Exchange-Coulomb interaction in resonating-group calculations

M. LeMere and Y. C. Tang

School of Physics, University of Minnesota, Minneapolis, Minnesota 55455

(Received 1 May 1978)

A simple, self-consistent procedure is proposed to approximately calculate the exchange-Coulomb kernel in a resonating-group formulation. By applying this procedure to $\alpha + \alpha$, $^3\text{He} + \alpha$, and light ion plus ^{16}O systems, it is found that satisfactory results can be obtained in all these cases.

[NUCLEAR REACTIONS Scattering theory, exchange-Coulomb interaction.]

I. INTRODUCTION

In resonating-group calculations,[1] the major task is to compute the various kernel functions which enter into the formulation through the use of totally antisymmetrized wave functions. By using a complex-generator-coordinate technique recently developed,[1] and by choosing functions of Gaussian dependence for both the spatial part of the cluster internal function and the spatial part of the nuclear interaction potential, it is straightforward, though tedious, to carry out an analytic evaluation of the normalization kernel and the kernels arising from the kinetic-energy operator and the nuclear part of the potential-energy operator. On the other hand, due to the fact that the Coulomb potential does not have a Gaussian spatial dependence, the evaluation of the exchange-Coulomb kernel frequently requires a considerably larger amount of computational effort. Therefore, it is desirable to devise a simple procedure by which this particular kernel may be approximately evaluated but is still accurate enough for practical purposes. In this investigation, we propose such a procedure which is based on the recognition that, because of the long-range nature of the Coulomb potential, the total Coulomb energy of a bound system may be computed in a good approximation by using only the unantisymmetrized part of the wave function.[2]

In the next section, we discuss the procedure for obtaining an approximate expression for the exchange-Coulomb kernel. To demonstrate that this expression is indeed useful in practical calculations, we consider in Sec. III $\alpha + \alpha$ and $^3\text{He} + \alpha$ systems where exact expressions for this kernel function have been derived. Here also, we shall describe the results obtained for the more complicated systems of d, ^3He, and α plus ^{16}O. Finally, in Sec. IV, concluding remarks will be made.

II. EXCHANGE-COULOMB KERNEL

Consider a single-channel resonating-group wave function given by[3]

$$\psi = \mathcal{Q}\bar{\psi}$$

$$= \mathcal{Q}[\phi_A \phi_B F(\vec{R}_A - \vec{R}_B)Z(\vec{R}_{\text{c.m.}})] , \tag{1}$$

where $\mathcal{Q}$ is an antisymmetrization operator, ϕ_A and ϕ_B describe the internal structures of clusters A and B, $F(\vec{R})$ describes the relative motion between the two clusters, and $Z(\vec{R}_{\text{c.m.}})$ is any normalizable function describing the motion of the total center of mass. By writing

$$\mathcal{Q} = \mathcal{Q}'\mathcal{Q}_A \mathcal{Q}_B , \tag{2}$$

where $\mathcal{Q}_A$ and $\mathcal{Q}_B$ are, respectively, antisymmetrization operators for the nucleons in clusters A and B, and $\mathcal{Q}'$ is an antisymmetrization operator which interchanges nucleons in different clusters, one obtains, by using the procedure discussed in Ref. 1, the following expression for the exchange-Coulomb kernel $K_C(\vec{R}', \vec{R}'')$:

$$K_C(\vec{R}', \vec{R}'') = \langle \phi_A \phi_B \delta(\vec{R} - \vec{R}')Z | \mathcal{U}_C |$$

$$\times \mathcal{Q}''[\hat{\phi}_A \hat{\phi}_B \delta(\vec{R} - \vec{R}'')Z] \rangle , \tag{3}$$

where

$$\mathcal{Q}'' = \mathcal{Q}' - 1 , \tag{4}$$

and $\hat{\phi}_K (K = A$ or $B)$ is an antisymmetrized cluster internal function given by

$$\hat{\phi}_K = \mathcal{Q}_K \phi_K . \tag{5}$$

Also, in Eq. (3), the quantities $\vec{R}'$ and $\vec{R}''$ are parameter coordinates on which antisymmetrization operators do not act, and $\mathcal{U}_C$ represents the total Coulomb interaction which has the form

$$\mathcal{U}_C = \sum_{i<j=1}^{N} V_{ij}^C , \tag{6}$$

with N being the total number of nucleons in the system and V_{ij}^C being the Coulomb potential between nucleons i and j. As was mentioned in the Introduction, the fact that V_{ij}^C possesses a non-Gaussian spatial dependence means that the evalu-

ation of K_C is particularly time consuming.

For a bound system described by the wave function of Eq. (1) with

$$F(\vec{R}) = \frac{1}{R} f_l(R) P_l(\cos\theta) ,\qquad (7)$$

the total Coulomb energy is

$$E_{Tl}^C = \frac{\langle \bar{\psi} | \mathbf{v}_C | \psi \rangle}{\langle \bar{\psi} | \psi \rangle}$$

$$= \frac{\langle \bar{\psi} | \mathbf{v}_C | \hat{\psi} \rangle + \langle \bar{\psi} | \mathbf{v}_C | \mathbf{\alpha}'' \hat{\psi} \rangle}{\langle \bar{\psi} | \hat{\psi} \rangle + \langle \bar{\psi} | \mathbf{\alpha}'' \hat{\psi} \rangle} \qquad (8)$$

with

$$\hat{\psi} = \mathbf{\alpha}_A \mathbf{\alpha}_B \bar{\psi} . \qquad (9)$$

Because the Coulomb potential V_{ij}^C is long ranged, it is a good approximation (see Chap. 6 of Ref. 2) to compute E_{Tl}^C by using only the unantisymmetrized part of ψ; that is, one can obtain a good estimate of the Coulomb energy by simply using the expression

$$E_{Tl}^C \approx \frac{\langle \bar{\psi} | \mathbf{v}_C | \hat{\psi} \rangle}{\langle \bar{\psi} | \hat{\psi} \rangle} . \qquad (10)$$

For example, in the [8]Be case where a translationally invariant shell-model function of the lowest configuration in a harmonic-oscillator well of width parameter $\alpha = 0.514$ fm[-2] is used,[4] the values of E_{Tl}^C calculated with Eqs. (8) and (10) are, respectively, equal to 4.26 and 4.06 MeV, which differ from each other by only about 5%.

By equating the expressions for E_{Tl}^C given by Eqs. (8) and (10), one finds

$$\langle \bar{\psi} | \mathbf{v}_C | \mathbf{\alpha}'' \hat{\psi} \rangle = E_{Tl}^C \langle \bar{\psi} | \mathbf{\alpha}'' \hat{\psi} \rangle . \qquad (11)$$

Using Eqs. (1) and (3) then yields

$$\int F^*(\vec{R}') K_C(\vec{R}', \vec{R}'') F(\vec{R}'') d\vec{R}' d\vec{R}''$$

$$= E_{Tl}^C \int F^*(\vec{R}') \mathfrak{N}_E(\vec{R}', \vec{R}'') F(\vec{R}'') d\vec{R}' d\vec{R}'' , \qquad (12)$$

where $\mathfrak{N}_E(\vec{R}', \vec{R}'')$ is the exchange-normalization kernel given by[1]

$$\mathfrak{N}_E(\vec{R}', \vec{R}'') = \langle \phi_A \phi_B \delta(\vec{R} - \vec{R}') Z |$$

$$\times \mathbf{\alpha}'' [\hat{\phi}_A \hat{\phi}_B \delta(\vec{R} - \vec{R}'') Z] \rangle . \qquad (13)$$

If one now makes the partial-wave expansions

$$K_C(\vec{R}', \vec{R}'') = \frac{1}{R' R''} \sum_{l,m} k_l^C(R', R'') Y_{lm}(\theta', \phi')$$

$$\times Y_{lm}^*(\theta'', \phi'') , \qquad (14)$$

$$\mathfrak{N}_E(\vec{R}', \vec{R}'') = \frac{1}{R' R''} \sum_{l,m} \mathfrak{N}_{El}(R', R'') Y_{lm}(\theta', \phi')$$

$$\times Y_{lm}^*(\theta'', \phi'') , \qquad (15)$$

then one obtains from Eqs. (7) and (12) the following equation:

$$\int_0^\infty \int_0^\infty f_l^*(R') k_l^C(R', R'') f_l(R'') dR' dR''$$

$$= E_{Tl}^C \int_0^\infty \int_0^\infty f_l^*(R') \mathfrak{N}_{El}(R', R'') f_l(R'') dR' dR'' . \qquad (16)$$

Since $f_l(R)$ is an arbitrary function, Eq. (16) implies that

$$k_l^C(R', R'') = E_{Tl}^C \mathfrak{N}_{El}(R', R'') . \qquad (17)$$

This is a useful, approximate expression for the partial-wave exchange-Coulomb kernel, because one can, in general, analytically evaluate the partial-wave exchange-normalization kernel $\mathfrak{N}_{El}$ in a relatively straightforward manner.

Next, we define the relative Coulomb energy E_{Rl}^C between the clusters by expressing E_{Tl}^C as

$$E_{Tl}^C = E_A^C + E_B^C + E_{Rl}^C . \qquad (18)$$

In the above equation, E_A^C and E_B^C are, respectively, the internal Coulomb energies of clusters A and B; these energies may be easily computed by using the expressions for the cluster internal functions $\hat{\phi}_A$ and $\hat{\phi}_B$. On the other hand, the relative Coulomb energy E_{Rl}^C is an *a priori* unknown quantity, but may be approximately determined by the use of a self-consistent procedure to be discussed below.

Before we discuss the self-consistent procedure, we wish to make the following remarks:
(i) If the cluster B is a neutron or a dineutron cluster and if each cluster (A or B) is described by a single Slater determinant of translationally invariant functions, then Eq. (17) is simply reduced to

$$k_l^C(R', R'') = E_A^C \mathfrak{N}_{El}(R', R'') , \qquad (19)$$

which is in fact an exact expression for the exchange-Coulomb kernel, as can be easily verified by an explicit calculation.[5]
(ii) For states in which the clusters penetrate into each other strongly, the mutual antisymmetrization between nucleons in different clusters is important. In such cases, there will be substantial cancellations between the individual terms in both the numerator and the denominator of Eq. (8), and it is a poor approximation to omit exchange-Coulomb contributions entirely by simply setting k_l^C equal to zero in the calculation.

For an approximate but self-consistent determi-

nation of E_{RI}^C, we use the following procedure. We consider a bound or a sharp resonance state having a certain definite value for the relative orbital angular momentum l and compute the separation energy of the clusters by solving the resonating-group integrodifferential equation

$$\left[\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dR'^2}-\frac{l(l+1)}{R'^2}\right)+E-V_N(R')-V_C(R')\right]f_l(R')$$

$$=\int_0^\infty [k_l^N(R',R'')+k_l^C(R',R'')]f_l(R'')dR'',$$
(20)

where V_N and V_C denote, respectively, the direct nuclear and the direct Coulomb potentials, and k_l^N contains the normalization kernel and the kernels arising from the kinetic-energy operator and the nuclear part of the potential-energy operator. Two separate calculations will be performed. In the first calculation, we choose an arbitrary but reasonable value for E_{RI}^C and obtain the separation energy E_S for the actual case where both clusters are charged. In the second calculation, we compute the separate energy E_S^0 for the reference case where the charge of the proton is assumed to be infinitesimally small. The difference

$$\Delta E_S = E_S^0 - E_S$$
(21)

is then a good estimate of the relative Coulomb energy. In general, the value of ΔE_S so determined will, of course, not be equal to the value of E_{RI}^C chosen initially. The procedure is thus to systematically repeat the calculation with different choices of E_{RI}^C until self-consistency, i.e., $E_{RI}^C = \Delta E_S$ is finally obtained. This self-consistent value of E_{RI}^C will then be used in Eqs. (17) and (18) to calculate binding energies and phase shifts in all states which are characterized by this particular l value.

In principle, one should determine the self-consistent values of E_{RI}^C for all l values of interest. In practice, however, this does not seem necessary and it is a good approximation to use the value determined for $l=0$ in all even-l states and the value determined for $l=1$ in all odd-l states. The reason why this simplification does yield satisfactory results is that in all states of a rotational band the intrinsic structures and, hence, the relative Coulomb energies are similar, and for those values of l for which no bound or sharp resonance states exist, the calculated values of the phase shifts are not expected to be greatly sensitive to the choice of E_{RI}^C appearing in the approximate expression for the exchange-Coulomb kernel.

It should be mentioned that there are other approximation methods which have been proposed to specifically handle the exchange-Coulomb prob-

lem.[6-9] In comparing with these, our method has the advantage of being exceedingly simple to apply. Also, as the discussion below shows, the results obtained are in good agreement with those obtained in cases where exact expressions for the exchange-Coulomb kernels have been derived.

III. EXAMPLES

A. $\alpha + \alpha$ system

To test the procedure described above, we consider the $\alpha+\alpha$ system where the exact exchange-Coulomb kernel is known.[10,11] For this test, we use the wave function of Eq. (1), with ϕ_A and ϕ_B being translationally invariant products of single-particle functions in harmonic-oscillator wells of width parameter $\alpha=0.514$ fm^{-2}. The nucleon-nucleon potential used is given by Eq. (5) of Ref. 5, with the spin-orbit part set as zero. The exchange-mixture parameter u in this potential is chosen to be 0.93, which yields a ^{8}Be, $l=0$ bound state having an α-particle separation energy of 0.748 MeV.

Using the self-consistent procedure for the $l=0$ ground state, we obtain a value of E_{RI}^C equal to 1.63 MeV. The corresponding value of the α-particle separation energy is 0.709 MeV, which is very close to the abovementioned value obtained with the exact exchange-Coulomb kernel. On the other hand, if the exchange-Coulomb interaction is neglected by setting $k_l^C=0$, then the separation energy becomes only 0.246 MeV, which is appreciably smaller than the correct value of 0.748 MeV quoted above.

In Table I, we compare the phase shifts δ_l, δ_l^A, and δ_l^N for $l=0$, 2, and 4 obtained, respectively, with the exact exchange-Coulomb kernel, with the approximate but self-consistent exchange-Coulomb kernel, and with k_l^C set as zero. Here it is seen that the approximation of omitting exchange-Coulomb effects leads to significant deviations from the exact result especially at energies near resonances, but the use of our simple, self-consistent procedure to take these effects approximately into account does yield satisfactory phase-shift values in all orbital-angular-momentum states.

To have a measure of the effectiveness of our proposed procedure, we define a quantity

$$\xi_l = \left|\frac{\delta_l^N-\delta_l}{\delta_l^A-\delta_l}\right|.$$
(22)

In Table I, the values of ξ_l are given in $l=0,2$, and 4 states at various energies. From this table one sees that its value is always appreciably larger than 1, indicating that the result obtained with the self-consistent exchange-Coulomb kernel is indeed greatly improved over that obtained by setting $k_l^C=0$.

TABLE I. Various phase shifts (in deg) as a function of E.

E (MeV)	$l=0$					$l=2$				$l=4$			
	δ_0	δ_0^A	δ_0^N	ξ_0	δ_2	δ_2^A	δ_2^N	ξ_2	δ_4	δ_4^A	δ_4^N	ξ_4
2	480.9	480.4	474.3	11.4	220.8	217.3	197.9	6.6	0	0	0	
4	435.8	435.0	428.7	9.2	311.5	310.3	296.0	12.3	0.6	0.6	0.6	
6	406.7	405.8	399.7	7.9	303.3	302.3	293.8	9.6	3.5	3.4	3.3	
8	385.3	384.4	378.5	7.0	294.2	293.2	286.0	8.2	12.4	12.3	11.1	8.4
10	368.4	367.3	361.8	6.3	286.0	285.0	278.5	7.2	37.2	36.1	30.0	6.4
12	354.2	353.1	347.9	5.7	278.8	277.7	271.8	6.5	83.8	80.6	65.1	5.9
14	342.0	340.9	336.0	5.2	272.3	271.2	265.7	6.0	115.2	112.3	97.8	6.0
16	331.3	330.1	325.6	4.8	266.3	265.2	260.1	5.5	129.1	126.7	115.9	5.6
18	321.7	320.5	316.3	4.5	260.8	259.6	255.0	5.1	136.5	134.4	125.8	5.1
20	312.9	311.8	307.9	4.2	255.6	254.5	250.2	4.7	141.1	139.2	132.1	4.8

B. ^{3}He + α system

Next, we study in the ^{3}He + α system the results obtained by using the approximate exchange-Coulomb kernel of Eq. (17) and the exact exchange-Coulomb kernel of Koepke et al.[12] This is a useful study because, in this system, both even-l and odd-l partial waves contribute but there exist no bound or sharp resonance states with even values of l. Thus, in the self-consistent procedure we shall consider only the ground state with $l=1$ and use the resultant value of E_{R1}^C for all orbital angular-momentum states.

The wave function used is again that of Eq. (1), with the cluster internal functions given by the lowest configurations in harmonic-oscillator wells characterized by a common width parameter of 0.45 fm^{-2}. The nucleon-nucleon potential is chosen to have a Serber exchange mixture (i.e., $u=1$) which results in a cluster separation energy of 2.058 MeV in the $l=1$ ground state when the exact exchange-Coulomb kernel is employed.

The self-consistent procedure, when applied to the $l=1$ ground state, yields a value of E_{R1}^C equal to 1.755 MeV. With this choice of E_{R1}^C, the resultant value of the ^{3}He separation energy is 2.032 MeV, which is rather close to the exact value mentioned above. As a comparison, we have also computed the separation energy in the case where k_I^C is set as zero. This turns out to be 2.450 MeV, which again differs appreciably from the value obtained with the exact exchange-Coulomb kernel.

Using the self-consistent value of E_{R1}^C so determined, we calculate the phase-shifts for $l=0$ to 5 at various energies. The results are shown in Fig. 1, together with those obtained with the exact exchange-Coulomb kernel and with $k_I^C=0$. As is seen, the phase-shift values in all l states obtained by our self-consistent procedure are indeed much closer to the exact values than those obtained by omitting exchange-Coulomb effects.

From Fig. 1 one also notes the interesting feature that in even-l states the phase-shift values obtained with $k_I^C=0$ are smaller than those obtained with the exact exchange-Coulomb kernel, while in odd-l states the opposite is true. This is a demonstration of the odd-even effect arising from antisymmetrization, which has been discussed in detail elsewhere.[1,13]

C. d, ^{3}H, ^{3}He, and $\alpha + {}^{16}$O systems

The self-consistent procedure discussed here has also been applied to the d, ^{3}H, ^{3}He, and α plus ^{16}O systems.[1] In these systems, because of the presence of p-shell nucleons, an analytic derivation of the exact expression for the exchange-Coulomb kernel becomes generally difficult and the use of an approximate procedure seems to be quite necessary.

In Table II, we list the values of E_{R1}^C obtained by applying the self-consistent procedure to the lowest $l=0$ and 1 states. From this table, one observes the following features:

(i) The values of E_{R0}^C are larger than the values of E_{R1}^C. This is consistent with the fact that in all these systems the ground states have $l=0$ and, hence, the intrinsic structures are expected to be more compact in $l=0$ states than in $l=1$ states.

(ii) Using the values of E_{R0}^C and E_{R1}^C, one estimates that in the $\alpha + {}^{16}$O case the mean separation distances between the clusters are equal to 3.8 and 4.5 fm in $l=0$ and 1 states, respectively. These values should be compared with the value of about 4.1 fm for the sum of the rms matter radii of the α and ^{16}O nuclei. From this comparison it is reasonable to state, in agreement with the conclusion reached by Matsuse et al.,[14] that the states in the ground-state band may have a rather shell-model-like character, while the states in the $K^\pi=0^-$ band with band head at 5.79 MeV are likely to have a strong $\alpha + {}^{16}$O molecule-like character.
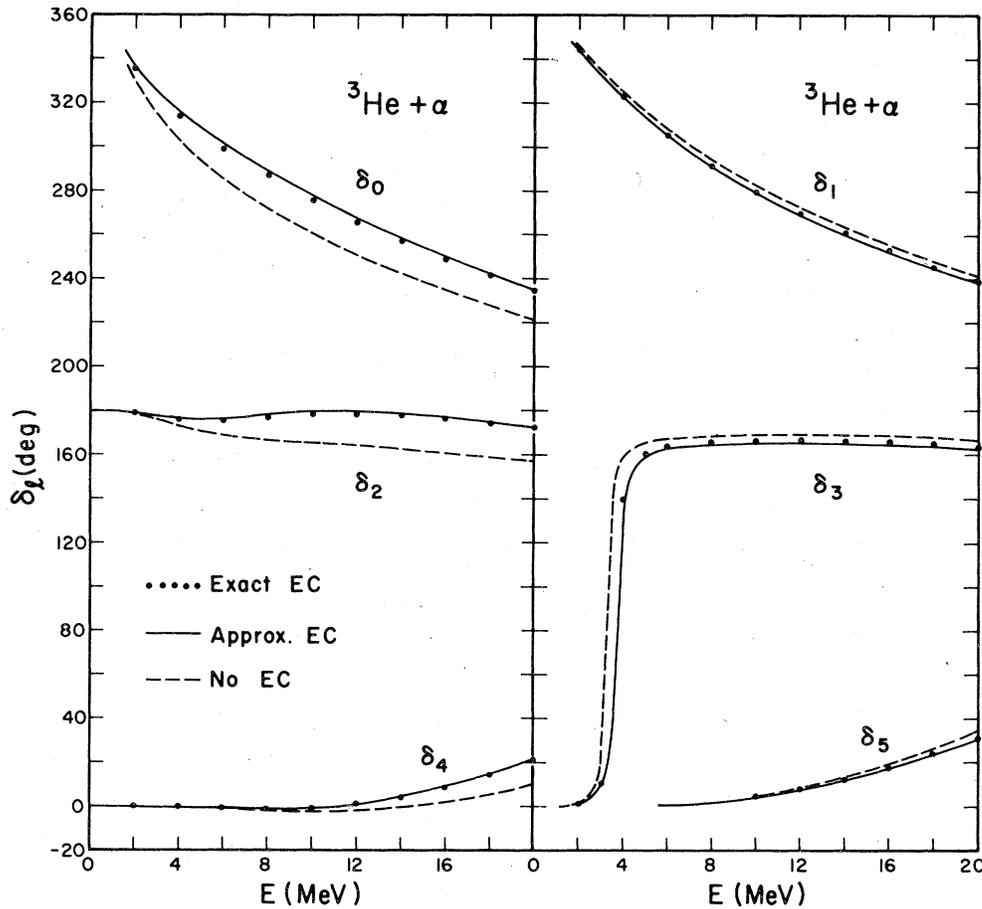
FIG. 1. Comparison of ^{3}He + α phase shifts calculated with the exact exchange-Coulomb kernel, with the approximate but self-consistent exchange-Coulomb kernel, and with k_I^C set as zero.

(iii) The value of E_{R0}^C in the ^{3}H + ^{16}O system is somewhat larger than one-half of that in the ^{3}He + ^{16}O system. This can be attributed to the fact that the ^{3}H separation energy in the ground state of ^{19}F is larger than the ^{3}He separation energy in the ground state of ^{19}Ne.

Because of these features, we are confident that, even though there is no comparison with results from exact exchange-Coulomb calculations, the binding energies and phase shifts obtained by our

TABLE II. Values of E_{R0}^C and E_{R1}^C.

System	E_{R0}^C (MeV)	E_{R1}^C (MeV)
$d + {}^{16}$O	3.38	2.42
^{3}H + ^{16}O	3.23	2.73
^{3}He + ^{16}O	6.34	5.38
$\alpha + {}^{16}$O	6.12	5.19

approximate procedure are likely to be reasonably correct.[1]

IV. CONCLUSION

In this investigation, we discuss a simple, self-consistent procedure which can be used to obtain an approximate expression for the exchange-Coulomb kernel in a resonating-group formulation. For this procedure the basic idea is that, because the Coulomb potential between two protons is long-ranged, the total Coulomb energy can be calculated to a good approximation by using only the unanti-symmetrized part of the resonating-group trial wave function.

By applying this procedure to $\alpha + \alpha$, ^{3}He + α, and light ions plus ^{16}O systems, we find that satisfactory results can be obtained in all these systems. From this we conclude that our procedure is likely to be useful in a general case involving complicated clusters. This is important, because already

for a two-cluster system where the clusters contain p-shell nucleons, the analytic derivation of the exchange-Coulomb kernel becomes difficult and an approximate procedure may have to be devised in order to make the corresponding resonating-group calculation computationally feasible.

[1]Y. C. Tang, M. LeMere, and D. R. Thompson, Phys. Rep. (to be published); Y. C. Tang, Fizika (Suppl. 3) 9, 91 (1977).

[2]K. Wildermuth and Y. C. Tang, *A Unified Theory of the Nucleus* (Vieweg, Braunschweig, 1977).

[3]For simplicity in presentation, the formulation is given in the case where both clusters have spin zero.

[4]The function $f_i(R)$ used in this case is $R^5\exp(-\alpha R^2)$.

[5]See, for example, the Appendix in a paper by I. Reichstein and Y. C. Tang, Nucl. Phys. A158, 529 (1970).

[6]H. Hutzelmeyer, Ph.D. thesis, Florida State University, 1968 (unpublished).

[7]M. Kamimura and T. Matsuse, Progr. Theor. Phys. 51, 438 (1974).

[8]H. Horiuchi, in Proceedings of the INS-IPCR Symposium on Cluster Structure of Nuclei and Transfer Reactions Induced by Heavy Ions, Tokyo, 1975 [IPCR Cyclotron Progress Report Supplement 4 (unpublished)], p. 685.

[9]L. F. Canto, Nucl. Phys. A279, 97 (1977).

[10]A. C. Butcher and J. M. McNamee, Proc. Phys. Soc. (London) 74, 529 (1959).

[11]D. R. Thompson, M. LeMere, and Y. C. Tang, Nucl. Phys. A286, 53 (1977).

[12]J. A. Koepke, R. E. Brown, Y. C. Tang, and D. R. Thompson, Phys. Rev. C 9, 823 (1974).

[13]M. LeMere and Y. C. Tang, Phys. Rev. C (to be published).

[14]T. Matsuse, M. Kamimura, and Y. Fukushima, Progr. Theor. Phys. 53, 706 (1975).