_{b(j)} \hat{A}_{b(j)d}, \quad (6.12a)$$

$$\sum_{b,j} \hat{A}_{b(j)d} = 0. \quad (6.12b)$$

Thus the  $\hat{A}$ 's are nonzero only when there are spurious (overcomplete or Pauli-forbidden) states. The canonical elements can be written

$$\hat{A}_{bd} = (\hat{N}_d / \hat{N}_b)^{1/2} \sum_a \tilde{Q}_{ba} \hat{B}_{ad} P_{d(0)}, \quad (6.13)$$

where the  $\hat{B}$ 's are arbitrary operators. The general expression for  $\hat{W}_{bd}$  is thus

$$\hat{W}_{bd} = P_{b(0)} \mathcal{P}^{-1} \hat{V}^d P_{d(0)} + (\hat{N}_d / \hat{N}_b)^{1/2} \sum_a \tilde{Q}_{ba} \hat{B}_{ad} P_{d(0)}. \quad (6.14)$$

From (6.14) we obtain the following expression for the  $\hat{U}$ 's:

$$\begin{aligned} \hat{U}_b^d - \delta_{bd} \hat{U}^d = & P_\pi \hat{V}_b^d P_{d(0)} - P_{b(0)} \mathcal{P}^{-1} \hat{V}^d P_{d(0)} \\ & - (\hat{N}_d / \hat{N}_b)^{1/2} \sum_a \tilde{Q}_{ba} \hat{B}_{ad} P_{d(0)}. \end{aligned} \quad (6.15)$$

To establish the identity with (4.5) we make the choice

$$\hat{B}_{ad} = -\delta_{ad} H_{d(0)}, \quad (6.16)$$

and substitute (6.14) into (6.2). This yields

In matrix form, the orthogonalized RGM equation (6.2) is

$$\underline{P}_0 \vec{\psi}_0^P = \vec{\Phi}_0 + \underline{P}_0 \underline{G}_0 \underline{\tilde{W}}_0 \underline{P}_0 \vec{\psi}_0^P, \quad (7.1)$$

where

$$(\underline{P}_0)_{bd} = P_{b(0)} \delta_{bd},$$

$$(\vec{\psi}_0)_b = \psi_{b(0)}(\alpha),$$

$$(\vec{\Phi}_0)_b = \Phi_{\alpha(0)} \delta_{b\alpha},$$

$$(\underline{G}_0)_{bd} = G_{b(0)} \delta_{bd},$$

and

$$(\underline{\tilde{W}}_0)_{bd} = (\hat{N}_b / \hat{N}_d)^{1/2} \hat{W}_{bd}.$$

Note that  $P_0$  projects only onto model-space states with two bound clusters, i.e.,  $P_{b(0)} \equiv 0$  if  $b(0)$  is not a two-cluster partition.

In this notation the exact equations (5.11) are

$$\vec{\psi}_0 = \vec{\Phi}_0 + \underline{G}_0(\vec{V}_0 + \vec{U}_0)\vec{\psi}_0, \quad (7.2)$$

where

$$(\vec{V}_0)_{bd} = (\hat{N}_b / \hat{N}_d)^{1/2} \hat{V}_b^d$$

and

$$(\vec{U}_0)_{bd} = (\hat{N}_b / \hat{N}_d)^{1/2} (\delta_{bd} \hat{U}^d - \hat{U}_b^d).$$

By writing  $\vec{\psi}_0 = P_0 \vec{\psi}_0 + Q_0 \vec{\psi}_0$ , where  $Q_0 = 1 - P_0$ , we can rewrite (7.2) as a pair of coupled equations for  $P_0 \vec{\psi}_0$  and  $Q_0 \vec{\psi}_0$ :

$$P_0 \vec{\psi}_0 = \vec{\Phi}_0 + P_0 \underline{G}_0 (\vec{V}_0 + \vec{U}_0) (P_0 \vec{\psi}_0 + Q_0 \vec{\psi}_0), \quad (7.3)$$

$$Q_0 \vec{\psi}_0 = Q_0 \underline{G}_0 (\vec{V}_0 + \vec{U}_0) (P_0 \vec{\psi}_0 + Q_0 \vec{\psi}_0).$$

With the distorting operators given by (6.14) and (6.15), we have

$$\begin{aligned} P_0 (\vec{V}_0 + \vec{U}_0) P_0 &= \vec{W}_0, \\ P_0 (\vec{V}_0 + \vec{U}_0) Q_0 &= P_0 \vec{V}_0 Q_0, \end{aligned} \quad (7.4)$$

$$Q_0 (\vec{V}_0 + \vec{U}_0) P_0 = Q_0 Q_\pi \vec{V}_0 P_0,$$

$$Q_0 (\vec{V}_0 + \vec{U}_0) Q_0 = Q_0 \vec{V}_0 Q_0,$$

where in the third equation,  $Q_\pi = 1 - P_\pi$ . Using (7.4) in (7.3) we obtain

$$P_0 \vec{\psi}_0 = \vec{\Phi}_0 + P_0 \underline{G}_0 \vec{W}_0 P_0 \vec{\psi}_0 + P_0 \underline{G}_0 \vec{V}_0 Q_0 \vec{\psi}_0, \quad (7.5a)$$

$$Q_0 \vec{\psi}_0 = Q_0 \underline{G}_0 Q_\pi \vec{V}_0 P_0 \vec{\psi}_0 + Q_0 \underline{G}_0 \vec{V}_0 Q_0 \vec{\psi}_0. \quad (7.5b)$$

Equation (7.5a) can be rewritten in terms of the solution of the RGM equation (7.1) and the RGM Green's functions  $\underline{G}_0^{\text{RGM}}$  defined by

$$\underline{G}_0^{\text{RGM}} = (\underline{G}_0^{-1} - \vec{W}_0)^{-1}. \quad (7.6)$$

This yields

$$P_0 \vec{\psi}_0 = P_0 \vec{\psi}_0^P + P_0 \underline{G}_0^{\text{RGM}} \vec{V}_0 Q_0 \vec{\psi}_0. \quad (7.7)$$

Equations (7.7) and (7.5b) achieve our goal of embedding the (orthogonalized) RGM in an exact theory. Note that if  $P_0$  does not contain all two-cluster channels (in canonical partitions) then some of the  $Q_{b(0)} \psi_{b(0)}$  will yield amplitudes for  $2 \rightarrow 2$  transitions as well as for  $2 \rightarrow m$  transitions with  $m > 2$ .

### VIII. THREE-CLUSTER BREAKUP CORRECTIONS

The pairs of equations (7.5a) and (7.5b) or (7.7) and (7.5b), supplemented by the usual boundary condition requirements, provide a unique solution to the identical particle collision problem. In principle, both  $m$ -cluster (breakup) contributions to  $P_0 \vec{\psi}_0$  and  $m$ -body transition amplitudes can be obtained from these pairs. In practice, however, calculations are likely to be restricted to the

$m=3$  case. This is due both to computational restrictions as well as to an expectation that the most important  $m$ -body corrections to a two-cluster approximation such as the RGM will come from three-cluster contributions. In this section, we will give a qualitative discussion of this case. The important conclusion we draw is that when the  $Q$  space is limited to one (or a few) three-body configuration(s), then  $Q_0 \vec{\psi}_0$  no longer obeys a connected kernel equation, and a Faddeev type of analysis must be initiated in order to obtain a unique solution. This is analogous to the procedure that must be followed in attempting to solve the three-cluster RGM-type equations advocated by Schmid.<sup>21</sup>

All  $m$ -cluster effects,  $m \geq 3$ , are contained in  $Q_0$  through  $Q_0 \vec{\psi}_0$ , which is related to  $P_0 \vec{\psi}_0$  of (7.7) by

$$Q_0 \vec{\psi}_0 = Q_0 \underline{G}_0 \vec{\mathcal{Z}}_0 P_0 \vec{\psi}_0. \quad (8.1)$$

The optical-potential-like<sup>22</sup> operator  $\vec{\mathcal{Z}}_0$  is given by

$$\vec{\mathcal{Z}}_0 = Q_\pi \vec{V}_0 + \vec{V}_0 Q_0 (\underline{G}_0^{-1} - Q_0 \vec{V}_0 Q_0)^{-1} Q_\pi \vec{V}_0, \quad (8.2)$$

which is the formal solution to

$$\vec{\mathcal{Z}}_0 = Q_\pi \vec{V}_0 + \vec{V}_0 Q_0 \underline{G}_0 \vec{\mathcal{Z}}_0. \quad (8.3)$$

Since we wish to focus on three-cluster terms, we write  $Q_0$  as

$$Q_0 = Q_0^{(3)} + Q_0', \quad (8.4)$$

where  $Q_0^{(3)}$  projects onto one or at most a few three-body continua, but not onto  $m$ -body breakup configurations  $m > 3$ . The assumption that corrections due to three-cluster contributions are the most important means that (8.4) is to be approximated by

$$Q_0 \cong Q_0^{(3)}. \quad (8.5)$$

For simplicity, we will also neglect the nonorthogonality corrections which arise from the occurrence of  $Q_\pi$  in (8.2), i.e., we set

$$Q_0^{(3)} Q_\pi \cong Q_0^{(3)}. \quad (8.6)$$

With these approximations it follows that

$$Q_0 \vec{\psi}_0 \cong Q_0^{(3)} \underline{G}_0 \vec{\mathcal{Z}}_0^{(3)} P_0 \vec{\psi}_0, \quad (8.7)$$

where

$$\begin{aligned} Q_0^{(3)} \vec{\mathcal{Z}}_0^{(3)} &= Q_0^{(3)} \vec{V}_0 + Q_0^{(3)} \vec{V}_0 Q_0^{(3)} \\ &\times (\underline{G}_0^{-1} - Q_0^{(3)} \vec{V}_0 Q_0^{(3)})^{-1} \vec{V}_0. \end{aligned} \quad (8.8)$$

This satisfies an equation analogous to (8.3):

$$Q_0^{(3)} \vec{\mathcal{Z}}_0^{(3)} = Q_0^{(3)} \vec{V}_0 + Q_0^{(3)} \vec{V}_0 \underline{G}_0 Q_0^{(3)} \vec{\mathcal{Z}}_0^{(3)}. \quad (8.9)$$

It is evident that (8.8) yields a "three-cluster" approximation to  $Q_0 \vec{\mathcal{Z}}_0$ . From (8.1) and (7.5a) we see that  $Q_0^{(3)} \vec{\mathcal{Z}}_0^{(3)}$  is the crucial ingredient in determining three-cluster corrections to  $P_0 \vec{\psi}_0 \cong P_0 \vec{\psi}_0^P$ , while from (8.7),  $Q_0^{(3)} \vec{\mathcal{Z}}_0^{(3)}$  is essential for obtaining three-body amplitudes, i.e., amplitudes describing processes of the form  $2 \rightarrow 3$ .

If, for computational simplicity, one retains only one three-cluster channel in  $Q_0^{(3)}$ , then (8.8) appears to define an approximation of the dominant-cluster-partition type<sup>23</sup>

in which the role of exchange symmetry is made explicit. While such a  $\underline{Q}_0^{(3)}\underline{\tilde{Q}}_0^{(3)}$  will satisfy (8.9), this latter equation alone cannot be used to calculate  $\underline{Q}_0^{(3)}\underline{\tilde{Q}}_0^{(3)}$ . The reason is that (8.9) is an integral equation with a disconnected kernel and therefore must be expected to yield nonunique solutions.<sup>24</sup> This lack of connectivity is a result of our using the combinatorial Benoist-Gueutal, L'Huillier, Redish, and Tandy (BLRT)<sup>20</sup> distribution scheme of Eqs. (5.3) and (5.4), as we will now demonstrate.

Equation (8.9) will be connected if its kernel  $\underline{Q}_0^{(3)}\underline{\tilde{V}}_0\underline{G}_0$  is connected after one or more iterations. Since  $\underline{G}_0$  contains free-particle Green's functions, the connectivity of the kernel is determined by the factor  $\underline{K}_0 = \underline{Q}_0^{(3)}\underline{\tilde{V}}_0$ . In the remaining discussion, therefore, we shall drop  $\underline{G}_0$  from our analysis and consider only the factor  $\underline{K}_0$  and its iterates. Despite the possibly unusual appearance of the resulting expressions, there is no loss of generality in this procedure.

The first iterate of this factor is

$$(\underline{K}_0 \underline{K}_0)_{ba} = \underline{Q}_{b(0)}^{(3)} \sum_d \tilde{V}_{b(0)}^{d(0)} \underline{Q}_{d(0)}^{(3)} \tilde{V}_{d(0)}^{a(0)}, \quad (8.10)$$

where  $\underline{Q}_{b(0)}^{(3)}$  and  $\underline{Q}_{d(0)}^{(3)}$  vanish, respectively, unless  $b(0)$  and  $d(0)$  are among the three-cluster partitions  $S_3$  contained in  $\underline{Q}_0^{(3)}$ . Hence, the sum on  $d$  in (8.8) is limited to one (or a few) three-cluster partition label(s). This limitation is the source of the problem. As Bencze and Redish have shown,<sup>14</sup> the connectivity property of quantities such as

$$(\underline{\tilde{V}}_0 \underline{\tilde{V}}_0)_{ba} = \sum_d \tilde{V}_{b(0)}^{d(0)} \tilde{V}_{d(0)}^{a(0)} \quad (8.11)$$

is related to the connectivity of the analogous unsymmetrized quantity, which here is

$$(\underline{V} \underline{V})_{b(0)a(0)} = \sum_{d,k} C_b V_{b(0)}^{d(k)} C_d V_{d(k)}^{a(0)}. \quad (8.12)$$

If (8.12) is connected, then so is (8.11).<sup>14</sup> In the case of the BLRT distribution, the analysis of Polyzou<sup>25</sup> clearly demonstrates that connectivity is generally achieved only if the  $d$  sum in (8.12) runs over all partition labels and not simply over three-cluster ones.

Applying this argument to (8.10) we see that it will be connected if

$$(\underline{K}_0 \underline{K}_0)_{ba} = \sum_{d,k} C_b V_{b(0)}^{d(k)} \underline{Q}_{d(k)}^{(3)} C_d V_{d(k)}^{a(0)} \quad (8.13)$$

is connected. But, the presence of  $\underline{Q}_{d(k)}^{(3)}$ , which allows only those  $d \in S_3$ , interrupts the full combinatorial sum needed to obtain connectivity. It is this limiting of  $d$  which is the source of the problem in the present case and also prevents  $(\underline{K}_0)^n$ ,  $n > 2$ , from being connected. It may prevent equations analogous to (8.9), but based on other coupling schemes, from being connected as well. [It is straightforward to establish the disconnectedness of (8.10) when the number of particles  $N$  is small, e.g.,  $N=4$  or  $5$ , since in these cases, momentum-conserving delta functions are relatively easily seen to occur in the relevant matrix elements.]

Given the lack of uniqueness to the solutions of (8.9)

that are associated with disconnectedness, it is clear that exact solutions to this equation are guaranteed only if the disconnectedness is removed. Since (8.9) involves only three-cluster contributions, i.e., does not allow for breakup of any one cluster, even in intermediate states, then the methods used in the three-particle problem should be applicable in the present case. Those latter methods are discussed, e.g., in Ref. 26, which may be consulted for details.

## IX. SUMMARY

In this paper we have treated the problems of nonorthogonality and possible overcompleteness in the resonating group method (RGM). Our analysis is based on explicitly symmetrized versions of the methods of Birse and Redish.<sup>10</sup> We have obtained orthogonalized versions of the RGM equations in which the effects of the NO kernel have been formally summed to all orders.

In Ref. 10 it was shown that CRC equations could be obtained as a bound-state (pole) approximation to distorted, connected-kernel equations with a suitable choice of distorting potentials. Here we have extended that result to the identical particle case. We have shown that one form of the orthogonalized RGM equations can be obtained as a pole approximation to the symmetrized versions<sup>11</sup> of the distorted  $N$ -body scattering equations of Levin.<sup>12</sup> We have shown how to embed the RGM in an exact multiparticle scattering theory and we have discussed problems that arise when our procedure is extended to include three-cluster (breakup) effects.

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## APPENDIX

In this appendix we give the proofs of relations (3.5)–(3.7). From (3.3) and the label transforming property of  $P_{b(j)}$ , we have

$$\begin{aligned} \hat{P} \mathcal{P} &= \hat{P} \sum_{b,j} P_{b(j)} \\ &= \sum_{b,j} P_{Pb(j)} \hat{P} \\ &= \mathcal{P} \hat{P}, \end{aligned} \quad (A1)$$

where  $\hat{P}$  is any permutation. Operating on this from right and left with  $\mathcal{P}^{-1}$ , we obtain

$$\mathcal{P}^{-1} \hat{P} P_\pi = P_\pi \hat{P} \mathcal{P}^{-1}. \quad (A2)$$

From (3.3), (3.4), and (2.7) we have

$$P_{b(j)} \mathcal{P}^{-1} = P_{b(j)} - \sum_{d,k} \delta_{b(j)d(k)} P_{b(j)} P_{d(k)} \mathcal{P}^{-1}. \quad (A3)$$

Hence, we write

$$\begin{aligned}
 P_{b(j)}\hat{P}\mathcal{P}^{-1} &= \hat{P}P_{P^{-1}b(j)}\mathcal{P}^{-1} \\
 &= \hat{P}P_{P^{-1}b(j)} - \sum_{d,k} \bar{\delta}_{P^{-1}b(j)d(k)} \\
 &\quad \times \hat{P}P_{P^{-1}b(j)}P_{d(k)}\mathcal{P}^{-1} \\
 &= \hat{P}P_{P^{-1}b(j)} + \hat{P}P_{P^{-1}b(j)}\mathcal{P}^{-1} \\
 &\quad - \sum_{d,k} \hat{P}P_{P^{-1}b(j)}P_{d(k)}\mathcal{P}^{-1} \\
 &= P_{b(j)}\hat{P} + P_{b(j)}\hat{P}\mathcal{P}^{-1} - P_{b(j)}\hat{P}P_{\pi}. \quad (A4)
 \end{aligned}$$

From (A4) we obtain

$$P_{b(j)}\hat{P} = P_{b(j)}\hat{P}P_{\pi}. \quad (A5)$$

Summing (A5) over  $b(j)$ , and then operating on the result from the left with  $\mathcal{P}^{-1}$ , yields

$$P_{\pi}\hat{P} = P_{\pi}\hat{P}P_{\pi}. \quad (A6)$$

Since this relation holds for any permutation, we also have

$$P_{\pi}\hat{P}^{-1} = P_{\pi}\hat{P}^{-1}P_{\pi}. \quad (A7)$$

Taking the transpose of both sides of (A7) yields

$$\begin{aligned}
 \hat{P}P_{\pi} &= P_{\pi}\hat{P}P_{\pi}, \\
 &= P_{\pi}\hat{P}. \quad (A8)
 \end{aligned}$$

Since  $\mathcal{P}^{-1}$  is nonzero only on the space of  $P_{\pi}$  by definition, we have, from (A2) and (A8), that

$$\hat{P}\mathcal{P}^{-1} = \mathcal{P}^{-1}\hat{P}. \quad (A9)$$

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