Resonating-group study of $N + {}^{16}O$ scattering with a generator-coordinate technique*

D. R. Thompson and Y. C. Tang

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

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The scattering of nucleons by ¹⁶O is studied with the resonating-group method. The ¹⁶O wave function used is a translationally invariant antisymmetrized product of single-particle wave functions of $(1 s)^4 (1 p)^{12}$ configuration in a harmonic-oscillator well having an appropriately chosen width parameter. A generatorcoordinate technique is employed to facilitate the computation of the nonlocal interaction between the nucleon and the ¹⁶O nucleus. This technique is discussed in some detail in order to demonstrate its utility in a nuclear problem involving a relatively large number of nucleons. Calculated results are compared with experimental data over a wide range of energies, and it is found that the agreement is in general quite satisfactory. Also, the result shows that in this particular problem the heavy-particle pickup process, which is properly taken into consideration by the use of a totally antisymmetric wave function, has a relatively small contribution.

> NUCLEAR REACTIONS ¹⁶O(N, N); calculated phase shifts, $\sigma(\theta)$, and $P(\theta)$. Resonating-group method with generator-coordinate technique.

I. INTRODUCTION

During the past years, the resonating-group method has been used with remarkable success to study elastic-scattering and reaction processes involving light nuclei.¹⁻³ This method employs a fully antisymmetric many-nucleon wave function and a nucleon-nucleon potential which fits reasonably well the low-energy scattering data, thus eliminating the ambiguities encountered in many phenomenological calculations. However, the explicit inclusion of these microscopic features necessarily means that the resonating-group calculation becomes quite complicated when the number of nucleons involved is large. In fact, it is primarily for this reason that earlier studies have been restricted to systems containing no more than ten nucleons.

Recently, however, a somewhat different computational procedure,⁴ known as the generator-coordinate technique,⁵ has been developed in order to extend the resonating-group method to heavier systems. Using this procedure, Sünkel and Wildermuth⁴ have been able to study the case of α +¹⁶O scattering and obtain rather good agreement with the experimentally observed rotational-band structure of ²⁰Ne and the α +¹⁶O differential scattering cross section.⁶

One of the successes of the investigation of Sünkel and Wildermuth⁴ is that the large backwardangle ($\geq 90^{\circ}$) cross sections observed experimentally are satisfactorily accounted for. This means that exchange processes,⁷ especially the heavyparticle pickup process, are quite important for a proper description of this particular scattering problem. On the other hand, for $p + {}^{40}$ Ca scattering at 30 MeV, where a resonating-group calculation is not yet available but a careful optical-model analysis has been made,⁸ it was found that even with the heavy-particle pickup process not explicitly included the experimental data can be well fitted up to a rather large angle of about 140°. This seems to indicate that the heavy-particle pickup process plays a relatively minor role in this case,⁹ in contrast with the finding from α + ¹⁶O scattering. To resolve this apparent contradiction, we study here the case of N + ¹⁶O scattering¹⁰ with the purpose of investigating further not only the importance of exchange processes but also the utility of the generator-coordinate technique in a rather large system.

A rather detailed description of the resonatinggroup calculation using the generator-coordinate technique is given in Sec. II, while in Sec. III we present and discuss the results of this calculation. As in the α + ¹⁶O case, we find that the agreement with experiment is again fairly satisfactory. Finally, in Sec. IV, we summarize the findings of the present study and mention other resonating-group calculations which are practicable and which will be useful for a better understanding of the importance of exchange effects.

II. FORMULATION

We begin this section with a description of the formulation of the single-channel resonating-group calculation. In particular, we shall indicate why this type of calculation can become rather tedious as the mass number becomes large. The generator-coordinate technique used by Sünkel and Wildermuth⁴ will then be discussed, and it will be shown how its use can significantly reduce the computational difficulty.

If we assume for clarity of discussion that the

nucleon-nucleon interaction is purely central,¹¹ then the wave function for the $p + {}^{16}O$ system can be written as

$$\Psi = \mathbf{\alpha}' [\phi_{16} \alpha(s_{17}) \pi(t_{17}) F(\vec{\mathbf{R}}) \chi(\vec{\mathbf{R}}_{c.m.})] , \qquad (1)$$

where α' is an operator which antisymmetrizes the wave function with respect to the interchange of the incident nucleon and the nucleons in the ¹⁶O cluster, and $\alpha(s_{17})$ and $\pi(t_{17})$ are the spin and isospin functions for the 17th nucleon, respectively. The translationally invariant function ϕ_{16} describes the behavior of the ¹⁶O cluster and is chosen to have the form

$$\phi_{16} = \mathbf{G}_{16} \left(\prod_{i=1}^{m} \left\{ h_i (\vec{\mathbf{r}}_i - \vec{\mathbf{R}}_{16}) \xi_i (s_i, t_i) \right. \\ \left. \times \exp\left[-\frac{1}{2} \alpha (\vec{\mathbf{r}}_i - \vec{\mathbf{R}}_{16})^2 \right] \right\} \right), \qquad (2)$$

where \mathfrak{A}_{16} is an antisymmetrization operator and \vec{R}_{16} denotes the ¹⁶O center-of-mass coordinate given by

$$\vec{\mathbf{R}}_{16} = \frac{1}{m} \sum_{i=1}^{m} \vec{\mathbf{r}}_{i}, \qquad (3)$$

with \vec{r}_i being the spatial coordinate of the *i*th particle and m=16. The functions $h_i(\vec{\eta})$ have the form

$$h_{i}(\hat{\eta}) = Y_{0}^{0}(\hat{\eta}) \quad (i = 1 - 4)$$

= $\eta Y_{1}^{1}(\hat{\eta}) \quad (i = 5 - 8)$
= $\eta Y_{1}^{0}(\hat{\eta}) \quad (i = 9 - 12)$
= $\eta Y_{1}^{-1}(\hat{\eta}) \quad (i = 13 - 16)$, (4)

while the spin-isospin functions $\xi_i(s, t)$ are given by

$$\xi_{i}(s,t) = \alpha(s)\pi(t) \quad (i = 1, 5, 9, 13)$$

$$= \alpha(s)\nu(t) \quad (i = 2, 6, 10, 14)$$

$$= \beta(s)\pi(t) \quad (i = 3, 7, 11, 15)$$

$$= \beta(s)\nu(t) \quad (i = 4, 8, 12, 16) \quad (5)$$

with $\alpha(s)$, $\beta(s)$, $\pi(t)$, and $\nu(t)$ denoting spin-up, spin-down, isospin-up, and isospin-down functions, respectively. The relative motion between the incident nucleon and the ¹⁶O cluster is described by the function $F(\vec{R})$ which is determined by the projection equation

$$\left< \delta \Psi \right| \left(H - E_t \right) \left| \Psi \right> = 0 \quad . \tag{6}$$

In this equation, the Hamiltonian H is given by

$$H = -\frac{\hbar^2}{2M} \sum_{i=1}^{17} \nabla_i^2 + \sum_{i \le j=1}^{17} V_{ij} - T_{c.m.}, \qquad (7)$$

with $T_{c.m.}$ being the total center-of-mass kineticenergy operator. The quantity E_t in Eq. (6) is the total energy of the system, given by

$$E_t = E_{16} + E , (8)$$

where E is the relative energy in the center-ofmass (c.m.) frame, and E_{16} is the internal energy of the ¹⁶O cluster obtained by computing the expectation value of the 16-particle Hamiltonian with respect to the function ϕ_{16} of Eq. (2).

We should mention that, since a translationally invariant Hamiltonian is employed in the calculation, the results do not depend on the motion of the center of mass of the entire system. The choice of the c.m. function $\chi(\vec{R}_{c.m.})$ in Eq. (1) is therefore arbitrary. At this point, we demand only that $\chi(\vec{R}_{c.m.})$ is normalizable. Later, in our discussion of the generator-coordinate technique, we shall choose a particular functional form for $\chi(\vec{R}_{c.m.})$ for computational convenience.

We now discuss briefly the meaning of the projection equation (6). If the function Ψ were not at all restricted, then solving Eq. (6) would, of course, be equivalent to solving exactly the Schrödinger equation for the 17-nucleon system. Since we have, in fact, restricted Ψ to the form given by Eq. (1) with all the freedom contained in the linear variational function $F(\mathbf{R})$ (single-channel approximation), we are only solving the Schrödinger equation in an approximate manner. It should be pointed out, however, that single-channel calculations have already been performed in many other systems and satisfactory results have been obtained. Therefore, we expect that the adoption of this approximation in the present study should also be a reasonable one.

In order to find the equation which the relativemotion function satisfies, we introduce the following parameter representation for $\delta \Psi$ and Ψ :

$$\begin{split} \delta\Psi &= \int \delta F(\vec{\mathbf{R}}') \mathbf{a}' [\phi_{16} \alpha(s_{17}) \pi(t_{17}) \\ &\times \delta(\vec{\mathbf{R}} - \vec{\mathbf{R}}') \chi(\vec{\mathbf{R}}_{c.m})] d \vec{\mathbf{R}}' , \quad (9) \\ \Psi &= \int F(\vec{\mathbf{R}}'') \mathbf{a}' [\phi_{16} \alpha(s_{17}) \pi(t_{17}) \\ &\times \delta(\vec{\mathbf{R}} - \vec{\mathbf{R}}'') \chi(\vec{\mathbf{R}}_{c.m})] d \vec{\mathbf{R}}'' , \quad (10) \end{split}$$

where $\delta F(\vec{\mathbf{R}}')$ represents an arbitrary variation of the function $F(\vec{\mathbf{R}}')$. It should be noted that in these equations, \mathfrak{A}' operates only on functions of the particle coordinates and does not operate on $\delta F(\vec{\mathbf{R}}')$ and $F(\vec{\mathbf{R}}'')$ which depend on the parameter coordinates $\vec{\mathbf{R}}'$ and $\vec{\mathbf{R}}''$. Next, we substitute Eqs. (9) and (10) into Eq. (6) and obtain the equation

$$\int \mathcal{K}(\vec{\mathbf{R}}',\vec{\mathbf{R}}'')F(\vec{\mathbf{R}}'')d\vec{\mathbf{R}}''=0$$
(11)

with $\Re(\vec{R}', \vec{R}'')$ given by

$$\mathcal{K}(\vec{R}',\vec{R}'') = \langle \phi_{16} \alpha(s_{17}) \pi(t_{17}) \delta(\vec{R}-\vec{R}') \chi(\vec{R}_{c.m}) | (H-E_t) | \alpha'[\phi_{16} \alpha(s_{17}) \pi(t_{17}) \delta(\vec{R}-\vec{R}'') \chi(\vec{R}_{c.m})] \rangle.$$
(12)

Equation (11) can be solved for $F(\vec{R}')$ from which scattering phase shifts can be determined. We should remark here that the single-channel approximation can be systematically improved by introducing distortion functions and reaction channels into the calculation, as has been done, for example, in the simpler case of $d + \alpha$ scattering.^{2, 12}

The computation of the kernel function $\mathfrak{K}(\vec{R}',\vec{R}'')$ involves integrations over the cluster coordinates

$$\vec{\eta}_{i} = \vec{r}_{i} - \vec{R}_{16} \quad (i = 1 - 16) ,$$

$$\vec{R} = \vec{R}_{16} - \vec{r}_{17} ,$$

$$\vec{R}_{c.m.} = \frac{1}{17} (16 \vec{R}_{16} + \vec{r}_{17})$$

$$(13)$$

subject to the restriction that

$$\sum_{i=1}^{16} \bar{\eta}_i = 0 .$$
 (14)

Because of the presence of the operator \mathfrak{G}' in Eq. (12) and the fact that a proper treatment of the total c.m. motion causes the appearance of cross terms involving $\overline{\eta}_i \cdot \overline{\eta}_j$ in Ψ , the integration over the cluster coordinates defined above can become very tedious when the number of nucleons is large. The generator-coordinate technique used by Sünkel and Wildermuth⁴ can significantly reduce the computational difficulty, especially if only two clusters are involved. This will be discussed in detail below.

For the application of the generator-coordinate technique, one writes Eq. (1) in the form

$$\Psi = \int F(\vec{\mathbf{R}}_{16}'' - \vec{\mathbf{R}}_{17}'') \chi \left[(16 \,\vec{\mathbf{R}}_{16}'' + \vec{\mathbf{R}}_{17}'') / 17 \right] \mathfrak{C}' \left[\phi_{16}(\vec{\mathbf{R}}_{16}'', \vec{\mathbf{a}}) \alpha(s_{17}) \pi(t_{17}) \delta(\vec{\mathbf{R}}_{16} - \vec{\mathbf{R}}_{16}'') \delta(\vec{\mathbf{r}}_{17} - \vec{\mathbf{R}}_{17}'') \right] d\vec{\mathbf{R}}_{16}'' d\vec{\mathbf{R}}_{17}'' , \qquad (15)$$

where two parameter coordinates \vec{R}_{16}'' and \vec{R}_{17}'' are introduced. In the above equation, the ¹⁶O wave function is written as

$$\phi_{16}(\vec{\mathbf{R}}_{16}'', \hat{\mathbf{a}}) = \mathbf{\mathcal{G}}_{16}\left(\prod_{i=1}^{m} \left\{ h_i(\vec{\mathbf{r}}_i - \vec{\mathbf{R}}_{16}'' + \hat{\mathbf{a}})\xi_i(s_i, t_i) \exp\left[-\frac{1}{2}\alpha(\vec{\mathbf{r}}_i - \vec{\mathbf{R}}_{16}'')^2\right] \right\} \right) .$$
(16)

It should be noted in Eq. (16) that a constant (independent of the particle coordinates \vec{r}_i) vector \vec{a} has been added to the argument of the function h_i . Owing to the presence of the antisymmetrization operator \mathbf{G}_{16} and the fact that we have restricted the 16 nucleons in the ¹⁶O cluster to occupy the lowest single-particle orbitals [see Eq. (4)], the addition of this vector \vec{a} does not affect the behavior of ϕ_{16} in any way and \vec{a} can be chosen arbitrarily.¹³ Here we indicate the existence of this freedom by explicitly including \vec{a} in the argument of ϕ_{16} . Later, we shall make a definite choice of \vec{a} for computational convenience.

We now introduce integral representations for the δ functions appearing in Eq. (15); they are

$$\delta(\vec{R}_{16} - \vec{R}_{16}'') = (1/2\pi)^3 \int \exp[i\vec{q}_1 \cdot (\vec{R}_{16} - \vec{R}_{16}'')] d\vec{q}_1$$
(17)

and

$$\delta(\mathbf{\vec{r}}_{17} - \mathbf{\vec{R}}_{17}'') = (\alpha/4\pi)^3 \int \exp\left[-\frac{1}{2}\alpha(\mathbf{\vec{r}}_{17} - \frac{1}{2}i\mathbf{\vec{S}}'')^2\right] \exp\left[\frac{1}{2}\alpha(\mathbf{\vec{R}}_{17}'' - \frac{1}{2}i\mathbf{\vec{S}}'')\right]^2 d\mathbf{\vec{S}}'' \quad . \tag{18}$$

Using these representations and the definition of \vec{R}_{16} given by Eq. (3), we obtain

$$\Psi = \left(\frac{\alpha}{8\pi^{2}}\right)^{3} \int \mathfrak{a}' \mathfrak{a}_{16} \left[\prod_{i=1}^{m} \left(h_{i} (\vec{\mathbf{r}}_{i} - \vec{\mathbf{R}}_{16}'' + \vec{\mathbf{a}}) \xi_{i} (s_{i}, t_{i}) \exp \left\{ -\frac{1}{2} \alpha \left[\vec{\mathbf{r}}_{i} - \left(\vec{\mathbf{R}}_{16}'' + \frac{i}{m \alpha} \vec{\mathbf{q}}_{1} \right) \right]^{2} \right\} \right) \\ \times \exp \left[-\frac{1}{2} \alpha (\vec{\mathbf{r}}_{17} - \frac{1}{2} i \vec{\mathbf{5}}'')^{2} \right] \alpha (s_{17}) \pi (t_{17}) \right] \\ \times F(\vec{\mathbf{R}}_{16}'' - \vec{\mathbf{R}}_{17}'') \chi \left(\frac{16 \vec{\mathbf{R}}_{16}'' + \vec{\mathbf{R}}_{17}''}{17} \right) \exp \left(-\frac{q_{1}^{2}}{2m \alpha} + \frac{1}{2} \alpha (\vec{\mathbf{R}}_{17}'' - \frac{1}{2} i \vec{\mathbf{5}}'')^{2} \right) d\vec{\mathbf{R}}_{16}'' d\vec{\mathbf{q}}_{1} d\vec{\mathbf{5}}'' \quad .$$
(19)

Under the coordinate transformations given by

$$\vec{R}'' = \vec{R}_{16}'' - \vec{R}_{17}'', \qquad \vec{R}_{c.m.}'' = \frac{1}{17} \left(16 \vec{R}_{16}'' + \vec{R}_{17}'' \right), \qquad \vec{q}_2 = \frac{1}{m\alpha} \vec{q}_1 - i \vec{R}_{16}'' , \qquad (20)$$

Eq. (19) takes the form

$$\Psi = \left(\frac{m\,\alpha^{2}}{8\,\pi^{2}}\right)^{3} \int \mathfrak{G}'\mathfrak{G}_{16} \left(\prod_{i=1}^{m} \left\{h_{i}(\vec{r}_{i}-\vec{a}_{1})\xi_{i}(s_{i},t_{i})\exp\left[-\frac{1}{2}\alpha(\vec{r}_{i}-i\vec{q}_{2})^{2}\right]\right\}\exp\left[-\frac{1}{2}\alpha(\vec{r}_{17}-\frac{1}{2}i\vec{S}'')^{2}\right]\alpha(s_{17})\pi(t_{17})\right) \\ \times \exp\left[-\frac{1}{2}(m\,\alpha)q_{2}^{2}-\frac{1}{8}\alpha S''^{2}+\frac{m\,\alpha}{2(m+1)}\left[\vec{R}''+i(\vec{q}_{2}-\frac{1}{2}\vec{S}'')\right]^{2}+\frac{m\,\alpha}{2(m+1)}(\vec{q}_{2}-\frac{1}{2}\vec{S}'')^{2}\right. \\ \left.-im\,\alpha\vec{R}_{c.m.}''\cdot\left(\vec{q}_{2}+\frac{1}{2m}\,\vec{S}''\right)+\frac{1}{2}(m+1)\alpha\vec{R}_{c.m.}''^{2}\right]\chi(\vec{R}_{c.m.}')F(\vec{R}'')d\vec{R}''d\vec{R}_{c.m.}'d\vec{S}''d\vec{q}_{2},$$
(21)

where we have further defined another constant vector \mathbf{a}_1 by the equation

$$\vec{a} = \vec{R}_{16}'' - \vec{a}_1$$
 (22)

To facilitate the computation, we make use of the fact that the choice of $\chi(\vec{R}''_{c.m.})$ is arbitrary and write

 $\chi(\vec{R}''_{c.m.}) = \exp\left[-\frac{1}{2}(m+1)\alpha \vec{R}''_{c.m.}\right] .$ (23)

With this particular choice for χ , the integration over $\vec{R}''_{c.m.}$ in Eq. (21) yields a factor $[2\pi/(m\alpha)]^{3\delta}(\vec{q}_2 + \vec{S}''/2m)$. After this is done, we can then integrate over \vec{q}_2 to obtain

$$\Psi = \left(\frac{\alpha}{4\pi}\right)^{3} \int \mathfrak{G}'\mathfrak{G}_{16} \left(\prod_{i=1}^{m} \left\{h_{i}(\vec{\mathbf{r}}_{i}-\vec{\mathbf{a}}_{i})\xi_{i}(s_{i},t_{i})\exp\left[-\frac{1}{2}\alpha\left(\vec{\mathbf{r}}_{i}+\frac{i}{2m}\vec{\mathbf{S}}''\right)^{2}\right]\right\} \exp\left[-\frac{1}{2}\alpha\left(\vec{\mathbf{r}}_{17}-\frac{1}{2}i\vec{\mathbf{S}}''\right)^{2}\right]\alpha(s_{17})\pi(t_{17})\right) \\ \times \exp\left[\frac{m\alpha}{2(m+1)}\left(\vec{\mathbf{R}}''+\frac{i(m+1)}{2m}\vec{\mathbf{S}}''\right)^{2}\right]F(\vec{\mathbf{R}}'')d\vec{\mathbf{R}}''d\vec{\mathbf{S}}'' \quad .$$

$$(24)$$

Although Eq. (24) appears more complicated than Eq. (1), it has the distinct advantage that Ψ is now expressed as an integral over an antisymmetrized product of single-particle functions of the particle coordinates \mathbf{r}_i . Consequently, cross terms of the form $\mathbf{r}_i \cdot \mathbf{r}_j$ no longer appear and the computation of $\mathcal{K}(\mathbf{R}', \mathbf{R}'')$ becomes significantly simplified.

Using the same procedure, we may write $\delta \Psi$ as

$$\delta \Psi = \left(\frac{\alpha}{4\pi}\right)^{3} \int \mathfrak{A}' \mathfrak{A}_{16} \left(\prod_{i=1}^{m} \left\{h_{i}(\vec{\mathbf{r}}_{i}-\vec{\mathbf{a}}_{1})\xi_{i}(s_{i},t_{i})\exp\left[-\frac{1}{2}\alpha\left(\vec{\mathbf{r}}_{i}+\frac{i}{2m}\vec{\mathbf{S}}'\right)^{2}\right]\right\} \exp\left[-\frac{1}{2}\alpha(\vec{\mathbf{r}}_{17}-\frac{1}{2}i\vec{\mathbf{S}}')^{2}\right]\alpha(s_{17})\pi(t_{17})\right) \\ \times \exp\left[\frac{m\alpha}{2(m+1)}\left(\vec{\mathbf{R}}'+\frac{i(m+1)}{2m}\vec{\mathbf{S}}'\right)^{2}\right]\delta F(\vec{\mathbf{R}}')d\vec{\mathbf{R}}'d\vec{\mathbf{S}}' \quad .$$

$$(25)$$

With the form for Ψ given by Eq. (24) and that for $\delta \Psi$ given by Eq. (25), the kernel function $\mathcal{K}(\vec{R}', \vec{R}'')$ of Eq. (11) becomes

$$\mathcal{H}\left(\vec{\mathbf{R}}',\vec{\mathbf{R}}''\right) = \left(\frac{\alpha}{4\pi}\right)^{6} \int \exp\left[\frac{m\alpha}{2(m+1)} \left(\vec{\mathbf{R}}' - \frac{i(m+1)}{2m}\vec{\mathbf{S}}'\right)^{2} + \frac{m\alpha}{2(m+1)} \left(\vec{\mathbf{R}}'' + \frac{i(m+1)}{2m}\vec{\mathbf{S}}''\right)^{2}\right] \\ \times \left\langle \prod_{i=1}^{m} \left\{ h_{i}(\vec{\mathbf{r}}_{i} - \vec{\mathbf{a}}_{1})\xi_{i}(s_{i}, t_{i})\exp\left[-\frac{1}{2}\alpha\left(\vec{\mathbf{r}}_{i} + \frac{i}{2m}\vec{\mathbf{S}}'\right)^{2}\right] \right\} \alpha(s_{17})\pi(t_{17})\exp\left[-\frac{1}{2}\alpha\left(\vec{\mathbf{r}}_{17} - \frac{1}{2}i\vec{\mathbf{S}}'\right)^{2}\right] \\ \times \left| (\mathbf{H} - E_{t}) \right| \mathcal{C}^{\prime} \mathcal{C}_{16}\left(\prod_{i=1}^{m} \left\{ h_{i}(\vec{\mathbf{r}}_{i} - \vec{\mathbf{a}}_{1})\xi_{i}(s_{i}, t_{i})\exp\left[-\frac{1}{2}\alpha\left(\vec{\mathbf{r}}_{i} + \frac{i}{2m}\vec{\mathbf{S}}''\right)^{2}\right] \right\} \\ \times \alpha(s_{17})\pi(t_{17})\exp\left[-\frac{1}{2}\alpha(\vec{\mathbf{r}}_{17} - \frac{1}{2}i\vec{\mathbf{S}}'')^{2}\right] \right\rangle d\vec{\mathbf{S}}'d\vec{\mathbf{S}}'' , \qquad (26)$$

where the angular brackets indicate integration over the particle coordinates \vec{r}_i (i = 1-17) and summation over the spin and isospin coordinates s_i and t_i (i = 1-17). We now make the transformation

$$\vec{\rho}_{i} = \vec{r}_{i} + (i/4m)(\vec{S}'' - \vec{S}') \quad (i = 1 - 17)$$
(27)

and choose

$$\vec{a}_1 = (i/4m)(\vec{S}' - \vec{S}'')$$
 (28)

Then, after some algebraic manipulation, Eq. (26) can be written as

$$\Im \left(\vec{\mathbf{R}}',\vec{\mathbf{R}}''\right) = \left(\frac{\alpha}{4\pi}\right)^{6} \int \exp\left[\frac{m\alpha}{2(m+1)} \left(\vec{\mathbf{R}}'-\frac{i(m+1)}{2m}\vec{\mathbf{S}}'\right)^{2} + \frac{m\alpha}{2(m+1)} \left(\vec{\mathbf{R}}''+\frac{i(m+1)}{2m}\vec{\mathbf{S}}''\right)^{2}\right] \Re \left(\vec{\mathbf{S}}',\vec{\mathbf{S}}''\right) d\vec{\mathbf{S}}' d\vec{\mathbf{S}}'' \quad , \tag{29}$$

where

$$\mathfrak{M}(\mathbf{\tilde{S}}', \mathbf{\tilde{S}}'') = \left\langle \prod_{i=1}^{m} \left\{ h_{i}(\mathbf{\tilde{\rho}}_{i})\xi_{i}(s_{i}, t_{i})\exp\left[-\frac{1}{2}\alpha\left(\mathbf{\tilde{\rho}}_{i} + \frac{i}{4m}\left(\mathbf{\tilde{S}}' + \mathbf{\tilde{S}}''\right)\right)^{2}\right] \right\} \alpha(s_{17})\pi(t_{17}) \\ \times \exp\left[-\frac{1}{2}\alpha\left(\mathbf{\tilde{\rho}}_{17} - \frac{i}{4m}\left[(2m+1)\mathbf{\tilde{S}}' - \mathbf{\tilde{S}}''\right]\right)^{2}\right] \\ \times \left| (H - E_{i}) \right| \alpha' \alpha_{16} \left(\prod_{i=1}^{m} \left\{ h_{i}(\mathbf{\tilde{\rho}}_{i})\xi_{i}(s_{i}, t_{i})\exp\left[-\frac{1}{2}\alpha\left(\mathbf{\tilde{\rho}}_{i} + \frac{i}{4m}\left(\mathbf{\tilde{S}}' + \mathbf{\tilde{S}}''\right)\right)^{2}\right] \right\} \\ \times \alpha(s_{17})\pi(t_{17})\exp\left[-\frac{1}{2}\alpha\left(\mathbf{\tilde{\rho}}_{17} - \frac{i}{4m}\left[(2m+1)\mathbf{\tilde{S}}'' - \mathbf{\tilde{S}}'\right]\right)^{2}\right] \right) \right\rangle.$$
(30)

In evaluating the quantity $\mathfrak{M}(\mathbf{\ddot{S}}',\mathbf{\ddot{S}}'')$, it is useful to observe that

$$\left\langle h_{i}(\vec{\rho})\xi_{i}(s,t)\exp\left[-\frac{1}{2}\alpha\left(\vec{\rho}+\frac{i}{4m}\left(\vec{S}'+\vec{S}''\right)\right)^{2}\right] \middle| h_{j}(\vec{\rho})\xi_{j}(s,t)\exp\left[-\frac{1}{2}\alpha\left(\vec{\rho}+\frac{i}{4m}\left(\vec{S}'+\vec{S}''\right)\right)^{2}\right] \right\rangle$$

$$= \begin{cases} \frac{1}{4\pi}\left(\frac{\pi}{\alpha}\right)^{3/2}\exp\left(\frac{\alpha}{16m^{2}}\left(\vec{S}'+\vec{S}''\right)^{2}\right)\delta_{ij} & (i=1-4; \ j=1-16) \\ \frac{1}{4\pi}\left(\frac{\pi}{\alpha}\right)^{3/2}\left(\frac{3}{2\alpha}\right)\exp\left(\frac{\alpha}{16m^{2}}\left(\vec{S}'+\vec{S}''\right)^{2}\right)\delta_{ij} & (i=5-16; \ j=1-16) . \end{cases}$$
(31)

The presence of this orthogonality relation means that $\mathfrak{M}(\vec{s}', \vec{s}'')$ is rather similar to matrix elements encountered in oscillator-shell-model calculations, and many of the well known shell-model techniques may be used to facilitate its evaluation.

In order to illustrate briefly the procedure for evaluating $\mathcal{K}(\vec{R}',\vec{R}'')$ we consider here the normalization term $\mathcal{K}^{N}(\vec{R}',\vec{R}'')$. This term has a form similar to Eq. (29) but with $\mathfrak{M}(\vec{S}',\vec{S}'')$ replaced by $\mathfrak{M}^{N}(\vec{S}',\vec{S}'')$, which contains a unity operator instead of the operator $(H - E_t)$ as in Eq. (30). After summing over spin and isospin coordinates, we obtain

$$\mathfrak{M}^{N}(\mathbf{\ddot{S}}',\mathbf{\ddot{S}}'') = \int \prod_{i=1}^{m} \left\{ h_{i}^{*}(\vec{\rho}_{i}) \exp\left[-\frac{1}{2} \alpha \left(\vec{\rho}_{i} - \frac{i}{4m} \left(\mathbf{\ddot{S}}' + \mathbf{\ddot{S}}''\right)\right)^{2}\right] \right\} \exp\left[-\frac{1}{2} \alpha \left(\vec{\rho}_{17} + \frac{i}{4m} \left[(2m+1)\mathbf{\ddot{S}}' - \mathbf{\ddot{S}}''\right]\right)^{2}\right] \\ \times (1 - P_{1,17}^{\rho} - P_{5,17}^{\rho} - P_{9,17}^{\rho} - P_{13,17}^{\rho}) \left(\prod_{i=1}^{m} \left\{h_{i}(\vec{\rho}_{i}) \exp\left[-\frac{1}{2} \alpha \left(\vec{\rho}_{i} + \frac{i}{4m} \left(\mathbf{\ddot{S}}' + \mathbf{\ddot{S}}''\right)\right)^{2}\right]\right\} \\ \times \exp\left[-\frac{1}{2} \alpha \left(\vec{\rho}_{17} - \frac{i}{4m} \left[(2m+1)\mathbf{\ddot{S}}'' - \mathbf{\ddot{S}}'\right]\right)^{2}\right] \right) d\tau ,$$
(32)

where $P_{i,j}^{\rho}$ is an operator which interchanges the spatial coordinates $\bar{\rho}_i$ and $\bar{\rho}_j$, and $d\tau$ signifies the integration over all the coordinates $\bar{\rho}_i$ (i = 1-17). The no-exchange term in $\mathfrak{M}^{N}(\mathbf{\tilde{S}}', \mathbf{\tilde{S}}'')$ is given by

$$\mathfrak{M}_{0}^{N}(\mathbf{\ddot{S}}',\mathbf{\ddot{S}}'') = \int \prod_{i=1}^{m} \left[|h_{i}(\mathbf{\ddot{\rho}}_{i})|^{2} \exp(-\alpha \rho_{i}^{2}) \right] \exp\left[-\alpha \left(\mathbf{\ddot{\rho}}_{17} + i \, \frac{m+1}{4m} \, (\mathbf{\ddot{S}}' - \mathbf{\ddot{S}}'') \right)^{2} \right] \exp\left(\frac{\alpha (m+1)}{16 \, m} \, (\mathbf{\ddot{S}}' + \mathbf{\ddot{S}}'')^{2} \right) d\tau$$

$$= \left(\frac{1}{4\pi} \right)^{16} \left(\frac{\pi}{\alpha} \right)^{51/2} \left(\frac{3}{2\alpha} \right)^{12} \exp\left(\frac{\alpha (m+1)}{16m} \, (\mathbf{\ddot{S}}' + \mathbf{\ddot{S}}'')^{2} \right) . \tag{33}$$

The term arising from the $P_{1,17}^{\rho}$ exchange is slightly more complicated; it has the form

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$$\begin{split} \mathfrak{M}_{1,17}^{N}(\mathbf{\ddot{5}}',\mathbf{\ddot{5}}'') &= \int \prod_{i=2}^{m} \left[|h_{i}(\mathbf{\ddot{\rho}}_{i})|^{2} \exp\left(-\alpha\rho_{i}^{2}\right) \right] h_{1}^{*}(\mathbf{\ddot{\rho}}_{1}) \exp\left[-\frac{1}{2}\alpha\left(\mathbf{\ddot{\rho}}_{1}-\frac{i}{4m}\left(\mathbf{\ddot{5}}'+\mathbf{\ddot{5}}''\right)\right)^{2}\right] \\ &\quad \times \exp\left[-\frac{1}{2}\alpha\left(\mathbf{\ddot{\rho}}_{17}+\frac{i}{4m}\left[(2m+1)\mathbf{\ddot{5}}'-\mathbf{\ddot{5}}''\right]\right)^{2}\right] h_{1}(\mathbf{\ddot{\rho}}_{17}) \exp\left[-\frac{1}{2}\alpha\left(\mathbf{\ddot{\rho}}_{17}+\frac{i}{4m}\left(\mathbf{\ddot{5}}'+\mathbf{\ddot{5}}''\right)\right)^{2}\right] \\ &\quad \times \exp\left[-\frac{1}{2}\alpha\left(\mathbf{\ddot{\rho}}_{1}-\frac{i}{4m}\left[(2m+1)\mathbf{\ddot{5}}''-\mathbf{\ddot{5}}'\right]\right)^{2}\right] \exp\left(\frac{\alpha(m-1)}{16m^{2}}\left(\mathbf{\ddot{5}}'+\mathbf{\ddot{5}}''\right)^{2}\right) d\tau \\ &= \left(\frac{1}{4\pi}\right)^{15} \left(\frac{\pi}{\alpha}\right)^{45/2} \left(\frac{3}{2\alpha}\right)^{12} \int \exp\left[-\alpha\left(\mathbf{\ddot{\rho}}_{1}-\frac{i(m+1)}{4m}\mathbf{\ddot{5}}'\right)^{2}\right] \\ &\quad \times \exp\left[-\alpha\left(\mathbf{\ddot{\rho}}_{17}+\frac{i(m+1)}{4m}\mathbf{\ddot{5}}'\right)^{2}\right] \\ &\quad \times \exp\left[-\alpha\left(\mathbf{\ddot{\rho}}_{17}+\frac{i(m+1)}{4m}\mathbf{\ddot{5}}'\right)^{2}\right] \\ &\quad = \left(\frac{1}{4\pi}\right)^{16} \left(\frac{\pi}{\alpha}\right)^{51/2} \left(\frac{3}{2\alpha}\right)^{12} \exp\left(\frac{\alpha(m+1)}{16m^{2}}\left[m(\mathbf{\ddot{5}}'^{2}+\mathbf{\ddot{5}}''^{2})-2\mathbf{\ddot{5}}'\cdot\mathbf{\ddot{5}}''\right]\right) d\mathbf{\ddot{\rho}}_{1}d\mathbf{\vec{\rho}}_{17} \end{split}$$
(34)

Similarly, the $P_{5,17}^{\rho}$ exchange term is

$$\mathfrak{M}_{5,17}^{N}(\mathbf{\ddot{S}}',\mathbf{\ddot{S}}'') = \left(\frac{1}{4\pi}\right)^{15} \left(\frac{\pi}{\alpha}\right)^{45/2} \left(\frac{3}{2\alpha}\right)^{11} \int \rho_{5} Y_{1}^{1*}(\hat{\rho}_{5}) \exp\left[-\alpha \left(\overline{\dot{\rho}_{5}} - \frac{i\left(m+1\right)}{4m},\mathbf{\ddot{S}}''\right)^{2}\right] \rho_{17} Y_{1}^{1}(\hat{\rho}_{17}) \\ \times \exp\left[-\alpha \left(\overline{\dot{\rho}_{17}} + \frac{i\left(m+1\right)}{4m},\mathbf{\ddot{S}}'\right)^{2}\right] \\ \times \exp\left(\frac{\alpha(m+1)}{16m^{2}} \left[m(\mathbf{\ddot{S}}'^{2} + \mathbf{\ddot{S}}''^{2}) - 2\mathbf{\ddot{S}}'\cdot\mathbf{\ddot{S}}''\right]\right) d\dot{\rho}_{5} d\dot{\rho}_{17} \\ = \left(\frac{1}{4\pi}\right)^{15} \left(\frac{\pi}{\alpha}\right)^{51/2} \left(\frac{3}{2\alpha}\right)^{11} \left(\frac{m+1}{4m}\right)^{2} \mathbf{S}' \mathbf{S}'' Y_{1}^{1*}(\mathbf{\ddot{S}}') \exp\left(\frac{\alpha(m+1)}{16m^{2}} \left[m(\mathbf{\ddot{S}}'^{2} + \mathbf{\ddot{S}}''^{2}) - 2\mathbf{\ddot{S}}'\cdot\mathbf{\ddot{S}}''\right]\right).$$

$$(35)$$

The $P_{9,17}^{\rho}$ and $P_{13,17}^{\rho}$ exchange terms are given by Eq. (35) but with $Y_1^{1*}(\hat{S}'')Y_1^{1}(\hat{S}')$ replaced by $Y_1^{0*}(\hat{S}'')Y_1^{0}(\hat{S}')$ and $Y_1^{-1*}(\hat{S}'')Y_1^{-1}(\hat{S})$, respectively. Now, by using the spherical-harmonic addition theorem, we can combine these latter three terms to give

$$\mathfrak{M}_{p,17}^{N}(\mathbf{\ddot{S}}',\mathbf{\ddot{S}}'') = \mathfrak{M}_{\mathbf{\bar{S}},17}^{N}(\mathbf{\ddot{S}}',\mathbf{\ddot{S}}'') + \mathfrak{M}_{9,17}^{N}(\mathbf{\ddot{S}}',\mathbf{\ddot{S}}'') + \mathfrak{M}_{13,17}^{N}(\mathbf{\ddot{S}}',\mathbf{\ddot{S}}'') \\ = \left(\frac{1}{4\pi}\right)^{16} \left(\frac{\pi}{\alpha}\right)^{51/2} \left(\frac{3}{2\alpha}\right)^{11} \frac{3(m+1)^{2}}{16m^{2}} \mathbf{\ddot{S}}' \cdot \mathbf{\ddot{S}}'' \exp\left(\frac{\alpha(m+1)}{16m^{2}} \left[m(\mathbf{\ddot{S}}'^{2}+\mathbf{\ddot{S}}''^{2})-2\mathbf{\ddot{S}}'\cdot\mathbf{\ddot{S}}''\right]\right).$$
(36)

The resultant expression for $\mathfrak{M}^{N}(\dot{\mathbf{S}}',\dot{\mathbf{S}}'')$ can now be used to calculate the normalization kernel $\mathfrak{K}^{N}(\dot{\mathbf{R}}',\dot{\mathbf{R}}'')$. The no-exchange term is given by

$$\mathfrak{K}_{0}^{N}(\vec{\mathsf{R}}',\vec{\mathsf{R}}'') = \left(\frac{\alpha}{4\pi}\right)^{6} \int \exp\left[\frac{m\alpha}{2(m+1)} \left(\vec{\mathsf{R}}' - \frac{i(m+1)}{2m}\vec{\mathsf{S}}'\right)^{2} + \frac{m\alpha}{2(m+1)} \left(\vec{\mathsf{R}}'' + \frac{i(m+1)}{2m}\vec{\mathsf{S}}''\right)^{2}\right] \mathfrak{M}_{0}^{N}(\vec{\mathsf{S}}',\vec{\mathsf{S}}'') d\vec{\mathsf{S}}' d\vec{\mathsf{S}}''. \tag{37}$$

To facilitate the evaluation of $\mathcal{K}_{0}^{N}(\vec{R}',\vec{R}'')$, we define

$$\dot{u} = \dot{S}' - \dot{S}'', \quad \dot{v} = \frac{1}{2} (\dot{S}' + \dot{S}'') .$$
 (38)

Substituting into Eq. (37) then yields

$$\mathcal{K}_{0}^{N}(\vec{\mathbf{R}}',\vec{\mathbf{R}}'') = \left(\frac{\alpha}{4\pi}\right)^{6} \left(\frac{1}{4\pi}\right)^{16} \left(\frac{\pi}{\alpha}\right)^{51/2} \left(\frac{3}{2\alpha}\right)^{12} \int \exp\left[-\frac{\alpha(m+1)}{16m} \left(\vec{\mathbf{u}} + \frac{i2m}{m+1} \left(\vec{\mathbf{R}}' + \vec{\mathbf{R}}''\right)\right)^{2} - \frac{\alpha i}{2} \vec{\mathbf{v}} \cdot \left(\vec{\mathbf{R}}' - \vec{\mathbf{R}}''\right) + \frac{m\alpha}{4(m+1)} \left(\vec{\mathbf{R}}' - \vec{\mathbf{R}}''\right)^{2}\right] d\vec{\mathbf{u}} d\vec{\mathbf{v}}$$
$$= \left(\frac{\alpha}{4\pi}\right)^{3} \left(\frac{1}{4\pi}\right)^{16} \left(\frac{\pi}{\alpha}\right)^{51/2} \left(\frac{3}{2\alpha}\right)^{12} \left(\frac{16m\pi}{\alpha(m+1)}\right)^{3/2} \delta(\vec{\mathbf{R}}' - \vec{\mathbf{R}}''). \tag{39}$$

In a similar manner, we obtain

$$\begin{aligned} \mathfrak{K}_{1,17}^{N}\left(\vec{\mathbf{R}}',\vec{\mathbf{R}}''\right) &= \left(\frac{\alpha}{4\pi}\right)^{6} \left(\frac{1}{4\pi}\right)^{16} \left(\frac{\pi}{\alpha}\right)^{51/2} \left(\frac{3}{2\alpha}\right)^{12} \\ &\times \int \exp\left[-\frac{\alpha(m+1)^{2}}{8m^{2}} \left(\vec{\mathbf{v}} + \frac{2m^{2}i}{(m+1)^{2}} \left(\vec{\mathbf{R}}' - \vec{\mathbf{R}}''\right)\right)^{2} - \frac{\alpha(m^{2}-1)}{32m^{2}} \left(\vec{\mathbf{u}} + \frac{4im^{2}}{m^{2}-1} \left(\vec{\mathbf{R}}' + \vec{\mathbf{R}}''\right)\right)^{2} \\ &- \frac{m^{2}\alpha}{2(m+1)^{2}} \left(\vec{\mathbf{R}}' - \vec{\mathbf{R}}''\right)^{2} - \frac{m^{2}\alpha}{2(m^{2}-1)} \left(\vec{\mathbf{R}}' + \vec{\mathbf{R}}''\right)^{2} + \frac{m\alpha}{2(m+1)} \left(R'^{2} + R''^{2}\right)\right] d\vec{\mathbf{u}} d\vec{\mathbf{v}} \\ &= \left(\frac{\alpha}{4\pi}\right)^{6} \left(\frac{1}{4\pi}\right)^{16} \left(\frac{\pi}{\alpha}\right)^{51/2} \left(\frac{3}{2\alpha}\right)^{12} \left(\frac{8m^{2}\pi}{\alpha(m+1)^{2}}\right)^{3/2} \left(\frac{32m^{2}\pi}{\alpha(m^{2}-1)}\right)^{3/2} \\ &\times \exp\left(-\frac{m(m^{2}+1)\alpha}{2(m+1)^{2}(m-1)} \left(R'^{2} + R''^{2}\right) - \frac{2m^{2}\alpha}{(m+1)^{2}(m-1)} \vec{\mathbf{R}}' \cdot \vec{\mathbf{R}}''\right), \end{aligned} \tag{40}$$

where the transformation of Eq. (38) has again been used. Finally, the *p*-shell exchange term is

$$\begin{split} \mathfrak{R} \mathcal{C}_{p,17}^{N}(\vec{\mathbf{R}}',\vec{\mathbf{R}}'') &= \left(\frac{\alpha}{4\pi}\right)^{6} \left(\frac{1}{4\pi}\right)^{16} \left(\frac{\pi}{\alpha}\right)^{51/2} \left(\frac{3}{2\alpha}\right)^{11} \frac{3(m+1)^{2}}{16m^{2}} \\ &\times \int \frac{1}{4} (4v^{2} - u^{2}) \exp\left[-\frac{\alpha(m+1)^{2}}{8m^{2}} \left(\vec{\mathbf{v}} + \frac{2m^{2}i}{(m+1)^{2}} \left(\vec{\mathbf{R}}' - \vec{\mathbf{R}}''\right)\right)^{2} - \frac{\alpha(m^{2} - 1)}{32m^{2}} \left(\vec{\mathbf{u}} + \frac{4im^{2}}{m^{2} - 1} \left(\vec{\mathbf{R}}' + \vec{\mathbf{R}}''\right)\right)^{2} \\ &- \frac{m^{2}\alpha}{2(m+1)^{2}} \left(\vec{\mathbf{R}}' - \vec{\mathbf{R}}''\right)^{2} - \frac{m^{2}\alpha}{2(m^{2} - 1)} \left(\vec{\mathbf{R}}' + \vec{\mathbf{R}}''\right)^{2} + \frac{m\alpha}{2(m+1)} \left(R'^{2} + R''^{2}\right)\right] d\vec{\mathbf{u}} d\vec{\mathbf{v}} \\ &= \left(\frac{\alpha}{4\pi}\right)^{6} \left(\frac{1}{4\pi}\right)^{16} \left(\frac{\pi}{\alpha}\right)^{51/2} \left(\frac{3}{2\alpha}\right)^{11} \left(\frac{8m^{2}\pi}{\alpha(m+1)^{2}}\right)^{3/2} \left(\frac{32m^{2}\pi}{\alpha(m^{2} - 1)}\right)^{3/2} \\ &\times \left(\frac{3m^{2}}{4(m-1)^{2}} \left(\vec{\mathbf{R}}' + \vec{\mathbf{R}}''\right)^{2} - \frac{3m^{2}}{4(m+1)^{2}} \left(\vec{\mathbf{R}}' - \vec{\mathbf{R}}''\right)^{2} - \frac{9}{2(m-1)\alpha}\right) \\ &\times \exp\left(-\frac{m(m^{2} + 1)\alpha}{2(m+1)^{2}(m-1)} \left(R'^{2} + R''^{2}\right) - \frac{2m^{2}\alpha}{(m+1)^{2}(m-1)} \vec{\mathbf{R}}' \cdot \vec{\mathbf{R}}''\right). \end{split}$$

The procedure for evaluating the potential-energy and kinetic-energy terms in $\mathcal{K}(\vec{R}',\vec{R}'')$ is similar to that described above for the normalization term, although more exchange terms are involved and the derivation is somewhat more complicated.

The computation of $\mathfrak{K}(\vec{\mathbf{R}}',\vec{\mathbf{R}}'')$ is quite tedious, but there is a simple way to test whether or not the resultant expression is correct. This is known as the redundant-solution test and is described in detail elsewhere.¹⁴ Briefly, the basis for this test is that the antisymmetric function

$$\Psi_{R} = \mathbf{G}'[\phi_{16}\alpha(s_{17})\pi(t_{17})F_{R}(\vec{R})\chi(\vec{R}_{c.m.})], \qquad (42)$$

where

$$\boldsymbol{F}_{R}(\vec{\mathbf{R}}) = c_{0} \frac{f_{0}(R)}{R} \boldsymbol{P}_{0}(\cos\theta) + c_{1} \frac{f_{1}(R)}{R} \boldsymbol{P}_{1}(\cos\theta)$$
(43)

with

$$f_0(R) = R \exp\left(-\frac{m\alpha}{2(m+1)}R^2\right) ,$$

$$f_1(R) = R^2 \exp\left(-\frac{m\alpha}{2(m+1)}R^2\right) ,$$
(44)

and c_0 and c_1 being arbitrary constants, is identically equal to zero. This means that Ψ_R is a trivial solution of Eq. (6); therefore, $F_R(\vec{R}'')$ must satisfy Eq. (11) if $\mathcal{K}(\vec{R}',\vec{R}'')$ has been derived cor-

rectly.

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This concludes our discussion of the application of the generator-coordinate technique to resonatinggroup calculations. We should mention that, although this discussion deals specifically with the case of $p + {}^{16}\text{O}$ elastic scattering, the generatorcoordinate technique in conjunction with the resonating-group method can also be used, with relatively minor modifications to the procedure outlined above, to study scattering and reaction problems involving two composite nuclei.

III. RESULTS

In this section, we discuss the results of an N + ¹⁶O calculation in which the procedure discussed in Sec. II is used. Since we intend to examine both differential cross-section and polarization data for N + ¹⁶O scattering, the nucleon-nucleon potential employed must contain a noncentral component. In this calculation, we choose to use a nucleonnucleon potential which has the same form as that used in a previous study of N + α scattering, ¹⁵ i.e.,

$$V_{ij} = \left[\frac{1}{2}(1+P_{ij}^{\sigma})V_{t} + \frac{1}{2}(1-P_{ij}^{\sigma})V_{s}\right] \left[\frac{1}{2}u + \frac{1}{2}(2-u)P_{ij}^{r}\right] \\ - \frac{1}{2\hbar}V_{\lambda} \exp\left[-\lambda(\vec{r}_{i}-\vec{r}_{j})^{2}\right](\vec{\sigma}_{i}+\vec{\sigma}_{j}) \cdot (\vec{r}_{i}-\vec{r}_{j}) \times (\vec{p}_{i}-\vec{p}_{j}) + \frac{e^{2}}{4|\vec{r}_{i}-\vec{r}_{j}|}(1+\tau_{iz})(1+\tau_{jz}).$$
(45)

In the above equation, V_t and V_s are, respectively, the s-wave triplet and singlet potentials which yield correct values for the two-nucleon effective-range parameters; they are given by

$$V_{t} = -V_{0t} \exp[-\kappa_{t}(\vec{r}_{i} - \vec{r}_{j})^{2}], \quad V_{s} = -V_{0s} \exp[-\kappa_{s}(\vec{r}_{i} - \vec{r}_{j})^{2}]$$
(46)

with

$$V_{ot} = 66.92 \text{ MeV}, \quad \kappa_t = 0.415 \text{ fm}^{-2}, \qquad V_{os} = 29.05 \text{ MeV}, \quad \kappa_s = 0.292 \text{ fm}^{-2}. \tag{47}$$

The choice of the parameters u, V_{λ} , and λ will be discussed below.

Since the potential V_{ij} has a noncentral component, we write the wave function as

$$\Psi = \mathbf{a}' \left(\phi_{16} \pi(t_{17}) \sum_{J=1/2}^{\infty} \sum_{l=J-1/2}^{J+1/2} \frac{1}{R} f_{Jl}(R) \mathcal{Y}_{Jl1/2}^{1/2}(\hat{R}, s_{17}) \chi(\vec{R}_{c.m.}) \right), \tag{48}$$

where $\mathcal{Y}_{JI_{1/2}}^{1/2}(\hat{R}, s_{17})$ is a normalized spin-angle function. The width parameter α in ϕ_{16} [see Eq. (2)] is chosen to yield the experimentally determined rms matter radius for ¹⁶O; its value is given by

$$\alpha = 0.32 \text{ fm}^{-2}$$
.

(49)

which corresponds to an rms radius of 2.6 fm. Also, we mention again that the procedure discussed in Sec. II can be extended in a straightforward way to include the case where Ψ is written in the form given by Eq. (48).

Using the wave function Ψ given by Eq. (48) and the nucleon-nucleon potential V_{ij} given by Eq. (45), we obtain the following integrodifferential equation for the function $f_{JI}(R')$:

$$\left[\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dR'^2} - \frac{l(l+1)}{R'^2}\right) + E - V_{\rm D}(R') - \eta_{Jl}V_{\rm so}(R') - V_{\rm C}(R')\right]f_{Jl}(R') = \int_0^\infty k_l(R',R'')f_{Jl}(R'')dR'', \tag{50}$$

where $V_{\rm D}(R')$, $V_{\rm so}(R')$, and $V_{\rm C}(R')$ are the direct nuclear central, the direct spin-orbit, and the direct Coulomb potentials, respectively. These potentials are given along with the kernel function $k_1(R', R'')$ in the Appendix. The quantity η_{JI} is given by

$$\eta_{l+1/2, l} = l, \quad \eta_{l-1/2, l} = -(l+1), \quad \eta_{1/2, 0} = 0.$$
(51)

In computing the Coulomb contribution, we have for simplicity omitted the exchange term by setting α' as unity in Eq. (48). As for the spin-orbit contribution, it is noted from a previous $N + \alpha$ calculation¹⁵ that the exchange term is not negligible compared to the direct term. In the present study, we have not computed the spin-orbit exchange term explicitly, but rather we have simply taken it crudely into account by adjusting the strength of $V_{so}(R')$. Based on the findings of our $N + \alpha$ investigation,¹⁵ this is not an unreasonable procedure. Furthermore, it was also found in the $N + \alpha$ calculation¹⁵ that the results were not sensitive to the value of the spin-orbit range parameter λ as long as this parameter was not chosen to have a very small value. Therefore, we have further simplified the present calculation by letting λ approach infinity. In this limit, the spin-orbit potential V_{so} is then characterized by a single quantity $V_{\lambda}\lambda^{-5/2}$ [see Eq. (A4) in the Appendix].

In order to determine the value of the exchangemixture parameter u in the nucleon-nucleon potential of Eq. (45), we solve Eq. (50) with bound-state boundary conditions for $f_{1/2,0}(R')$ and adjust uuntil the calculation yields the experimental value of 3.26 MeV¹⁶ for the separation energy of the first $J^{\pi} = \frac{1}{2}^+$ excited state in ¹⁷O. The resultant value of u is 0.825, which is fairly close to the value required in the case of $\alpha + \alpha$ scattering.¹⁷

With the value of u determined as explained above, we next choose the strength $V_{\lambda}\lambda^{-5/2}$ of the spin-orbit potential to be equal to 48 MeV fm⁵. With this value, the calculation yields reasonable magnitudes for the p +¹⁶O polarization in the energy region between 30 and 50 MeV, and also a value of 4.50 MeV for the splitting between the $\frac{5}{2}^+$ ground state and the first $\frac{3}{2}^+$ excited state in ¹⁷O. This latter value compares quite favorably with the experimental value of about 5 MeV.¹⁶

Our calculation yields separation energies of 4.00, 3.26, and -0.50 MeV, respectively, for the lowest $\frac{5}{2}^+$, $\frac{1}{2}^+$, and $\frac{3}{2}^+$ states in ¹⁷O. The fact that the positions of the $\frac{5}{2}^+$ and $\frac{3}{2}^+$ states relative to the $\frac{1}{2}^+$ state agree quite well with experiment means that the structure of the ground-state rotational band is given correctly. Also, in Fig. 1 we show



FIG. 1. Calculated phase shifts for $n + {}^{16}\text{O}$ scattering. The symbols δ_1^+ and δ_1^- denote phase shifts in states with $J = l + \frac{1}{2}$ and $J = l - \frac{1}{2}$, respectively.

the calculated $n + {}^{16}$ O phase shifts as a function of the c.m. energy. Here one sees that the $\frac{3}{2}^+$ state appears as a narrow resonance in the δ_2^- phase shift. In addition, it should be noted that the calculation yields fairly broad l=3 resonances. Quite clearly, these resonances will have a significant effect on the behavior of the elastic scattering in the energy region between about 10 and 30 MeV.

We have examined $n + {}^{16}O$ elastic scattering at various energies below the $\alpha + {}^{13}C$ threshold at E =2.21 MeV.¹⁶ There are several excited states in this energy region in ¹⁷O. Except for the first $\frac{3}{2}^+$ state, all the other states in this region cannot be adequately described by a neutron plus an ¹⁶O (ground state) cluster configuration. Therefore, only energies at which no sharp levels exist have been chosen for this examination. For example, such an energy is E = 1.647 MeV, and a comparison of the calculated and experimental¹⁸ differential cross sections is shown in Fig. 2. It is seen from this figure that the agreement is indeed quite satisfactory. Also, we have computed total cross sections at several other such energies in this region, and we find again that the agreement with experiment¹⁹ is good.

For energies above reaction thresholds we account for reaction effects in an approximate manner by the addition of a phenomenological imaginary potential W(R') into our resonating-group formulalation. In other words, we replace $V_D(R')$ in Eq. (50) by $V_D(R') + iW(R')$. At energies of 28.33, 37.4, and 46.57 MeV, the imaginary potentials used are simply those determined by van Oers and Cameron²⁰ from an optical-model analysis of p+¹⁶O scattering, and no further adjustment is made. In Figs. 3 and 4 the calculated differential cross sections and polarizations at these energies



FIG. 2. Comparison of calculated and experimental differential cross sections for $n+{}^{16}O$ scattering at an energy of 1.647 MeV.

are shown by solid curves, while the experimental data²¹⁻²⁵ are represented by solid circles. From these figures one can see that the agreement at 28.33 MeV is noticeably worse than that at the two higher energies. A probable reason for this is that at 28.33 MeV the excitation of the compound system is still low enough such that the influence of individual compound-nucleus resonances remains important at particular energies.²⁴ On the other hand, at 37.4 and 46.57 MeV, it is seen that the agreement is fairly good for angles up to about 130°. Beyond 130°, the calculation does correctly predict a rise in the cross section, but a detailed agreement is not obtained.

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To understand the cause of this discrepancy at large angles, we have made a careful examination of the behavior of the kernel function $k_l(R', R'')$ in Eq. (50). The results of this examination indicate that the contribution to the scattering amplitude at backward angles from the heavy-particle pickup process⁷ is not only relatively small, but also similar to that from direct processes. Therefore, because of the interference between direct and exchange processes, even minor deficiencies in the calculation can cause the observed discrepancy in the backward angular region.

In an optical-model study of $p + {}^{40}Ca$ scattering,³ it was found that the incorporation of an odd-even orbital angular-momentum dependence into the imaginary potential can significantly improve the agreement with experiment at backward angles. To see if a similar feature might also be required here, we have made a calculation in which W(R')is multiplied by a factor $[1+C_{I}(-1)^{i}]$. The results obtained with C_I equal to 0.2, 0.03, and 0.01 at 28.33, 37.4, and 46.57 MeV, respectively, are shown by the dashed curves in Figs. 3 and 4. As expected, the inclusion of this odd-even dependence has little effect on the forward-angle cross sections, but does have significant influence at backward angles. This indicates that the behavior in the large-angle region is determined by a coherent admixture of small amplitudes and a proper description of the scattering in this angular region is



FIG. 3. Comparison of calculated and experimental differential cross sections for $p + {}^{16}$ O scattering at energies of 28.33, 37.4, and 46.57 MeV.



FIG. 4. Comparison of calculated and experimental polarizations for $p + {}^{16}$ O scattering at energies of 28.33, 37.4, and 46.57 MeV.

rather difficult.

We have also examined $n + {}^{16}O$ scattering at E =14.04 MeV. As mentioned above, it is expected that compound-nucleus effects can be important at this energy. However, one can see from Fig. 9 of Ref. 19 that the $n + {}^{16}O$ total cross section does vary smoothly with energy in the energy region around 14 MeV. Thus, the use of an imaginary potential to account for open reaction channels should yield reasonable results. At 14.04 MeV, we have adopted the pure-surface form factor for W(R') used by van Oers and Cameron²⁰ at 28.33 MeV and adjusted the strength (no odd-even dependence) to obtain a best agreement with experimental data.¹⁸ The result of our calculation using a strength of 1.8 MeV is shown in Fig. 5, where one sees that the agreement is indeed quite good. No polarization data exist at this energy, but we have shown the calculated polarization result for interest.



FIG. 5. Comparison of calculated and experimental differential cross sections for $n + {}^{16}O$ scattering at an energy of 14.04 MeV. Experimental data for polarizations are not yet available at this energy; therefore, only the calculated curve is shown.

In a previous communication,¹⁰ we have briefly examined the importance of the antisymmetrization operator \boldsymbol{a}' . There we have stated that the heavy-particle pickup process becomes less important in nucleon-nucleus scattering as the target mass increases. To make this statement more clear, we examine here the neutron-nucleus scattering cross sections for two different-mass target nuclei at large angles where the heavy-particle pickup process has its largest amplitude.⁷ In Fig. 6, the differential cross sections for $n + {}^{16}O$ and n $+\alpha$ scattering, calculated at the same value of 1.65 fm^{-1} for the wave number and with the spinorbit potential set as zero, are depicted. From this figure, it is indeed seen that the backward-tofoward ratio $\sigma(180^\circ)/\sigma(0^\circ)$ for $n + \alpha$ scattering is more than 100 times larger than that for $n + {}^{16}O$ scattering.

The above finding shows that the heavy-particle pickup amplitude is sensitively dependent upon the ratio of the mass of the cluster being picked up to the mass of the cluster which does the pickup. This explains therefore the observation, as mentioned in the Introduction, that the heavy-particle



FIG. 6. Comparison of $n+\alpha$ and $n+{}^{16}\text{O}$ differential cross sections, calculated at the same value of 1.65 fm⁻¹ for the wave number.

pickup process seems to be important in the α +¹⁶O problem, but much less so in the p +⁴⁰Ca problem. To make even more certain, we are at present also examining the case of n +⁴⁰Ca scattering using the resonating-group method in order to understand even better the dependence of the heavy-particle pickup amplitude on the mass of the target nucleus.

IV. CONCLUSION

We have shown in this investigation that the resonating-group method, which has been quite successful in previous studies of light nuclear systems, can be extended in a straightforward way to study heavier systems. This extension is accomplished through the use of a generator-coordinate technique which simplifies considerably the computation for systems involving a rather large number of nucleons. In this work, we have outlined the use of this technique in a relatively simple resonating-group calculation of the $N+^{16}O$ system. However, as the discussion of this technique shows, it can also be applied to more complicated scattering and reaction problems involving larger composite particles.

The results of our $N + {}^{16}$ O calculation have been compared with experimental data over a wide range of energies. From this comparison it is found that these results are, in general, quite satisfactory.

Since a fully antisymmetric wave function is employed in the calculation, the importance of various exchange processes can be examined. For example, we have found evidence from this study that the heavy-particle pickup process in nucleonnucleus scattering becomes less important as the mass of the target nucleus increases. As resonating-group calculations can now be performed in even rather heavy systems, one can proceed to examine in a systematic manner the importance of antisymmetrization in many nuclear scattering and reaction problems, such as the scattering of α particles by Ca isotopes, the reaction ¹⁶O(t, α)-¹⁵N, and so on. In this way, it is hoped that reliable approximation methods can eventually be devised for systems where a direct application of the resonating-group method may still be impracticable.

APPENDIX: EXPRESSIONS FOR THE DIRECT POTENTIALS AND THE KERNEL FUNCTION

The explicit expressions for the direct potentials $V_{\rm D}$, $V_{\rm so}$, and $V_{\rm C}$, and the kernel function k_i are given in this Appendix. We give these rather lengthy expressions here, because they will be very useful if one wishes to study the effects of the Pauli principle in a scattering problem, as has been done previously in the simpler case of $N + \alpha$ scattering.⁷

The direct nuclear central potential has the form

$$V_{\mathrm{D}}(\vec{\mathrm{R}}') = -\sum_{i=1}^{2} V_{0i} \gamma_{i} \left(\frac{m\alpha}{m\alpha + (m-1)\kappa_{i}}\right)^{3/2} \left(\frac{4m\alpha + (m-4)\kappa_{i}}{m\alpha + (m-1)\kappa_{i}} + \frac{2m^{2}\alpha\kappa_{i}^{2}}{[m\alpha + (m-1)\kappa_{i}]^{2}}R'^{2}\right) \exp\left(-\frac{m\alpha\kappa_{i}}{m\alpha + (m-1)\kappa_{i}}R'^{2}\right), \tag{A1}$$

where

$$V_{01} = V_{0t}, \quad V_{02} = V_{0s}, \quad \kappa_1 = \kappa_t, \quad \kappa_2 = \kappa_s \quad , \tag{A2}$$

and

$$\gamma_1 = \frac{1}{4} (9u - 6), \quad \gamma_2 = \frac{1}{4} (u + 2) , \quad (A3)$$

with m=16 and u being the exchange-mixture parameter in the nucleon-nucleon potential of Eq. (45). The direct spin-orbit potential is given by

$$V_{so}(\vec{R}') = -\frac{1}{8} V_{\lambda} \lambda^{-5/2} \left(\frac{m\alpha}{m-1}\right)^{3/2} \left(\frac{2m^4 \alpha^2}{(m-1)^3} R'^2 - \frac{m^2(m-4)\alpha}{(m-1)^2}\right) \exp\left(-\frac{m\alpha}{m-1} R'^2\right),$$
(A4)

while the direct Coulomb potential is given by

$$V_{\rm C}(\vec{\rm R}') = zz'e^2 \left\{ \frac{1}{R'} \Phi\left[\left(\frac{m\alpha}{m-1} \right)^{1/2} R' \right] - \frac{1}{2} \left(\frac{m}{m-1} \right)^{3/2} \left(\frac{\alpha}{\pi} \right)^{1/2} \exp\left(-\frac{m\alpha}{m-1} R'^2 \right) \right\},$$
(A5)

where

$$\Phi(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2) dt$$
(A6)

and z and z' are the atomic numbers of the ¹⁶O nucleus and the incident nucleon, respectively.

For the partial-wave kernel function $k_1(R', R'')$ we write it in terms of the function $K(\vec{R}', \vec{R}'')$ as

$$k_{I}(R',R'') = 2\pi R' R'' \int_{-1}^{1} K(\vec{R}',\vec{R}'') P_{I}(\cos\theta) d(\cos\theta) , \qquad (A7)$$

where

$$\cos\theta = \frac{1}{R'R''} \vec{R}' \cdot \vec{R}'' \quad . \tag{A8}$$

The function $K(\vec{\mathbf{R}}', \vec{\mathbf{R}}'')$ is in turn written as

$$K(\vec{\mathbf{R}}',\vec{\mathbf{R}}'') = \frac{\hbar^2}{2M} \,\mathcal{T} - \sum_{i=1}^2 V_{0i} \mathcal{U}_i + E_t \mathcal{H} \,, \tag{A9}$$

which contains the quantities \mathcal{T} , \mathcal{V}_i , and \mathfrak{X} , representing the kinetic-energy, potential-energy, and normalization kernels, respectively. In Eq. (A9), M is the nucleon mass and

$$E_t = E + E_{16}$$
 (A10)

The ¹⁶O internal energy E_{16} is given by

$$E_{16} = \frac{\hbar^2}{2M} \frac{69\alpha}{2} - \sum_{i=1}^2 \left\{ V_{0i} \left(\frac{\alpha}{\alpha + 2\kappa_i} \right)^{3/2} \left[6\delta_i + 2\epsilon_i \frac{3\alpha^2 + 6\alpha\kappa_i + 5\kappa_i^2}{(\alpha + 2\kappa_i)^2} + 4\omega_i \frac{3\alpha\kappa_i + 11\kappa_i^2}{(\alpha + 2\kappa_i)^2} + 12\gamma_i \frac{\alpha + \kappa_i}{\alpha + 2\kappa_i} \right] \right\}$$

$$+ \frac{83e^2}{2} \left(\frac{\alpha}{\pi} \right)^{1/2} , \qquad (A11)$$

with

$$\delta_1 = \delta_2 = \frac{1}{2} , \qquad \epsilon_1 = \frac{1}{2} (9u - 3), \qquad \epsilon_2 = \frac{1}{2} (u + 5) , \qquad \omega_1 = \frac{1}{4} (-9u + 12), \qquad \omega_2 = \frac{1}{4} (-u + 4) .$$
(A12)

The normalization kernel $\mathfrak A$ is given by

$$\mathfrak{N} = C_N \left(\frac{m-4}{m-1} + \frac{m^2 \alpha}{2(m-1)^2} \left(\vec{\mathbf{R}}' + \vec{\mathbf{R}}'' \right)^2 - \frac{m^2 \alpha}{2A^2} \left(\vec{\mathbf{R}}' - \vec{\mathbf{R}}'' \right)^2 \right) \exp\left(-a_1 R'^2 - b_1 R''^2 - c_1 \vec{\mathbf{R}}' \cdot \vec{\mathbf{R}}'' \right) , \tag{A13}$$

where

$$C_{N} = \left(\frac{\alpha}{4\pi}\right)^{3} \left(\frac{16m^{3}\pi}{\alpha A^{2}(m-1)}\right)^{3/2} ,$$
 (A14)

$$a_1 = b_1 = \frac{m(m^2 + 1)\alpha}{2A^2(m - 1)} \quad , \tag{A15}$$

$$c_1 = \frac{2m^2 \alpha}{A^2(m-1)} ,$$
 (A16)

with A = m+1. The kinetic-energy kernel \mathcal{T} is given by

$$\mathcal{T} = C_{N} \left(d_{k} + h_{k} (\vec{\mathbf{R}}' + \vec{\mathbf{R}}'')^{2} + f_{k} (\vec{\mathbf{R}}' - \vec{\mathbf{R}}'')^{2} + \frac{m^{4} \alpha^{3}}{4(m-1)^{4}} (\vec{\mathbf{R}}' + \vec{\mathbf{R}}'')^{4} - \frac{m^{4} (m-1) \alpha^{3}}{4A^{5}} (\vec{\mathbf{R}}' - \vec{\mathbf{R}}'')^{4} - \frac{m^{4} \alpha^{3}}{2A^{3}(m-1)^{2}} (\vec{\mathbf{R}}' + \vec{\mathbf{R}}'')^{2} (\vec{\mathbf{R}}' - \vec{\mathbf{R}}'')^{2} \right) \exp(-a_{1} R'^{2} - b_{1} R''^{2} - c_{1} \vec{\mathbf{R}}' \cdot \vec{\mathbf{R}}'') ,$$
(A17)

with

$$d_{k} = -\frac{\alpha}{2A(m-1)^{2}} (5m^{4} - 12m^{3} - 21m^{2} + 29m - 56) ,$$

$$h_{k} = -\frac{m^{2}\alpha^{2}}{4A(m-1)^{3}} (5m^{3} + 2m^{2} + 9m + 24) ,$$

$$f_{k} = \frac{m^{2}\alpha^{2}}{4A^{3}(m-1)} (5m^{3} + 6m^{2} - 15m + 24) .$$
(A18)

Finally, the potential-energy kernel $\boldsymbol{\upsilon}_i$ has the form

$$\mathcal{U}_{i} = \sum_{j=1}^{20} v_{ij},$$
(A19)

with

$$\begin{split} v_{i_{1}} &= -C_{N} \Big(\frac{\alpha}{\alpha + 2\kappa_{i}} \Big)^{5/2} \Big(3b_{1} + 2b_{1} \frac{3a^{2} + 5\alpha\kappa_{i} + 5\kappa_{i}^{2}}{(\alpha + 2\kappa_{i})^{2}} + \omega_{i} \frac{3\alpha\kappa_{i} + 38\kappa_{i}^{2}}{(\alpha + 2\kappa_{i})^{2}} + 9\gamma_{i} \frac{\alpha + \kappa_{i}}{\alpha + 2\kappa_{i}} \Big) \\ &\times \exp(-a_{1}R^{\prime 2} - b_{1}R^{\prime 2} - c_{1}\vec{R}^{\prime} \cdot \vec{R}^{\prime\prime}), \\ v_{i_{2}} &= -C_{N} \Big(\frac{\alpha}{\alpha + 2\kappa_{i}} \Big)^{5/2} \Big(b_{1}^{\prime} + b_{1}^{\prime} - \frac{3a^{2}}{3(\alpha + 2\kappa_{i})^{2}} + \omega_{i} \frac{33\alpha\kappa_{i} + 116\kappa_{i}^{2}}{3(\alpha + 2\kappa_{i})^{2}} + 11\gamma_{i} \frac{\alpha + \kappa_{i}}{\alpha + 2\kappa_{i}} \Big) \\ &\times \Big(\frac{m^{3}\alpha}{2(m-1)^{2}} (\vec{R}^{\prime} + \vec{R}^{\prime\prime}) - \frac{m^{2}\alpha}{2A^{2}} (\vec{R}^{\prime} - \vec{R}^{\prime\prime})^{2} - \frac{3}{m-1} \Big) \exp(-a_{1}R^{\prime 2} - b_{1}R^{\prime 2} - c_{1}\vec{R}^{\prime} \cdot \vec{R}^{\prime\prime}), \\ v_{i_{3}} &= C_{\mu}\alpha_{i}\exp(-a_{2}R^{\prime 2} - b_{2}R^{\prime 2} - c_{2}\vec{R}^{\prime} \cdot \vec{R}^{\prime\prime}), \\ v_{i_{4}} &= C_{\mu}\alpha_{i}\exp(-a_{2}R^{\prime 2} - b_{3}R^{\prime 2} - c_{3}\vec{R}^{\prime} \cdot \vec{R}^{\prime\prime}), \\ v_{i_{5}} &= -3C_{\mu}C_{\nu}b_{1}\exp(-a_{3}R^{\prime 2} - b_{3}R^{\prime 2} - c_{3}\vec{R}^{\prime} \cdot \vec{R}^{\prime\prime}), \\ v_{i_{6}} &= -3C_{\mu}C_{\nu}\gamma_{i} \Big(\frac{3(m-1)\alpha - \kappa_{i}}{1(m-1)\alpha + (m-2)\kappa_{i}} + \frac{2m^{2}\alpha\kappa_{i}^{2}}{A^{2}(m-1)\alpha + (m-2)\kappa_{i}} + P_{1}(\vec{R}^{\prime}, \vec{R}^{\prime\prime}) \Big) \exp(-a_{3}R^{\prime 2} - b_{3}R^{\prime 2} - c_{3}\vec{R}^{\prime} \cdot \vec{R}^{\prime\prime}), \\ v_{i_{7}} &= -C_{\mu}C_{\nu}\gamma_{i} \Big(-\frac{3(\alpha + \kappa_{i})}{1(m-1)\alpha + (m-2)\kappa_{i}} + \frac{2m^{2}\alpha(\alpha + \kappa_{i})}{A^{2}(m-1)\alpha + (m-2)\kappa_{i}} + P_{1}(\vec{R}^{\prime}, \vec{R}^{\prime\prime}) \Big) \exp(-a_{3}R^{\prime 2} - b_{3}R^{\prime 2} - c_{3}\vec{R}^{\prime} \cdot \vec{R}^{\prime}), \\ v_{i_{1}i} &= -C_{\mu}C_{\nu}\gamma_{i} \Big(-\frac{3(\alpha + \kappa_{i})}{1(m-1)\alpha + (m-2)\kappa_{i}} + \frac{2m^{2}\alpha(\alpha + \kappa_{i})}{A^{2}(m-1)\alpha + (m-2)\kappa_{i}} + P_{2}(\vec{R}^{\prime}, \vec{R}^{\prime\prime}) \Big) \exp(-a_{3}R^{\prime 2} - b_{3}R^{\prime 2} - c_{3}\vec{R}^{\prime} \cdot \vec{R}^{\prime}), \\ v_{i_{1}i} &= -C_{\mu}C_{\nu}\gamma_{i} \Big(-\frac{3(\alpha + \kappa_{i})}{1(m-1)\alpha + (m-2)\kappa_{i}} + \frac{2m^{2}\alpha(\alpha + \kappa_{i})\kappa_{i}}{A^{2}(m-1)\alpha + (m-2)\kappa_{i}} + P_{2}(\vec{R}^{\prime}, \vec{R}^{\prime\prime}) \Big) \exp(-a_{3}R^{\prime 2} - b_{3}R^{\prime 2} - c_{3}\vec{R}^{\prime} \cdot \vec{R}^{\prime}), \\ v_{i_{1}i} &= -C_{\mu}C_{\nu}\omega_{i} \Big(-\frac{3\kappa_{i}}{1(m-1)\alpha + (m-2)\kappa_{i}} + \frac{2m^{2}\alpha(\alpha + \kappa_{i})\kappa_{i}}{A^{2}(m-1)\alpha + (m-2)\kappa_{i}} + \frac{2m^{2}\alpha(\alpha + \kappa_{i})\kappa_{i}}{A^{2}(m-1)\alpha + (m-2)\kappa_{i}} + \frac{2m^{2}\alpha(\alpha + \kappa_{i})\kappa_{i}}{R^{\prime}}, \vec{R}^{\prime}) \Big) \exp(-a_{3}R^{\prime 2} - b_{3}R^{\prime$$

 $v_{i,20} = v_{i,19}$ with $\vec{\mathbf{R}}' \leftrightarrow \vec{\mathbf{R}}''$.

In the above equations, we have used the following definitions:

$$\begin{split} P_{1}(\vec{\mathbf{R}}',\vec{\mathbf{R}}'') &= (m\vec{\mathbf{R}}'+\vec{\mathbf{R}}'')^{2}, \\ P_{2}(\vec{\mathbf{R}}',\vec{\mathbf{R}}'') &= m(\alpha+2\kappa_{i})R'^{2} + \left[m\alpha+(m-1)\kappa_{i}\right]R''^{2} + \left[(m^{2}+1)\alpha+(m^{2}-m+2)\kappa_{i}\right]\vec{\mathbf{R}}'\cdot\vec{\mathbf{R}}'', \\ C_{V} &= \left(\frac{(m-1)\alpha}{(m-1)\alpha+(m-2)\kappa_{i}}\right)^{3/2}, \\ a_{2} &= b_{2} = \frac{m}{2A^{2}(m-1)}\left[(m^{2}+1)\alpha+2m(m-1)\kappa_{i}\right], \quad c_{2} = \frac{2m^{2}}{A^{2}(m-1)}\left[\alpha-(m-1)\kappa_{i}\right], \\ a_{3} &= \frac{m\alpha[(m^{2}+1)\alpha+(3m^{2}+m+2)\kappa_{i}]}{2A^{2}[(m-1)\alpha+(m-2)\kappa_{i}]}, \quad b_{3} = \frac{m\alpha[(m^{2}+1)\alpha+(m^{2}-m+2)\kappa_{i}]}{2A^{2}[(m-1)\alpha+(m-2)\kappa_{i}]}, \quad c_{3} = \frac{2\alpha m^{2}(\alpha+2\kappa_{i})}{A^{2}[(m-1)\alpha+(m-2)\kappa_{i}]}. \end{split}$$

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