Convergence of the orthogonalized resonating group method

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In the conventional coupled channels resonating group approach it is difficult to investigate the convergence of the solution with increasing number of distortion channels because of the nonorthogonality (and linear dependency) of channel spaces and because of nonuniqueness of the coupled channels solution. The orthogonalized version of the resonating group method allows us to study convergence. It is presently done for the n-channels case with one open channel and $n-1$ (closed) distortion channels. It is found that the relative motion solutions and distortion amplitudes determined by the approximate equations converge pointwise towards values determined by the Schrödinger equation. The converged set of equations defines the effective interaction of two clusters in the elastic energy region; if one cluster is a single particle this definition goes over into Feshbach's definition of the optical potential in the elastic energy region.

I. INTRODUCTION

There has been increasing interest in the resonating group model[1,2] since it became apparent that this model can be applied not only to nuclear and atomic physics but also to the nonrelativistic constituent quark model. Bencze, Chandler, and Gibson[3] investigated the resonating group model in relation to the two-Hilbert space formalism and showed that coupled channels equations with only two-cluster channels cannot be equivalent to the Schrödinger equation. Adhikari, Birse, Kozack, and Levin[4] showed how the resonating group method can be embedded into a rigorous integral equations approach. The trouble arising from the nonorthogonality of channel spaces has also been widely discussed, both in the coupled reaction channels method[5,6] and in the resonating group model. A method of orthogonalizing and renormalizing coupled channels equations has been proposed by one of us.[7] It involves diagonalization of the full norm operator. A more general but similar treatment, based on Penrose's generalized inverse of the full norm operator, has been given by Birse and Redish.[8] The latter approach has been applied to the resonating group model in Ref. 4. Besides practical difficulties involved in inverting large matrices, all these methods have the disadvantage of mixing channel spaces rather than separating them during orthogonalization. For this reason, and for the reason of easier practical use, another orthogonalization and renormalization procedure has been introduced.[9] In this latter method channels are ordered according to their physical importance and the Gram-Schmidt orthonormalization rule is applied. Only the norm operator of one channel has to be diagonalized, at each step of the recursive procedure, which is comparatively easy. All other operations are multiplications of operators. The resulting orthogonalized resonating group equation is Hermitian. All zero-norm states which eventually arise by overcompleteness and by the Pauli principle appear as solutions of the equation at a chosen unphysical (negative or large positive) energy.

Intuitively one expects the resonating group approach to be convergent when all necessary distortion corrections are included in the wave function ansatz.[2] In the ordinary resonating group approach, however, it seems to be rather difficult to study the convergence properties because of the nonorthogonality of the channel spaces. One might run into overcompleteness, and consequently into nonuniqueness of the solution, before one reaches a converged result.

Nonorthogonality and even linear dependency of a test function space is not at all harmful to the orthogonalized resonating group method, as has been demonstrated by an example in Ref. 9. This encourages us to consider the question of convergence in this model. As a start we consider a simple case, namely an A-particle two-cluster system in the elastic energy range. The elastic channel is open, all other channels are closed. The closed channels are represented by a set of square integrable states which are coupled to the elastic channel via the coupled channels resonating group equation. We will investigate convergence with respect to increasing number of square integrable states, the latter being taken from the harmonic oscillator shell model. The orthogonalization scheme we use is the one given in Ref. 9.

In Sec. II the orthonormalization of function spaces and the orthogonalized resonating group equation will be discussed. The question of convergence is studied in Sec. III. Concluding remarks are made in Sec. IV.

II. THE ORTHOGONALIZATION PROCEDURE

The general formalism of orthogonalizing the resonating group equation has been given earlier.[9] A recursion relation has been given which leads from the ordinary resonating group equation to a resonating group equation in which the elements of the matrix Hamiltonian are defined in orthogonalized and renormalized function spaces. The recursion relation uses only objects which appear explicitly in the ordinary resonating group equation. The theory presented in Ref. 9 applies to coupled two-, three-, and multicluster channels, with and without distortion corrections.

Presently we are interested in the question of whether the solution of the orthogonalized and renormalized resonating group equation converges towards the true solution of the Schrödinger equation, when the number of distortion corrections is increased. We restrict our investigation to the case in which only one two-cluster channel is open. The distortion corrections are then square integrable A-particle states. We use the name "channel" also for these distortion corrections because of their formal similarity to closed channels.

In the resonating group model, the A-particle Schrödinger equation

$$(H-E)|\psi\rangle=0 \tag{1}$$

is projected into the restricted function space

$$|\Psi\rangle=\sum_{i=1}^{n}\mathcal{A}|\phi_i^{(0)}\rangle|\chi_i^{(0)}\rangle\ . \tag{2}$$

We let the first channel $i=1$ be a two-cluster channel, which means that the internal motion state $\phi_1^{(0)}$ is a product of (exact) ground states of the two clusters, while $\chi_1^{(0)}$ is a state of relative motion of the two clusters; the operator $\mathcal{A}$ denotes antisymmetrization. For $2\le i\le n$, the $\phi_i^{(0)}$ are A-particle shell model states and the $\chi_i^{(0)}$ are amplitudes. The total center of mass component is subtracted out of H and factored out of Ψ. We choose the harmonic oscillator shell model for $\phi_2^{(0)},\dots,\phi_n^{(0)}$, because separating out the center of mass motion is easy in this model.

From (1) and (2) we get the ordinary resonating group equation by variation of the relative motion function $\chi_1^{(0)}$ as well as of the amplitudes $\chi_i^{(0)}$, $2\le i\le n$, in

$$\langle\delta\Psi|(H-E)|\Psi\rangle=0\ . \tag{3}$$

We get

$$\sum_{j=1}^{n}\langle\phi_i^{(0)}|\mathcal{A}(H-E)\mathcal{A}|\phi_j^{(0)}\rangle|\chi_j^{(0)}\rangle \equiv\sum_{j=1}^{n}(\tilde{H}_{ij}^{(0)}-E\tilde{N}_{ij}^{(0)})|\chi_j^{(0)}\rangle=0 \quad \text{for } i=1,\dots,n\ . \tag{4}$$

The upper index (0) indicates that no orthogonalization, or renormalization has as yet been performed. The tilde reminds us that the function space used may have zero-norm components. The quantities $\tilde{H}_{ij}^{(0)}$ and $\tilde{N}_{ij}^{(0)}$ are either numbers or operators, depending on how many variables are integrated over by $\langle\phi_i^{(0)}|$ and $|\phi_j^{(0)}\rangle$.

The orthogonalized and renormalized resonating group equation reads

$$\sum_{j=1}^{n}(H_{ij}^{(n)}-E)|\chi_j^{(n)}\rangle=0 \quad \text{for } i=1,\dots,n\ . \tag{5}$$

The upper index (n) indicates that orthogonalization and renormalization have been carried out with respect to all n channels. In this paper we do not want to calculate the quantities $H_{ij}^{(n)}$ by the recursion relation of Ref. 9. We want to obtain them as matrix elements of H taken between orthogonalized channel states, with a special treatment of zero-norm states.

We start with the first channel, $i=1$. The states forming the channel space are $\mathcal{A}|\phi_1^{(0)}\rangle|\mathbf{r}\rangle$, where $\mathbf{r}$ is the c.m. distance of the two clusters. These states do not form an orthonormal set, because their scalar products are the norm kernel in $\mathbf{r}$ space, $\tilde{N}_{11}^{(0)}(\mathbf{r},\mathbf{r}')$, which is not a delta function. In order to orthonormalize the $i=1$ space, we solve the eigenvalue equation

$$\tilde{N}_{11}^{(0)}|u_{1,\nu}\rangle=\tilde{\eta}_{1,\nu}|u_{1,\nu}\rangle\ . \tag{6}$$

The operator $\tilde{N}_{11}^{(0)}$ is not compact. It is the sum of the unit operator plus a compact operator. Whenever compactness becomes relevant, we will have to use this latter form and treat the unit operator separately. The problem at the moment is to calculate the inverse of $\tilde{N}_{11}^{(0)}$. Since we have assumed rigorous cluster ground states, we do not expect that $\tilde{N}_{11}^{(0)}$ has eigenvalues equal to zero. But in order to standardize our treatment, we allow also for zero eigenvalues, say $\tilde{\eta}_{1,1}=\cdots=\tilde{\eta}_{1,m}=0$. The orthonormalization should not affect the zero-norm eigenstates. Therefore we replace, in the eigenstate representation of the norm kernel, $\tilde{\eta}_{1,\nu}$ by $\eta_{1,\nu}$, with

$$\begin{aligned}&\eta_{1,1}=\cdots=\eta_{1,m}=1 \quad \text{and}\\ &\eta_{1,\nu}=\tilde{\eta}_{1,\nu} \quad \text{for } m+1\le\nu\ .\end{aligned} \tag{7}$$

With these new eigenvalues we define $N_{11}^{(0)}$ by

$$N_{11}^{(0)}=\sum_{\nu}|u_{1,\nu}\rangle\eta_{1,\nu}\langle u_{1,\nu}|\ . \tag{8}$$

The inverse of $N_{11}^{(0)}$, as well as the square root of the inverse, obviously exist. The orthonormalized basis of the $i=1$ space can now be written as

$$\mathcal{A}|\phi_1^{(1)}\rangle|\mathbf{r}\rangle=\mathcal{A}|\phi_1^{(0)}\rangle(N_{11}^{(0)})^{-1/2}|\mathbf{r}\rangle \tag{9}$$

[to evaluate the expression on the right-hand side one inserts the unit operator $\int|\mathbf{r}'\rangle\langle\mathbf{r}'|d^3r'$ between $|\phi_1^{(0)}\rangle$ and $(N_{11}^{(0)})^{-1/2}$]. With the orthonormalized $i=1$ basis we define the projector P_1 onto the $i=1$ space,

$$P_1=\mathcal{A}|\phi_1^{(1)}\rangle\langle\phi_1^{(1)}|\mathcal{A}=\mathcal{A}|\phi_1^{(0)}\rangle(N_{11}^{(0)})^{-1}\langle\phi_1^{(0)}|\mathcal{A}\ . \tag{10}$$

With this operator we can now remove from channels $i=2,3,\dots$ all overlaps with the $i=1$ channel. We get

$$\begin{aligned}&\mathcal{A}|\phi_2^{(1)}\rangle=(\mathbf{1}-P_1)\mathcal{A}|\phi_2^{(0)}\rangle\ ,\\ &\qquad\vdots\\ &\mathcal{A}|\phi_n^{(1)}\rangle=(\mathbf{1}-P_1)\mathcal{A}|\phi_n^{(0)}\rangle\ .\end{aligned} \tag{11}$$

This completes the transition from upper index (0) to upper index (1).

Next we renormalize $\mathcal{A}|\phi_2^{(1)}\rangle$. We calculate

$$N_{22}^{(1)}=\langle\phi_2^{(1)}|\mathcal{A}|\phi_2^{(1)}\rangle\ , \tag{12}$$

which is just a number. When it is zero, we leave everything as it is and replace the upper index (1) by (2), everywhere. When it is nonzero, we renormalize $\mathcal{A}|\phi_2^{(1)}\rangle$,

$$\mathcal{A}|\phi_2^{(2)}\rangle=\mathcal{A}|\phi_2^{(1)}\rangle(N_{22}^{(1)})^{-1/2}\ . \tag{13}$$

The projector on $i=2$ space (consisting of only one state) becomes

$$P_2=\mathcal{A}|\phi_2^{(2)}\rangle\langle\phi_2^{(2)}|\mathcal{A}\ . \tag{14}$$

Taking out overlaps with $\mathcal{A}|\phi_2^{(2)}\rangle$ from the higher channel states leads to

$$\begin{aligned}\mathcal{A}|\phi_3^{(2)}\rangle&=(\mathbf{1}-P_2)\mathcal{A}|\phi_3^{(1)}\rangle\ ,\\ &\ \vdots\\ \mathcal{A}|\phi_n^{(2)}\rangle&=(\mathbf{1}-P_2)\mathcal{A}|\phi_n^{(1)}\rangle\ .\end{aligned} \tag{15}$$

The $i=1$ space remains as it is, but nevertheless we replace its upper index (1) by (2). This then completes the transition from upper index (1) to (2).

We continue in the same way. The last step will be the renormalization of $\mathcal{A}|\phi_n^{n-1}\rangle$ and replacement of all upper indices $(n-1)$ by (n). We then have constructed an $i=1$ space consisting of a continuous set of functions $\mathcal{A}|\phi_1^{(n)}\rangle|\mathbf{r}\rangle$ and the $i=2,i=3,\ldots,i=n$ spaces $\mathcal{A}|\phi_2^{(n)}\rangle,\mathcal{A}|\phi_3^{(n)}\rangle,\ldots,\mathcal{A}|\phi_n^{(n)}\rangle$ consisting of only one state each. All basis states are orthogonal and have either unit norm or zero norm; so far, the number of zero-norm states is finite.

In terms of the orthogonalized basis states, the elements of the matrix Hamiltonian of (5) are defined in the following way:[9]

$$\begin{aligned}H_{11}^{(n)}&=\langle\phi_1^{(n)}|\mathcal{A}H\mathcal{A}|\phi_1^{(n)}\rangle+\sum_{\nu=1}^{m}|u_{1,\nu}\rangle\epsilon\langle u_{1,\nu}|\ ,\\ H_{ii}^{(n)}&=\left\{\begin{matrix}\epsilon\ \text{ when }\langle\phi_i^{(n)}|\mathcal{A}|\phi_i^{(n)}\rangle=0\\ \langle\phi_i^{(n)}|\mathcal{A}H\mathcal{A}|\phi_i^{(n)}\rangle\ \text{ otherwise}\end{matrix}\right\}\ \text{for } 2\le i\le n\ ,\\ H_{ij}^{(n)}&=\langle\phi_i^{(n)}|\mathcal{A}H\mathcal{A}|\phi_j^{(n)}\rangle,\ \text{ for } i\neq j\ .\end{aligned} \tag{16}$$

With this definition, Eq. (5) has the following properties.

(1) The diagonal elements $H_{ii}^{(n)}$ of the matrix Hamiltonian consist of two parts. In the first part the microscopic Hamiltonian is represented on the basis of states with nonzero norm. The second part is ϵ times the projector onto zero-norm eigenstates of the channel. Either the first or the second part is missing when the channel space consists of only one state. The energy ϵ is chosen to lie outside the energy spectrum of interest, which means that ϵ has either a large positive value, or a value which is more negative than the ground state energy of the system.

(2) The channel coupling Hamiltonians are either physical transition amplitudes, i.e., transition amplitudes of the microscopic Hamiltonian, taken with normalized states, or they are zero.

(3) Equation (5) is Hermitian. Solutions at different energies are orthogonal to each other.

(4) The solutions of the coupled channels Eqs. (5) are related to the microscopic state of the resonating group ansatz (2) by

$$|\Psi\rangle=\sum_{i=1}^{n}\mathcal{A}|\phi_i^{(n)}\rangle|\chi_i^{(n)}\rangle\ . \tag{17}$$

(5) The zero-norm states which have been detected during the orthogonalization process appear as solutions of (5) at $E=\epsilon$. At $E\neq\epsilon$ the solutions of (5) are orthogonal to the zero-norm solutions.

III. CONVERGENCE WITH INCREASING NUMBER OF DISTORTION STATES

Linear dependency is not harmful to the orthonormalized resonating group equation. We want to take advantage of this feature and enlarge our ansatz (2) in such a way that it will always form a complete space. We simply add the complete space as an additional channel. Instead of (2) we write

$$|\Psi\rangle=\sum_{i=1}^{n+1}\mathcal{A}|\phi_i^{(0)}\rangle|\chi_i^{(0)}\rangle \tag{18}$$

with

$$|\phi_{n+1}^{(0)}\rangle=1\ . \tag{19}$$

The symbol 1 at the right-hand side of (19) means that there is no internal motion state at all in this channel while $\chi_{n+1}^{(0)}$ is a function of all particle coordinates. Without the first n channels, $\chi_{n+1}^{(0)}$ would just be the microscopic state ψ, and Ψ would be $\mathcal{A}\psi$. Our goal is now to show that the $i=n+1$ channel becomes less and less important as n increases.

We shall proceed in five steps. (1) We derive the orthonormalized resonating group equation for the new ansatz (18) and (19). (2) We show that the solution of the Schrödinger equation, when decomposed into channel states, satisfies the new resonating group equation and that (3) the microscopic state obtained from the solution of the new equation satisfies the Schrödinger equation (1). (4) We use the completeness relation of harmonic oscillator shell model states to show that, with increasing n, the norm of $\chi_{n+1}^{(n+1)}$ goes to zero. (5) We show that the difference of the solution of the n-channels equation and the solution of the $(n+1)$-channels equation converges pointwise to zero.

Step 1

We orthonormalize channels space (18). Equations (9) and (10) remain unchanged, (11) is replaced by

$$\begin{aligned}\mathcal{A}|\phi_2^{(1)}\rangle&=(\mathbf{1}-P_1)\mathcal{A}|\phi_2^{(0)}\rangle\ ,\\ &\ \vdots\\ \mathcal{A}|\phi_{n+1}^{(1)}\rangle&=(\mathbf{1}-P_1)\mathcal{A}|\phi_{n+1}^{(0)}\rangle\ .\end{aligned} \tag{20}$$

Equations (12)–(14) remain unchanged while (15) is replaced by

$$\mathcal{A}|\phi_3^{(2)}\rangle=(\mathbf{1}-P_2)\mathcal{A}|\phi_3^{(1)}\rangle ,$$
$$\vdots \tag{21}$$
$$\mathcal{A}|\phi_{n+1}^{(2)}\rangle=(\mathbf{1}-P_2)\mathcal{A}|\phi_{n+1}^{(1)}\rangle .$$

The subtraction process continues until the projector P_n has been formed and the $i=n$ channel state has been projected out from the $i=n+1$ space, provided that the $i=n$ channel state is not a zero-norm state.

In the last step, which leads from upper index (n) to $(n+1)$, the depleted $i=n+1$ space is renormalized. The eigenvalue equation

$$\tilde{N}^{(n)}_{n+1,n+1}|u_{n+1,\nu}\rangle=\tilde{\eta}_{n+1,\nu}|u_{n+1,\nu}\rangle \tag{22}$$

is solved and zero-norm eigenstates are detected. This equation has a simple structure. The original norm operator $N^{(0)}_{n+1,n+1}$ has been the unit operator in A-particle space (except for the total c.m. degrees of freedom), and $\tilde{N}^{(n)}_{n+1,n+1}$ has been obtained by subtracting out all states which are included in the first n channels. All these latter states are now zero-norm eigenstates of (22), and all other states are unit-norm eigenstates of (22). No renormalization is needed and we can just replace the upper index (n) by $(n+1)$. The projector onto $i=n+1$ channel space is

$$P_{n+1}=\mathbf{1}-\sum_{i=1}^{n}P_i . \tag{23}$$

The $(n+1)$-channels orthonormalized resonating group equation, which follows from ansatz (18) and (19) becomes

$$\sum_{j=1}^{n+1}(H_{ij}^{(n+1)}-E\delta_{ij})|\chi_j^{(n+1)}\rangle=0 . \tag{24}$$

For values of i and j between 1 and n, the elements $H_{ij}^{(n+1)}$ are identical to those given by (16),

$$H_{ij}^{(n+1)}=H_{ij}^{(n)} \quad \text{for } 1\le i,j\le n . \tag{25}$$

In addition we have

$$\begin{aligned} H_{n+1,j}^{(n+1)}&=\langle\phi_{n+1}^{(n+1)}|\mathcal{A}H\mathcal{A}|\phi_j^{(n+1)}\rangle \quad \text{for } j\le n ,\\ H_{j,n+1}^{(n+1)}&=\langle\phi_j^{(n+1)}|\mathcal{A}H\mathcal{A}|\phi_{n+1}^{(n+1)}\rangle \quad \text{for } j\le n ,\\ H_{n+1,n+1}^{(n+1)}&=\langle\phi_{n+1}^{(n+1)}|\mathcal{A}H\mathcal{A}|\phi_{n+1}^{(n+1)}\rangle+\epsilon\sum_{i=1}^{n}P_i . \end{aligned} \tag{26}$$

Let us recall again our somewhat unconventional notation. In order to be able to write down orthogonalized multichannels equations in a concise way we have introduced the quantities $|\phi_j^{(i)}\rangle$. They are not internal motion states in the ordinary sense because they contain projection operators operating on the relative motion states $|\chi_j^{(i)}\rangle$. A somewhat extreme case in terms of notation is $|\phi_{n+1}^{(n+1)}\rangle$, which is purely a projection operator.

Step 2

Suppose we had found a rigorous solution ψ of the Schrödinger equation (1), at an energy $E<E_0$, where E_0 is the energy of the first inelastic threshold. In order to insert this solution ψ into (24) we have to decompose it into channel states by means of our projection operators. We get the vector of states

$$|\chi_i^{(n+1)}\rangle=\langle\phi_i^{(n+1)}|\mathcal{A}P_i|\psi\rangle+\sum_\nu{}' c_{i\nu}|u_{i,\nu}^{(n+1)}\rangle . \tag{27}$$

The prime at the sum symbol indicates that the sum includes only zero-norm states. The coefficients $c_{i\nu}$ are arbitrary; $|u_{i,\nu}^{(n+1)}\rangle=1$ for $2\le i\le n$. Inserting (27) into (24) and using (25) and (26) we get

$$\begin{aligned}\sum_{j=1}^{n+1}(H_{ij}^{(n+1)}-E\delta_{ij})|\chi_j^{(n+1)}\rangle&=\sum_{j=1}^{n+1}\langle\phi_i^{(n+1)}|\mathcal{A}(H-E)\mathcal{A}|\phi_j^{(n+1)}\rangle\langle\phi_j^{(n+1)}|\mathcal{A}P_j|\psi\rangle+(\epsilon-E)\sum_\nu{}' c_{i,\nu}|u_{i,\nu}\rangle\\ &=\langle\phi_i^{(n+1)}|\mathcal{A}(H-E)\mathcal{A}|\psi\rangle=0 ,\end{aligned} \tag{28a}$$

provided that

$$c_{i,\nu}=0 \quad \text{for } E\neq\epsilon . \tag{28b}$$

Here, we have used (23) and the fact that, according to our definition of the projection operators, $\mathcal{A}|\phi_j^{(n+1)}\rangle\langle\phi_j^{(n+1)}|\mathcal{A}$ is equal to P_j. Since $\epsilon\neq E$ is assumed to be true for all physical energies E, the coefficients $c_{i,\nu}$ must be zero. The transition from a microscopic solution ψ of the Schrödinger equation to the vector of channel states or amplitudes $|\chi_i^{(n+1)}\rangle$ is unique, and this vector of channel states or amplitudes satisfies the orthonormalized $(n+1)$-channels resonating group equation (24).

Step 3

Suppose we had found a vector of states or amplitudes $|\chi_i^{(n+1)}\rangle$ which satisfies (24) at an energy $E<E_0$. The corresponding microscopic state is

$$|\Psi\rangle=\sum_{i=1}^{n+1}\mathcal{A}|\phi_i^{(n+1)}\rangle|\chi_i^{(n+1)}\rangle . \tag{29}$$

Together with (25) and (26), (24) becomes

$$\sum_{j=1}^{n+1}\langle\phi_i^{(n+1)}|\mathcal{A}(H-E)\mathcal{A}|\phi_j^{(n+1)}\rangle|\chi_j^{(n+1)}\rangle =\langle\phi_i^{(n+1)}|\mathcal{A}(H-E)\mathcal{A}|\Psi\rangle=0 . \tag{30}$$

The ϵ terms have not been written because no zero-norm components are present in the column vector $(|\chi_i^{(n+1)}\rangle)$. Each one of the equations (30) tells us that $(H-E)|\Psi\rangle$ is zero when projected onto a channel space. Since, according to (23), the sum of all projectors is unity in the complete space, and since $|\Psi\rangle$ satisfies all $(n+1)$ equations (30), it also satisfies the Schrödinger equation (1). It follows that the solutions of (24), inserted into (29), yield solutions of the Schrödinger equation (1). Our way of detecting zero-norm states has given us *all* zero-norm states. Therefore the solution vector $(|\chi_i^{(n+1)}\rangle)$ is unique for $E \neq \epsilon$, provided that the solutions of the Schrödinger equation are uniquely determined by the boundary conditions.

Step 4

Suppose we had found a solution of (24) at an energy $E<E_0$. We consider the last component of the vector $(|\chi_i^{(n+1)}\rangle)$ and calculate its norm,

$$\langle \chi_{n+1}^{(n+1)}|\chi_{n+1}^{(n+1)}\rangle^{1/2} = \langle \chi_{n+1}^{(n+1)}|\langle \phi_{n+1}^{(n+1)}|\mathcal{A}|\phi_{n+1}^{(n+1)}\rangle|\chi_{n+1}^{(n+1)}\rangle^{1/2}$$

$$= \langle \psi|P_{n+1}|\psi\rangle^{1/2} = \langle \psi| \left[\mathbf{1} - \sum_{i=1}^{n} P_i \right] |\psi\rangle^{1/2} . \tag{31}$$

We know that ψ is a solution of the Schrödinger equation at $E<E_0$. Hence $(\mathbf{1}-P_1)|\psi\rangle$ is a square integrable state. From the last term of (31) we see that $n-1$ further states are projected out of this state. As a consequence of the completeness of harmonic oscillator shell model states the norm of the remaining state, which is the norm of $|\chi_{n+1}^{(n+1)}\rangle$, goes to zero with increasing n,

$$\lim_{n\to\infty} \langle \chi_{n+1}^{(n+1)}|\chi_{n+1}^{(n+1)}\rangle = 0 . \tag{32}$$

Later on we will need some information on the rate of convergence. We may ask which are the largest coefficients in an harmonic oscillator expansion of $|\chi_{n+1}^{(n+1)}\rangle$ and from which part of the compound state wave function do they arise? Large coefficients of states with many harmonic oscillator quantz can arise either from singularities, from discontinuities, or from a long range of the expanded function. We have assumed smooth potentials and have excluded resonances of approximately zero width. Our compound state is a smooth and bounded function. Slightly below the inelastic threshold E_0, however, it has a long range because there will be an exponential tail reaching far into the inelastic channel. At $E=E_0-\Delta$, with Δ being a small positive energy, this tail will be proportional to $\exp(-\kappa r)$, with $\kappa=(2\mu\Delta/\hbar^2)^{1/2}$. The harmonic oscillator expansion coefficients C_{NLM} of such an asymptotic function are known from the algebraic version of the resonating group method.[10] With L and M being the orbital partial wave quantum numbers of the inelastic channel and N being the radial harmonic oscillator quantum number we have

$$C_{NLM} \rightarrow \text{const}(4N+2L+3)^{-1/4} \times \exp[-\kappa r_0(4N+2L+3)^{1/2}] , \tag{33}$$

where r_0 is the width of the harmonic oscillator basis, $r_0=\sqrt{\hbar/(\mu\omega)}$. The exponential decrease of these coefficients will become important in our further considerations.

Step 5

We want to compare, for given boundary conditions, the solutions $(|\chi_j^{(n)}\rangle)$ of (5) with the solutions $(|\chi_j^{(n+1)}\rangle)$ of (24). Equation (5) can be obtained from (24) by dropping the last row and column of the matrix $(H_{ij}^{(n+1)})$ and by dropping the last element of the column vector $(|\chi_j^{(n+1)}\rangle)$. Intuitively one might think that this dropping of terms cannot make much difference when n is large, because of (32). That this intuition might be wrong, can easily be demonstrated by an example: When the spectrum of (24) contains a resonance of zero width and when the width of the corresponding resonance of (5) approaches zero only as n goes to infinity, then the solutions of (5) and (24) can differ rather much in the vicinity of the resonance, for any given n.

Before we go on we have to make some restrictions. We assume that we are dealing with a *physical* system which means that no resonance state has infinite lifetime (zero width) and we assume that all microscopic potentials are bounded operators (no hard core). In order to compare the solutions of (5) with those of (24) we formally solve these two equations. We do this in two steps. First we diagonalize the submatrix $(H_{ij}^{(n+1)})$, $2\le i,j\le n$; recall (25). The many zeros obtained by this diagonalization enable us to construct, in the second step, the Green's function needed for the formal solution. When quantities are affected by the diagonalization of the submatrix we denote it by a hat. Equation (5) then becomes

$$\sum_{j=1}^{n} (\hat{H}_{ij}^{(n+1)} - E\delta_{ij})|\hat{\chi}_j^{(n)}\rangle = 0 ; \tag{34}$$

here we have used (25) which allowed us to replace the superscript (n) at the Hamiltonian matrix by $(n+1)$. Equation (24) becomes

$$\sum_{j=1}^{n+1} (\hat{H}_{ij}^{(n+1)} - E\delta_{ij})|\hat{\chi}_j^{(n+1)}\rangle = 0 . \tag{35}$$

We compare the solutions of (34) and (35) with each other and then go back to (5) and (24).

In Appendix A we derive the matrix Green's function $(\hat{G}_{ij}^{(n+1)})$ of the operator appearing in (34). The element $\hat{G}_{11}^{(n+1)}(E;\mathbf{r},\mathbf{r}')$ is the usual Green's function which corresponds to the equation which is obtained from (34) by formal elimination of channels $i=2,\ldots,n$. In terms of this Green's function the other elements of $(\hat{G}_{ij}^{(n+1)})$ are

$$\hat{G}_{1j}^{(n+1)}=\hat{G}_{11}^{(n+1)}\hat{H}_{1j}^{(n+1)}\frac{1}{E-\hat{H}_{jj}^{(n+1)}},\quad 2\le j\le n\ ,$$

$$\hat{G}_{i1}^{(n+1)}=\frac{1}{E-\hat{H}_{ii}^{(n+1)}}\hat{H}_{i1}^{(n+1)}\hat{G}_{11}^{(n+1)},\quad 2\le i\le n\ , \tag{36}$$

$$\hat{G}_{ij}^{(n+1)}=\frac{1}{E-\hat{H}_{ii}^{(n+1)}}\hat{H}_{i1}^{(n+1)}\hat{G}_{11}^{(n+1)}\times\hat{H}_{1j}^{(n+1)}\frac{1}{E-\hat{H}_{jj}^{(n+1)}}-\delta_{ij}\frac{1}{E-\hat{H}_{ii}^{(n+1)}},\quad 2\le i,j\le n\ .$$

Operating with this matrix Green's function on the matrix equation formed by the first n equations of the set of equations (35) we get

$$|\chi_1^{(n+1)}\rangle-|\chi_1^{(n)}\rangle=-\hat{G}_{11}^{(n+1)}\left[\hat{H}_{1,n+1}^{(n+1)}+\sum_{j=2}^{n}\hat{H}_{1j}^{(n+1)}\frac{1}{E-\hat{H}_{jj}^{(n+1)}}\hat{H}_{j,n+1}^{(n+1)}\right]|\chi_{n+1}^{(n+1)}\rangle\ , \tag{37a}$$

$$|\chi_i^{(n+1)}\rangle-|\chi_i^{(n)}\rangle=-\frac{1}{E-\hat{H}_{ii}^{(n+1)}}\hat{H}_{i1}^{(n+1)}\hat{G}_{11}^{(n+1)}\left[\hat{H}_{1,n+1}^{(n+1)}+\sum_{j=2}^{n}\hat{H}_{1j}^{(n+1)}\frac{1}{E-\hat{H}_{jj}^{(n+1)}}\hat{H}_{j,n+1}^{(n+1)}\right]|\chi_{n+1}^{(n+1)}\rangle+\frac{1}{E-\hat{H}_{ii}^{(n+1)}}\hat{H}_{i,n+1}^{(n+1)}|\chi_{n+1}^{(n+1)}\rangle,\quad 2\le i\le n\ . \tag{37b}$$

We want to show that the right-hand sides of (37a) and (37b) go to zero as n goes to infinity. This is not a trivial consequence of the fact that the norm of $\chi_{n+1}^{(n+1)}$ tends to zero, because some of the factors in front of $\chi_{n+1}^{(n+1)}$ are unbounded. We have to consider three types of unboundedness.

(a) A finite number of energies $\hat{H}_{ii}^{(n+1)}$ may lie in the elastic region. When E approaches one of them, say $E\to\hat{H}_{kk}^{(n+1)}$, then $(E-\hat{H}_{kk}^{(n+1)})^{-1}$ goes to infinity. In order to show that $\hat{G}_{11}^{(n+1)}\hat{H}_{1k}^{(n+1)}$ compensates this pole, we follow the treatment given in Sec. 9.2 of Ref. 2. We need a Green's function $\hat{G}_{11}^{(n+1),k}(E;\mathbf{r},\mathbf{r}')$ which is defined similarly to $\hat{G}_{11}^{(n+1)}(E;\mathbf{r},\mathbf{r}')$ but with omitted elimination potential $\hat{H}_{1k}^{(n+1)}\hat{H}_{k1}^{(n+1)}/(E-\hat{H}_{kk}^{(n+1)})$ of the kth channel. From the resolvent equations

$$\hat{G}_{11}^{(n+1)}=\hat{G}_{11}^{(n+1),k}-\hat{G}_{11}^{(n+1)}\frac{\hat{H}_{1k}^{(n+1)}\hat{H}_{k1}^{(n+1)}}{E-\hat{H}_{kk}^{(n+1)}}\hat{G}_{11}^{(n+1),k}\ , \tag{38a}$$

$$\hat{G}_{11}^{(n+1)}=\hat{G}_{11}^{(n+1),k}-\hat{G}_{11}^{(n+1),k}\frac{\hat{H}_{1k}^{(n+1)}\hat{H}_{k1}^{(n+1)}}{E-\hat{H}_{kk}^{(n+1)}}\hat{G}_{11}^{(n+1)} \tag{38b}$$

we get

$$\hat{G}_{11}^{(n+1)}\frac{\hat{H}_{1k}^{(n+1)}}{E-\hat{H}_{kk}^{(n+1)}}=\hat{G}_{11}^{(n+1),k}\frac{\hat{H}_{1k}^{(n+1)}}{E-\hat{H}_{kk}^{(n+1)}+\hat{H}_{k1}^{(n+1)}\hat{G}_{11}^{(n+1),k}\hat{H}_{1k}^{(n+1)}}\ , \tag{39a}$$

$$\frac{\hat{H}_{k1}^{(n+1)}}{E-\hat{H}_{kk}^{(n+1)}}\hat{G}_{11}^{(n+1)}=\frac{\hat{H}_{k1}^{(n+1)}}{E-\hat{H}_{kk}^{(n+1)}+\hat{H}_{k1}^{(n+1)}\hat{G}_{11}^{(n+1),k}\hat{H}_{1k}^{(n+1)}}\hat{G}_{11}^{(n+1),k}\ . \tag{39b}$$

Inserting (39a) into (37a) we get

$$|\chi_1^{(n+1)}\rangle-|\chi_1^{(n)}\rangle=-\hat{G}_{11}^{(n+1)}\left[\hat{H}_{1,n+1}^{(n+1)}+\sum_{\substack{j=2\\ j\neq k}}^{n}\hat{H}_{1j}^{(n+1)}\frac{1}{E-\hat{H}_{jj}^{(n+1)}}\hat{H}_{j,n+1}^{(n+1)}\right]|\chi_{n+1}^{(n+1)}\rangle+\hat{G}_{11}^{(n+1),k}\frac{\hat{H}_{1,n+1}^{(n+1)}}{E-\hat{H}_{kk}^{(n+1)}+\hat{H}_{k1}^{(n+1)}\hat{G}_{11}^{(n+1),k}\hat{H}_{1k}^{(n+1)}}|\chi_{n+1}^{(n+1)}\rangle\ . \tag{40a}$$

As is shown in Sec. 9.2 of Ref. 2 the quantity $\hat{H}_{k1}^{(n+1)}\hat{G}_{11}^{(n+1),k}\hat{H}_{1k}^{(n+1)}$ appearing in the denominator is a complex number. Its imaginary part is essentially the width of a Breit-Wigner-type resonance. Since we have excluded resonances of zero width, the factor in front of $|\chi_{n+1}^{(n+1)}\rangle$ in the last term of the right-hand side of (40a) remains bounded. The singularity at $E=\hat{H}_{kk}^{(n+1)}$ disappears when $\hat{H}_{kk}^{(n+1)}$ is a nondegenerate eigenvalue. It also disappears when $\hat{H}_{kk}^{(n+1)}$ is a degenerate eigenvalue, because we can apply (39a) to each of the degenerate terms.

The same sum over j which is present in (37a) is also present in (37b). For $E\to\hat{H}_{kk}^{(n+1)}$ with $i\neq k$ and $\hat{H}_{kk}^{(n+1)}\neq\hat{H}_{ii}^{(n+1)}$ we repeat the treatment which has led from (37a) to (40a) and get the same conclusion. For $E\to\hat{H}_{ii}^{(n+1)}$ we apply (39a) and (39b) in the following way:

$$-\frac{\hat{H}_{i1}^{(n+1)}}{E-\hat{H}_{ii}^{(n+1)}}\hat{G}_{11}^{(n+1)}\hat{H}_{1,n+1}^{(n+1)}|\chi_{n+1}^{(n+1)}\rangle=-\frac{\hat{H}_{i1}^{(n+1)}}{E-\hat{H}_{ii}^{(n+1)}+\hat{H}_{i1}^{(n+1)}\hat{G}_{11}^{(n+1),i}\hat{H}_{1i}^{(n+1)}}\hat{G}_{11}^{(n+1),k}\hat{H}_{1,n+1}^{(n+1)}|\chi_{n+1}^{(n+1)}\rangle\;,$$

$$\begin{aligned}-\frac{\hat{H}_{i1}^{(n+1)}}{E-\hat{H}_{ii}^{(n+1)}}\hat{G}_{11}^{(n+1)}\frac{\hat{H}_{1i}^{(n+1)}}{E-\hat{H}_{ii}^{(n+1)}}\hat{H}_{i,n+1}^{(n+1)}|\chi_{n+1}^{(n+1)}\rangle+\frac{1}{E-\hat{H}_{ii}^{(n+1)}}\hat{H}_{i,n+1}^{(n+1)}|\chi_{n+1}^{(n+1)}\rangle\\
=\left[-\frac{\hat{H}_{i1}^{(n+1)}\hat{G}_{11}^{(n+1),i}\hat{H}_{1i}^{(n+1)}}{(E-\hat{H}_{ii}^{(n+1)}+\hat{H}_{i1}^{(n+1)}\hat{G}_{11}^{(n+1),i}\hat{H}_{1i}^{(n+1)})(E-\hat{H}_{ii}^{(n+1)})}+\frac{1}{E-\hat{H}_{ii}^{(n+1)}}\right]\hat{H}_{i,n+1}^{(n+1)}|\chi_{n+1}^{(n+1)}\rangle\\
=\frac{\hat{H}_{i,n+1}^{(n+1)}}{E-\hat{H}_{ii}^{(n+1)}+\hat{H}_{i1}^{(n+1)}\hat{G}_{11}^{(n+1),i}\hat{H}_{1i}^{(n+1)}}|\chi_{n+1}^{(n+1)}\rangle\;,\end{aligned}$$

and

$$\begin{aligned}-\frac{\hat{H}_{i1}^{(n+1)}}{E-\hat{H}_{ii}^{(n+1)}}\hat{G}_{11}^{(n+1)}\hat{H}_{1j}^{(n+1)}\frac{1}{E-\hat{H}_{jj}^{(n+1)}}\hat{H}_{j,n+1}^{(n+1)}|\chi_{n+1}^{(n+1)}\rangle\\
=-\frac{\hat{H}_{i1}^{(n+1)}}{E-\hat{H}_{ii}^{(n+1)}+\hat{H}_{i1}^{(n+1)}\hat{G}_{11}^{(n+1),i}\hat{H}_{1i}^{(n+1)}}\hat{G}_{11}^{(n+1),i}\hat{H}_{1j}^{(n+1)}\frac{1}{E-\hat{H}_{jj}^{(n+1)}}\hat{H}_{j,n+1}^{(n+1)}|\chi_{n+1}^{(n+1)}\rangle,\quad j\neq i\;.\end{aligned}$$

Inserting these relations into (37b) we get

$$\begin{aligned}|\chi_i^{(n+1)}\rangle-|\chi_i^{(n)}\rangle=&-\frac{\hat{H}_{i1}^{(n+1)}}{E-\hat{H}_{ii}^{(n+1)}+\hat{H}_{i1}^{(n+1)}\hat{G}_{11}^{(n+1),i}\hat{H}_{1i}^{(n+1)}}\hat{G}_{11}^{(n+1),k}\hat{H}_{1,n+1}^{(n+1)}|\chi_{n+1}^{(n+1)}\rangle\\
&-\frac{\hat{H}_{i1}^{(n+1)}}{E-\hat{H}_{ii}^{(n+1)}+\hat{H}_{i1}^{(n+1)}\hat{G}_{11}^{(n+1),i}\hat{H}_{1i}^{(n+1)}}\hat{G}_{11}^{(n+1),i}\\
&\times\sum_{\substack{j=2\\j\neq i}}^{n}\hat{H}_{1j}^{(n+1)}\frac{1}{E-\hat{H}_{jj}^{(n+1)}}\hat{H}_{j,n+1}^{(n+1)}|\chi_{n+1}^{(n+1)}\rangle\\
&+\frac{\hat{H}_{i,n+1}^{(n+1)}}{E-\hat{H}_{ii}^{(n+1)}+\hat{H}_{i1}^{(n+1)}\hat{G}_{11}^{(n+1),i}\hat{H}_{1i}^{(n+1)}}|\chi_{n+1}^{(n+1)}\rangle\;.\end{aligned}\tag{40b}$$

Again we see that the singularity at $E=\hat{H}_{ii}^{(n+1)}$ disappears and the factor in front of $|\chi_{n+1}^{(n+1)}\rangle$ remains bounded. This is true also when $\hat{H}_{kk}^{(n+1)}=\hat{H}_{ii}^{(n+1)}$ for some $k\neq i$, because (39a) and (39b) allow us quite generally to replace a denominator $(E-\hat{H}_{kk}^{(n+1)})$ by a resonance denominator $E-\hat{H}_{kk}^{(n+1)}+\hat{H}_{k1}^{(n+1)}G\hat{H}_{1k}^{(n+1)}$ with an appropriate Green's function G.

(b) In Appendix B it is shown that the kinetic energy part of H does not contribute to the elements $\hat{H}_{1j}^{(n+1)}$, $2\leq j\leq n+1$ of the matrix Hamiltonian. For bounded potentials these operators are bounded. The term $\hat{G}_{11}^{(n+1)}\hat{H}_{1,n+1}^{(n+1)}|\chi_{n+1}^{(n+1)}\rangle$ of (37a) goes to zero when n goes to infinity, for every value of $\mathbf{r}$ in $\hat{G}_{11}^{(n+1)}(\mathbf{r},\mathbf{r}')$. The other terms on the right-hand sides of Eqs. (37a) and (37b) contain the operators $\hat{H}_{j,n+1}^{(n+1)}$, $2\leq j\leq n$. These operators contain coupling matrix elements of the kinetic energy part of H. The kinetic energy operator can couple harmonic oscillator states which differ by two excitation quanta. The relevant matrix elements are

$$T_{N,N+1}^{L}=\sqrt{N(N+L+1/2)}\frac{\hbar\omega}{2}\;.\tag{41}$$

For given angular momentum L and large radial quantum number N this matrix element increases approximately proportional to N. We have to show that, nevertheless, $\hat{H}_{j,n+1}^{(n+1)}|\chi_{n+1}^{(n+1)}\rangle$ goes to zero when N goes to infinity. Let us choose our basis of harmonic oscillator shell model states such that it includes all states up to a given (large) number of excitation quanta and excludes all states with more excitation quanta. And let us choose the worst possible case for our coupled channels equation. Let us consider an energy E which is just slightly below the first inelastic threshold E_0. At this energy highly excited harmonic oscillator states are needed to represent the long exponential tail of the wave function reaching into the first inelastic channel. The largest harmonic oscillator amplitudes which we present in $|\hat{\chi}_{n+1}^{(n+1)}\rangle$ will come from this tail. Their dependence on the number of excitation quanta is given by (33). We see that the exponential decrease with $\sqrt{N}$ of these amplitudes overrides the linear increase with N which is present in $\hat{H}_{j,n+1}^{(n+1)}$, for all values of j. At $E=E_0$ convergence has to break down because the compound state part of the wave function is no longer normalizable. In (33) this feature is expressed by the fact that κ becomes zero at $E=E_0$.

(c) The number $(n-1)$ of harmonic oscillator shell model states can be much larger than the maximum number N of excitation quanta. Up to now we have only shown that in (37a) and (37b) the individual terms in the sums over j go to zero. We still have to show that they go to zero fast enough to override the increasing number of terms in the sum. This is easily shown. For A particles the number of Cartesian (or Jacobi) coordinates is $3A$ (or less, if we separate out the center of mass motion). If we distribute up to $(2N+L)$ harmonic oscillator quanta over $3A$ oscillators we find that there are fewer than $(2N+L)^{3A}$ possibilities. This factor is clearly overridden by the exponential decrease of the terms in the sum.

This completes our investigation of the convergence property of the orthogonalized n-channels resonating group equation (34). The result is equally valid for Eq. (5), because (5) and (34) differ only by a unitary transformation in the closed channels subspace. We have found that with increasing number of distortion channels the appropriate relative motion wave function $\hat{\chi}_1^{(n)}(\mathbf{r})$ converges to the true wave function, for every value of $\mathbf{r}$, and that the compound state or distortion amplitudes $\hat{\chi}_i^{(n)}$, $i\geq 2$, converge to their true values, for all i.

We hesitate to call our findings a convergence proof in the sense of rigorous mathematics. We are physicists rather than mathematicians. But we felt that, after 50 years of successful applications of the resonating group method, its convergence properties (with rigorous cluster ground states) should be investigated.

IV. CONCLUSION

The Gram-Schmidt orthogonalization procedure, supplemented by a special treatment of zero-norm states, has been applied to the coupled channels resonating group equation with one open channel and $n-1$ (closed) distortion channels. When the orthogonal complement of the n-channels space is added as space of an $(n+1)$th channel, an orthogonalized $(n+1)$-channels equation is obtained which is fully equivalent to the microscopic Schrödinger equation. It is seen that the norm of the $(n+1)$th component of the solution vector goes to zero as n increases. It is also seen that the relative motion wave function of the elastic channel converges pointwise to the corresponding wave function component of the true Schrödinger solution when n goes to infinity. The distortion amplitudes also converge to the corresponding amplitudes which are present in the true Schrödinger solution. The converged set of equations defines the effective interaction of two clusters in the elastic energy region;[9] if one cluster is a single particle this definition goes over into Feshbach's definition of the optical potential in the elastic energy region.

APPENDIX A

We want to solve the equation

$$\sum_{j=1}^{n}(\hat{H}_{ij}^{(n+1)}-E\delta_{ij})|\hat{\chi}_j^{(n+1)}\rangle=-\hat{H}_{i,n+1}^{(n+1)}|\hat{\chi}_{n+1}^{(n+1)}\rangle \quad \text{for } 1\leq i\leq n\ , \tag{A1}$$

by introducing a matrix Green's function for the matrix operator $(\hat{H}_{ij}^{(n+1)}-E\delta_{ij})$ such that

$$|\hat{\chi}_i^{(n+1)}\rangle=|\hat{\chi}_i^{(n)}\rangle-\sum_{j=1}^{n}\hat{G}_{ij}^{(n+1)}\hat{H}_{j,n+1}^{(n+1)}|\hat{\chi}_{n+1}^{(n+1)}\rangle\ . \tag{A2}$$

We formally eliminate from (A1) the equations with $i\geq 2$, i.e., we insert the formal solutions (recall that $\hat{H}_{ij}^{(n+1)}$, $2\leq i,j\leq n$, is diagonal)

$$|\hat{\chi}_i^{(n+1)}\rangle=\frac{1}{E-\hat{H}_{ii}^{(n+1)}}(\hat{H}_{i1}^{(n+1)}|\hat{\chi}_1^{(n+1)}\rangle+\hat{H}_{i,n+1}^{(n+1)}|\hat{\chi}_{n+1}^{(n+1)}\rangle) \quad \text{for } 2\leq i\leq n\ , \tag{A3}$$

into the first one of the set of Eqs. (A1). We get

$$\left[\hat{H}_{11}^{(n+1)}-E+\sum_{j=2}^{n}\hat{H}_{1j}^{(n+1)}\frac{1}{E-\hat{H}_{jj}^{(n+1)}}\hat{H}_{j1}^{(n+1)}\right]|\hat{\chi}_1^{(n+1)}\rangle=-\left[\hat{H}_{1,n+1}^{(n+1)}+\sum_{j=2}^{n}\hat{H}_{1j}^{(n+1)}\frac{1}{E-\hat{H}_{jj}^{(n+1)}}\hat{H}_{j,n+1}^{(n+1)}\right]|\hat{\chi}_{n+1}^{(n+1)}\rangle\ . \tag{A4}$$

The operator appearing on the left-hand side is well known.[2] It has an ordinary three-dimensional Green's function which we denote by $\hat{G}_{11}^{(n+1)}$. By formally solving (A4) with this Green's function we get

$$|\hat{\chi}_1^{(n+1)}\rangle=|\hat{\chi}_1^{(n)}\rangle-\hat{G}_{11}^{(n+1)}\left[\hat{H}_{1,n+1}^{(n+1)}+\sum_{j=2}^{n}\hat{H}_{1j}^{(n+1)}\frac{1}{E-\hat{H}_{jj}^{(n+1)}}\hat{H}_{j,n+1}^{(n+1)}\right]|\hat{\chi}_{n+1}^{(n+1)}\rangle\ . \tag{A5}$$

We insert $|\hat{\chi}_1^{(n+1)}\rangle$ from this equation into (A3) and get

$$|\hat{\chi}_i^{(n+1)}\rangle=|\hat{\chi}_i^{(n)}\rangle-\frac{1}{E-\hat{H}_{ii}^{(n+1)}}\hat{H}_{i1}^{(n+1)}\hat{G}_{11}^{(n+1)}\left[\hat{H}_{1,n+1}^{(n+1)}+\sum_{j=2}^{n}\hat{H}_{1j}^{(n+1)}\frac{1}{E-\hat{H}_{jj}^{(n+1)}}\hat{H}_{j,n+1}^{(n+1)}\right]|\hat{\chi}_{n+1}^{(n+1)}\rangle$$
$$+\frac{1}{E-\hat{H}_{ii}^{(n+1)}}\hat{H}_{i,n+1}^{(n+1)}|\hat{\chi}_{n+1}^{(n+1)}\rangle \quad \text{for } 2\le i\le n \ . \qquad \text{(A6)}$$

By comparing (A5) and (A6) with (A2) we get the matrix Green's function $(\hat{G}_{ij}^{(n+1)})$ in terms of $\hat{G}_{11}^{(n+1)}$,

$$\hat{G}_{1j}^{(n+1)}=\hat{G}_{11}^{(n+1)}\hat{H}_{1j}^{(n+1)}\frac{1}{E-\hat{H}_{jj}^{(n+1)}} \quad \text{for } 2\le j\le n \ ,$$

$$\hat{G}_{i1}^{(n+1)}=\frac{1}{E-\hat{H}_{ii}^{(n+1)}}\hat{H}_{i1}^{(n+1)}\hat{G}_{11}^{(n+1)} \quad \text{for } 2\le i\le n \ ,$$

$$\hat{G}_{ij}^{(n+1)}=\frac{1}{E-\hat{H}_{ii}^{(n+1)}}\hat{H}_{i1}^{(n+1)}\hat{G}_{11}^{(n+1)} \times\hat{H}_{1j}^{(n+1)}\frac{1}{E-\hat{H}_{jj}^{(n+1)}} -\frac{1}{E-\hat{H}_{ii}^{(n+1)}}\delta_{ij} \quad \text{for } 2\le i,j\le n \ . \qquad \text{(A7)}$$

APPENDIX B

We want to show that the elements $H_{1j}^{(n+1)}$, $j\ge 2$, of our matrix Hamiltonian $(H_{ij}^{(n+1)})$ do not contain any contribution from the microscopic kinetic energy operator. We consider a two-channel equation with an elastic two-cluster channel, as first channel, and any other channel as second channel. Using either the orthogonalization procedure outlined in Sec. II, or the recursion relation given in Ref. 9, we get

$$H_{12}^{(2)}=(N_{11}^{(0)})^{-1/2}H_{12}^{(0)}(N_{22}^{(1)})^{-1/2} -(N_{11}^{(0)})^{-1/2}H_{11}^{(0)}(N_{11}^{(0)})^{-1}N_{12}^{(0)}(N_{22}^{(1)})^{-1/2} \ . \qquad \text{(B1)}$$

The norm operator $N_{11}^{(0)}$ of the first channel, expressed in its eigenstates basis, is

$$N_{11}^{(0)}=\sum_{\nu}|u_\nu\rangle\eta_\nu\langle u_\nu| \ . \qquad \text{(B2)}$$

Let $|v_\mu\rangle$ be the eigenstates of the norm operator $N_{22}^{(0)}$ of the second channel. Then $N_{12}^{(0)}$ can be expanded as

$$N_{12}^{(0)}=\sum_{\mu,\nu}|u_\mu\rangle n_{\mu\nu}\langle v_\nu| \ . \qquad \text{(B3)}$$

The microscopic kinetic energy operator, when acting in the first channel, decomposes into three parts. Two of them operate in the internal motion space of the two clusters, the third one operates in the relative motion space. The former two parts, together with cluster-internal potentials, convert into binding energy of the two clusters. The latter part has the Hilbert space representation

$$T=\sum_{\mu,\nu}|u_\mu\rangle T_{\mu\nu}\langle u_\nu| \ . \qquad \text{(B4)}$$

We get

$$H_{11}^{(0)}=\sum_{\mu,\nu}|u_\mu\rangle\langle u_\mu|\langle\phi_1^{(0)}|T\mathcal{A}|\phi_1^{(0)}\rangle|u_\nu\rangle\langle u_\nu| + \text{terms not containing } T$$
$$=\sum_{\mu,\nu}|u_\mu\rangle T_{\mu\nu}\eta_\nu\langle u_\nu|+\cdots \ . \qquad \text{(B5)}$$

In (B5), the decision to put $\mathcal{A}$ to the right-hand side of T has been made *before* decomposing H into pieces which are not exchange symmetric. Similarly we get

$$H_{12}^{(0)}=\sum_{\mu,\nu,\tau}|u_\mu\rangle T_{\mu\nu}n_{\nu\tau}\langle v_\tau|+\cdots \ . \qquad \text{(B6)}$$

This operator appears in the first term of the right-hand side of (B1). In the second term appears the product $H_{11}^{(0)}(H_{11}^{(0)})^{-1}N_{12}^{(0)}$ which becomes

$$H_{11}^{(0)}(N_{11}^{(0)})^{-1}N_{12}^{(0)}=\sum_{\mu,\nu,\tau}|u_\mu\rangle T_{\mu\nu}n_{\nu\tau}\langle v_\tau|+\cdots$$
$$=H_{12}^{(0)}+\cdots \ . \qquad \text{(B7)}$$

Therefore the two terms at the right-hand side of (B1) cancel, except for contributions not arising from T.

Now, the second channel has been arbitrary, in this consideration. It can consist of one of our shell model states $|\phi_i^{(0)}\rangle$, $2\le i\le n$, or it can be the complete space $|\phi_i^{(0)}\rangle$, $i=n+1$. The feature which has been essential for getting our result was that the second channel is orthogonalized with respect to the first channel and that the space of the first channel contains the complete representation space of the kinetic energy operator of relative motion. We conclude that our result is true for $H_{1j}^{(n+1)}$, $j\ge 2$. Only the potential operator contributes to $H_{1j}^{(n+1)}$, $j\ge 2$. For bounded potentials the operators $H_{1j}^{(n+1)}$, $2\le j\le n+1$ are therefore bounded.

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