Problem of Antisymmetrization in Heavy-Ion Scattering*

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A general formalism for the scattering of heavy ions, which is especially convenient to study the antisymmetrization effects, is developed. Antisymmetrization effects are investigated by expanding the completely antisymmetrized wave function according to the number of exchanged nucleons. The particle-core model for the scattering of nuclei with loosely bound nucleons is presented. A formula for the additional contribution to the effective potential due to antisymmetrization effects is obtained by calculating the expectation value of the Hamiltonian with intrinsic wave functions. Application of the formalism is illustrated for the $^{14}N+^{14}N$ scattering problem and its usefulness is demonstrated.

I. INTRODUCTION

In the scattering of two identical light nuclei, such as ^{12}C, ^{14}N, ^{16}O, or ^{18}O, the elastic excitation functions reveal prominent gross structures with widths of 2–3 MeV.[1-5] Furthermore, in the excitation functions for the elastic scattering of ^{12}C on ^{12}C and ^{16}O on ^{16}O, the intermediate structures of width ~0.3 MeV are superimposed over the gross structure, while the ^{14}N-^{14}N and ^{18}O-^{18}O cross sections seem to show no intermediate structure. This different behavior may be explained as due to a stronger absorption of high partial waves in the cases of ^{14}N and ^{18}O.[4,6] This is because both nuclei have loosely bound nucleons outside the closed shells and, therefore, inelastic surface reaction processes are more probable than in the case of the closed-shell nuclei ^{12}C and ^{16}O. In the ^{14}N-^{14}N scattering a further smoothing effect of the gross structure arises due to the spin, $I=1$, of the ^{14}N nuclei since the scattering wave function has to be symmetrized differently compared to the case of two identical spin-zero nuclei.[7]

The scattering of two ^{14}N or ^{18}O nuclei is interesting to study in many respects. In this paper we examine mainly the effects due to the antisymmetrization between the nuclei. It is customary to treat two identical nuclei with integer spin as bosons and to symmetrize the wave function for the exchange of the whole nuclei.[1] The scattering wave function, then, consists of two terms, the so-called *direct* and *total exchange* terms which can be transformed into one another by replacing the nucleons of nucleus 1 by the nucleons of nucleus 2 and vice versa. But these two terms represent only a part of the full antisymmetrization. In an exact treatment the antisymmetrized wave function may be generated from the direct term by successively interchanging the nucleons between the nuclei.[8] When the maximum number of particles is exchanged, the total exchange term is obtained again.

For identical nuclei the total exchange term has the same intrinsic wave function as the direct term, i.e., both terms have maximum overlap, if one integrates over the intrinsic nucleon coordinates only. All other exchange terms have a smaller intrinsic overlap with the direct term. The overlap decreases with the number of nucleons exchanged and vanishes asymptotically for large separations of the nuclei.

The scattering amplitude depends on the interaction between the direct and exchange terms in the wave function.[8] If the different terms do not overlap, no antisymmetrization would be required and the direct term alone would describe the scattering correctly. In the surface region, where the nuclei come into contact, the overlap of the direct and the exchange terms decreases rapidly with the number of exchanged nucleons. Since most of the observed structure in the cross sections is produced in the surface region, effects due to the Pauli principle can be analyzed with wave functions which are expanded according to the number of exchanged nucleons. This method is convenient and useful because the additional nucleus-nucleus potentials arising from the antisymmetrization give only small contributions in the surface region and decrease rapidly with the number of exchanged particles. With increasing overlap of the nuclei,

i.e., inside the surface region, the absorption from the elastic channel increases strongly. Hence no information about the real potential at short distances can be obtained from the elastic cross section alone. One needs inelastic excitation functions also.

We investigate the effects of antisymmetrization between two nuclei in the framework of the particle-core model in which nuclei are considered to be composed of inert cores surrounded by loosely bound extracore nucleons. The total scattering system is, therefore, described by two cores to which a few extracore particles are bound. This picture is quite familiar in molecular physics[9] and was introduced first by von Oertzen[10,11] into heavy-ion physics.

The particle-core model circumvents the problems which arise in the antisymmetrization of the relative coordinate between the two nuclear mass centers. The relative coordinate is unsymmetrical in the particle coordinates and, therefore, affected by the antisymmetrization procedure. This leads to nonlocalities in the effective differential equations for the scattering amplitude.[12] One way to avoid the difficulties is to define a scattering coordinate which is symmetrical in the nuclear coordinates. For example, one could set the scattering coordinate proportional to the square root of the quadrupole moment of the nucleus-nucleus system.[13,14] In the particle-core model the relative distance between the centers of the cores serves naturally as the scattering coordinate. It is affected by the antisymmetrization procedure only if the cores are exchanged, i.e., all antisymmetrization effects between the individual nucleons of the cores are neglected. This approximation is applicable for reactions proceeding mainly in the surface region where the cores do not overlap and behave like inert spectators.

It is useful to describe the motion of the extracore particles in an intrinsic coordinate system. The symmetry axis of the intrinsic system is the line connecting the centers of the cores which are assumed to be spherical. This method corresponds to the strong coupling limit of the Nilsson model because the core system can be considered as a strongly deformed compound system.[15] The average potential for the extracore particles is generated by the cores and depends on their relative distance. The potential may be chosen to be the two-center oscillator potential which was proposed originally as a shell-model potential to describe fission processes.[16-18]

In this paper a general consideration of the scattering of heavy ions and the antisymmetrization problem is first discussed in Sec. II on the basis of the theory of coupled equations. Next the particle-core model for the scattering of nuclei with loosely bound nucleons is developed in Sec. III. In Sec. IV, the effects of antisymmetrization on the potentials are investigated and the application of the formalism is illustrated for the ^{14}N-^{14}N scattering problem.

II. GENERAL CONSIDERATIONS FOR THE SCATTERING OF HEAVY IONS

When two nuclei are scattered various reaction processes, such as transfer reactions and compound-nucleus formation, will occur in addition to the elastic scattering and the inelastic excitation of the two nuclei. For simplicity we restrict our considerations to the case when the nucleus-nucleus system breaks up into only two parts after the collision. Thereby, we avoid the complicated three- and many-body problems of continuum wave functions in the outgoing channels.

The asymptotic wave functions may be expanded according to the different partitions in which the A nucleons of the total system can be divided. The different partitions are characterized by two specifications. The first specifies which two nuclei can be measured in which nuclear states in the asymptotic region; the second specifies the various partitions of nucleons in the various states in the two nuclei. Here we consider the protons and neutrons as nucleons in different isospin states. The second specification of the asymptotic wave function cannot be distinguished by measurement and is obviously related to the antisymmetrization of the wave functions.[12]

A. Definition of the Coordinates

Let us assume that the nucleus-nucleus system splits into two nuclei with A_1 and $A_2 = A - A_1$ particles. Further let us assign the particles with numbers $i \leq A_1$ to nucleus 1 and the particles with numbers $i > A_1$ to nucleus 2. To describe the scattering of these nuclei it is convenient to introduce the center-of-mass coordinate

$$\vec{R} = \frac{1}{A} \sum_{i=1}^{A} \vec{r}_i , \tag{1}$$

and the relative coordinate between the mass centers of the nuclei,

$$\vec{r}_{A_1 A_2} = \vec{R}_{A_1} - \vec{R}_{A_2} , \tag{2}$$

with

$$\vec{R}_{A_1} = \frac{1}{A_1} \sum_{i=1}^{A_1} \vec{r}_i ,$$

$$\vec{R}_{A_2} = \frac{1}{A_2} \sum_{i=A_1+1}^{A} \vec{r}_i ,$$

and the sets of $3A_1 - 3$ and $3A_2 - 3$ independent intrinsic coordinates abbreviated by $\{\alpha_{A_1}\}$ and $\{\alpha_{A_2}\}$. The relative coordinates $\vec{r}_i - \vec{R}_{A_1}$ for $1 \leq i \leq A_1$ and $\vec{r}_i - \vec{R}_{A_2}$ for $A_1 + 1 \leq i \leq A$ are not independent, but are functions of the intrinsic coordinates $\{\alpha_{A_1}\}$ and $\{\alpha_{A_2}\}$, respectively (see Fig. 1).

The relative coordinate $\vec{r}_{A_1A_2}$ depends on the distribution of the particles in the two nuclei. There are $A!/A_1!A_2!$ different possible choices of the relative coordinate depending upon to which nucleus each particle belongs.[8] We choose the above partition of the particles as our basic or direct partition,

$$A_1\{1, 2, \ldots, A_1\}, \quad A_2\{A_1+1, A_1+2, \ldots, A\}. \tag{3}$$

The numbers in the curly brackets in (3) denote the assignment of the particles to the nuclei. If particles are successively exchanged between the two nuclei all relative coordinates are generated. For an l-particle exchange the relative coordinate becomes

$$\vec{r}'_{A_1A_2} = \vec{r}_{A_1A_2} - \left(\frac{1}{A_1} + \frac{1}{A_2}\right) \sum_{k=1;\, i_k \leq A_1 < j_k}^{k=l} (\vec{r}_{i_k} - \vec{r}_{j_k}). \tag{4}$$

In the special case when all nucleons of two nuclei with equal mass numbers are exchanged, i.e., $A_1 = A_2 = l$, we have $\vec{r}'_{A_1A_2} = -\vec{r}_{A_1A_2}$. To every partition of the particles we can construct two sets of $3A_1 - 3$ and $3A_2 - 3$ independent coordinates, as already explained for the basic partition (3). For convenience we abbreviate the relative coordinates by $\vec{r}_{S,A_1A_2}$ and the sets of intrinsic coordinates by $\{\alpha_{S,A_1}\}$ and $\{\alpha_{S,A_2}\}$ in the following discussion. The index S denotes different partitions of the particles in the two nuclei with A_1 and A_2 nucleons.

B. Derivation of the Coupled Equations

The Hamiltonian can be written in the coordinates defined above as

$$\begin{aligned} H &= \sum_i t_i + \sum_{i<j} V_{ij} \\ &= T_{\text{c.m.}} + T_{A_1A_2}(\vec{r}_{S,A_1A_2}) + H_{A_1}(\alpha_{S,A_1}) \\ &\quad + H_{A_2}(\alpha_{S,A_2}) + V_{A_1A_2}(\vec{r}_{S,A_1A_2}; \alpha_{S,A_1}, \alpha_{S,A_2}), \end{aligned} \tag{5}$$

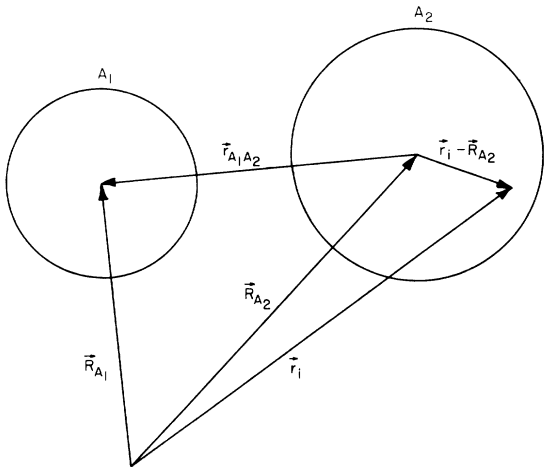

FIG. 1. General definition of the coordinates.

where the kinetic energy of the center of mass is denoted by $T_{\text{c.m.}}$ and that of the relative motion by $T_{A_1A_2}$. The Hamiltonians describing the individual nuclei and the residual interaction are given, e.g., for the partition according to (3), by

$$\begin{aligned} H_{A_1}(\alpha_{A_1}) &= \sum_{i=1}^{A_1} t_i - T_{A_1}(\vec{R}_{A_1}) + \sum_{j>i\geq 1}^{A_1} V_{ij}, \\ H_{A_2}(\alpha_{A_2}) &= \sum_{i=A_1+1}^{A} t_i - T_{A_2}(\vec{R}_{A_2}) + \sum_{j>i\geq A_1+1}^{A} V_{ij}, \end{aligned} \tag{6}$$

and

$$V_{A_1A_2}(\vec{r}_{A_1A_2}; \alpha_{A_1}, \alpha_{A_2}) = \sum_{i=1}^{A_1} \sum_{j=A_1+1}^{A} V_{ij}. \tag{7}$$

Let us assume that we have already solved the eigenequations

$$H_{A_\beta}(\alpha_{A_\beta}) \Phi_{n_{A\beta}}(\alpha_{A_\beta}) = \epsilon_{n_{A\beta}} \Phi_{n_{A\beta}}(\alpha_{A_\beta}), \quad \beta = 1, 2, \tag{8}$$

where n_{A_β} denotes the set of quantum numbers of the states. The states $\Phi_{n_{A\beta}}$ are the intrinsic eigenstates of the nuclei A_1 and A_2 for large separations $\vec{r}_{A_1A_2}$. Then the asymptotic wave function can be expanded in terms of these eigenstates:

$$\psi = \psi_{\text{c.m.}}(\vec{R}) \mathcal{A} \sum_{n_{A1}, n_{A2}, A_1, (A_2 = A - A_1)} \varphi_{n_{A1}n_{A2}}(\vec{r}_{A_1A_2}) \Phi_{n_{A1}}(\alpha_{A_1}) \Phi_{n_{A2}}(\alpha_{A_2}). \tag{9}$$

We assume that the intrinsic wave functions Φ are already antisymmetrized. Therefore, we only need to antisymmetrize between the nuclei A_1 and A_2, which is carried out by the antisymmetrization operator $\mathcal{A}$. It will be done by expanding the antisymmetrized wave function according to the number of particles exchanged between the nuclei.[8] Introducing the abbreviation

$$\Phi_d(n_{A_1}, n_{A_2}) = \varphi_{n_{A1}n_{A2}}(\vec{r}_{A_1A_2}) \Phi_{n_{A1}}(\alpha_{A_1}) \Phi_{n_{A2}}(\alpha_{A_2}), \tag{10}$$

the one-particle-exchange function is generated by interchanging two particles belonging to different nuclei,

e.g.,

$$\Phi_{\mathrm{ex},1}(1,\ldots,i,\ldots,A_1;A_1+1,\ldots,j,\ldots,A)=\Phi_d(1,\ldots,j,\ldots,A_1;A_1+1,\ldots,i,\ldots,A)\,, \tag{11}$$

and analogously for $\Phi_{\mathrm{ex},l}$. The index d stands for direct; it characterizes the basic or direct partition. There are A_1A_2 wave functions of the one-exchange type, and in general, $\binom{A_1}{l}\binom{A_2}{l}$ wave functions of the l-exchange type. Thus, we obtain

$$\Psi=\sum_{A_1,n_{A1},n_{A2}}\left[\Phi_d(n_{A_1},n_{A_2})+\sum_l(-)^l\sum_S\Phi^{(S)}_{\mathrm{ex},l}(n_{A_1},n_{A_2})\right], \tag{12a}$$

where we have omitted the center-of-mass function $\psi_{\mathrm{c.m.}}$, which is not important in the following discussion. The summation over S denotes different possible l-exchange functions. Equation (12a) is identical with the following expression using the above notation:

$$\Psi=\sum_{A_1,n_{A1},n_{A2}}\sum_S(-)^{l_S}\varphi_{n_{A1}n_{A2}}(\vec{\mathrm{r}}_{S,A_1A_2})\Phi_{n_{A1}}(\alpha_{S,A_1})\Phi_{n_{A2}}(\alpha_{S,A_2})\,, \tag{12b}$$

where l_S denotes that l particles are exchanged in partition S (see Sec. II A). If the wave functions $\Phi_{n_{A\beta}}$ are restricted to the set of bound-state functions only, all functions in the expansion are orthogonal in the asymptotic region where the fragments do not overlap. On the other hand, in the interaction region the different terms of the wave function (12a) are nonorthogonal in general.

By projecting with the intrinsic functions $\Phi_{n_{A1}}(\alpha_{A_1})\Phi_{n_{A2}}(\alpha_{A_2})$ we can replace the Schrödinger equation by an infinite system of coupled integrodifferential equations which depend only on the relative coordinates $\vec{\mathrm{r}}_{A_1A_2}$. The set of intrinsic coordinates $\{\alpha_{A_1},\alpha_{A_2}\}$ corresponds to the basic partition given by (3). Hence, we have

$$\int\Phi^*_{n_{A1}}(\alpha_{A_1})\Phi^*_{n_{A2}}(\alpha_{A_2})(H-E-T_{\mathrm{c.m.}})\Psi d\alpha_{A_1}d\alpha_{A_2}=0\,, \tag{13}$$

where $d\alpha_{A_1}d\alpha_{A_2}$ denotes the volume element of the intrinsic coordinates. Using Ψ given by (12), and the Hamiltonian (5), and introducing the difference function Ψ' by

$$\Psi'_{n_{A1}n_{A2}}=\Psi-\varphi_{n_{A1}n_{A2}}(\vec{\mathrm{r}}_{A_1A_2})\Phi_{n_{A1}}(\alpha_{A_1})\Phi_{n_{A2}}(\alpha_{A_2})\,, \tag{14}$$

we obtain from (13)

$$\begin{aligned}[T_{A_1A_2}(\vec{\mathrm{r}}_{A_1A_2})+\epsilon_{n_{A1}}+\epsilon_{n_{A2}}+V_{n_{A1}n_{A2}}(\vec{\mathrm{r}}_{A_1A_2})-E]\varphi_{n_{A1}n_{A2}}(\vec{\mathrm{r}}_{A_1A_2})\\ =-[T_{A_1A_2}(\vec{\mathrm{r}}_{A_1A_2})+\epsilon_{n_{A1}}+\epsilon_{n_{A2}}-E]\int\Phi^*_{n_{A1}}(\alpha_{A_1})\Phi^*_{n_{A2}}(\alpha_{A_2})\Psi'_{n_{A1}n_{A2}}d\alpha_{A_1}d\alpha_{A_2}\\ -\int\Phi^*_{n_{A1}}(\alpha_{A_1})\Phi^*_{n_{A2}}(\alpha_{A_2})V_{A_1A_2}(\vec{\mathrm{r}}_{A_1A_2},\alpha_{A_1},\alpha_{A_2})\Psi'_{n_{A1}n_{A2}}d\alpha_{A_1}d\alpha_{A_2}\,,\end{aligned} \tag{15}$$

with the potential $V_{n_{A1}n_{A2}}$ given by

$$V_{n_{A1}n_{A2}}(\vec{\mathrm{r}}_{A_1A_2})=\int\Phi^*_{n_{A1}}(\alpha_{A_1})\Phi^*_{n_{A2}}(\alpha_{A_2})V_{A_1A_2}(\vec{\mathrm{r}}_{A_1A_2},\alpha_{A_1},\alpha_{A_2})\Phi_{n_{A1}}(\alpha_{A_1})\Phi_{n_{A2}}(\alpha_{A_2})d\alpha_{A_1}d\alpha_{A_2}\,. \tag{16}$$

The right-hand side of Eq. (15), which vanishes in the asymptotic region, contains the various couplings to other channels. The coupling potentials arise from several sources, namely due to the nuclear forces, the nonorthogonality of the channel functions in the interaction region, and the antisymmetrization of the wave function.

C. Formal Solution for the Nonlocal Coupling Potentials

The system of equations (15) can be formally solved by determining first the eigenvalues of the integral equations[19]

$$\int\Phi^*_{n_{A1}}(\alpha_{A_1})\Phi^*_{n_{A2}}(\alpha_{A_2})(H-E-T_{\mathrm{c.m.}})\sum_S{}'(-)^{l_S}\Phi_{n_{A1'}}(\alpha_{S,A_1'})\Phi_{n_{A2'}}(\alpha_{S,A_2'})v^{(m)}_{\lambda\lambda'}(\vec{\mathrm{r}}_{S,A_1'A_2'})d\alpha_{A_1}d\alpha_{A_2}=V^{(m)}_{\lambda\lambda'}v^{(m)}_{\lambda\lambda'}(\vec{\mathrm{r}}_{A_1A_2})\,, \tag{17}$$

where $\lambda=(n_{A_1},n_{A_2})$ and $\lambda'=(n_{A_1'},n_{A_2'})$. Note that, in Eq. (17), one integrates over the intrinsic coordinates of the basic partition. The coordinates of the different fragmentations A_1' and A_2' have to be expressed in terms of the coordinates of the basic partition. The different eigenfunctions $v^{(m)}_{\lambda\lambda'}$ and their corresponding

eigenvalues $V^{(m)}_{\lambda\lambda'}$ are specified by the superscript m. The prime on the summation sign indicates that the basic partition (3) does not occur for $\lambda=\lambda'$. Therefore, the eigenfunctions $v^{(m)}_{\lambda\lambda'}$ are restricted to the interaction region. The eigenvalues $V^{(m)}_{\lambda\lambda'}$ are energy-dependent. From (17) one can obtain the following relation concerning the orthogonality of the eigenfunctions:

$$0=(V^{(m)*}_{\lambda\lambda'}-V^{(m')}_{\lambda'\lambda})\int v^{(m)*}_{\lambda\lambda'}(\vec{r})v^{(m')}_{\lambda'\lambda}(\vec{r})d^3\gamma\,. \tag{18}$$

It is possible to order the eigenvalues so that

$$V^{(m)}_{\lambda\lambda'}=V^{(m)*}_{\lambda'\lambda}\,. \tag{19}$$

Then the eigenfunctions can be normalized as follows:

$$\int v^{(m)*}_{\lambda\lambda'}(\vec{r})v^{(m')}_{\lambda'\lambda}(\vec{r})d^3\gamma=\delta_{mm'}\,. \tag{20}$$

In the special case when $\lambda=\lambda'$, the eigenvalues are real. Using these results, Eq. (15) becomes

$$[T_{A_1A_2}(\vec{r})+V_{n_{A1}n_{A2}}(\vec{r})+\epsilon_{n_{A1}}+\epsilon_{n_{A2}}-E]\varphi_\lambda(\vec{r})=-\sum_{\lambda'}\int K_{\lambda\lambda'}(\vec{r},\vec{r}';E)\varphi_{\lambda'}(\vec{r}')d\tau'\,, \tag{21}$$

with the energy-dependent kernel $K_{\lambda\lambda'}$ given by

$$K_{\lambda\lambda'}(\vec{r},\vec{r}';E)=\sum_m V^{(m)}_{\lambda\lambda'}v^{(m)}_{\lambda\lambda'}(\vec{r})v^{(m)*}_{\lambda'\lambda}(\vec{r}')\,. \tag{22}$$

Equations (21) and (22) show explicitly the nonlocality of the coupling potentials.

D. Effects of the Spurious Center-of-Mass Motion

One usually describes the nuclear states with shell-model wave functions which depend on all particle coordinates. These functions contain a spurious center-of-mass motion. In the following we discuss the effect of the spurious center-of-mass motion on the calculation of the matrix elements of Eq. (15).

For many-body wave functions which are constructed from single-particle wave functions of the harmonic oscillator, the center-of-mass part can be separated with the transformation to the center-of-mass and intrinsic coordinates. For the product of an A_1-particle oscillator function concentrated around the center at $\underline{\vec{R}}_{A_1}$ and A_2-particle oscillator function concentrated around the second center at $\underline{\vec{R}}_{A_2}$, it yields

$$\chi_{n_{A1}}(\vec{r}_1-\underline{\vec{R}}_{A_1},\ldots,\vec{r}_{A_1}-\underline{\vec{R}}_{A_1})\chi_{n_{A2}}(\vec{r}_{A_1+1}-\underline{\vec{R}}_{A_2},\ldots,\vec{r}_A-\underline{\vec{R}}_{A_2})$$

$$=\left(\frac{\mu_{A_1}\mu_{A_2}}{\pi^2}\right)^{3/4}\exp[-\tfrac{1}{2}\mu_{A_1}(\vec{R}_{A_1}-\underline{\vec{R}}_{A_1})^2]\exp[-\tfrac{1}{2}\mu_{A_2}(\vec{R}_{A_2}-\underline{\vec{R}}_{A_2})^2]\Phi_{n_{A1}}(\alpha_1)\Phi_{n_{A2}}(\alpha_2)\,. \tag{23}$$

The oscillator length a_{A_β} for the center of mass is given by

$$a_{A_\beta}=(\mu_{A_\beta})^{-1/2}=\left(\frac{\hbar}{MA_\beta\omega_{A_\beta}}\right)^{1/2},\quad \beta=1,2\,. \tag{24}$$

The centers of mass of the nuclei are bound with an uncertainty of a_{A_1} and a_{A_2}, respectively, to the positions $\vec{\underline{R}}_{A_1}$ and $\vec{\underline{R}}_{A_2}$. This uncertainty in the positions of the centers of mass is small compared to the nuclear dimensions because $a_A\sim 1.0A^{-1/3}$ F with $\hbar\omega=41A^{-1/3}$ MeV.[15] Therefore, the wave functions (23) can be used for an approximative calculation of matrix elements which appear in Eq. (15) and which connect the basic partition of fragmentation n_{A_1}, n_{A_2} with a specific fragmentation $n_{A_1'}$, $n_{A_2'}$ and partition S:

$$I(\vec{r}_{A_1A_2})=\int\Phi^*_{n_{A1}}(\alpha_1)\Phi^*_{n_{A2}}(\alpha_2)\left(\sum_{i\le A_1<j}V_{ij}\right)\Phi_{n_{A1'}}(\alpha_{S,A_1'})\Phi_{n_{A2'}}(\alpha_{S,A_2'})\varphi_{n_{A1'}n_{A2'}}(\vec{r}_{S,A_1'A_2'})d\alpha_1d\alpha_2\,. \tag{25}$$

Replacing the functions Φ_n which depend solely on the intrinsic coordinates by the functions χ_n we obtain

the analogous approximative expression:

$$I_0 = \int \chi^*_{n_{A1}}(\vec{r}_1 - \underline{\vec{R}}_{A_1}, \ldots, \vec{r}_{A_1} - \underline{\vec{R}}_{A_1}) \chi^*_{n_{A2}}(\vec{r}_{A_1+1} - \underline{\vec{R}}_{A_2}, \ldots, \vec{r}_A - \underline{\vec{R}}_{A_2})$$

$$\times \left(\sum_{i \le A_1 < j} V_{ij} \right) \chi_{n_{A1'}}(\vec{r}_{S,1} - \underline{\vec{R}}_{S,A_1'}, \ldots) \chi_{n_{A2'}}(\vec{r}_{S,A_1+1} - \underline{\vec{R}}_{S,A_2'}, \ldots) \varphi_{n_{A1'}, n_{A2'}}(\vec{r}_{S,A_1'A_2'}) \prod_{\nu=1}^{A} d\tau_\nu . \tag{26}$$

In the following we consider further how Eq. (26) can be related to Eq. (25). For this purpose we connect the position parameters $\underline{\vec{R}}_{S,A_1'}$, $\underline{\vec{R}}_{S,A_2'}$ and $\underline{\vec{R}}_{A_1}$, $\underline{\vec{R}}_{A_2}$ by the following coordinate dependent transformation:

$$\begin{aligned} \underline{\vec{R}}_{S,A_1'} &= \underline{\vec{R}}_{A_1} + \vec{R}_{S,A_1'} - \vec{R}_{A_1} , \\ \underline{\vec{R}}_{S,A_2'} &= \underline{\vec{R}}_{A_2} + \vec{R}_{S,A_2'} - \vec{R}_{A_2} . \end{aligned} \tag{27}$$

Then we are able to integrate over the coordinate of the total center of mass in Eq. (26). The coordinate of the center of mass is given by

$$\vec{R} = \frac{1}{A}(A_1 \vec{R}_{A_1} + A_2 \vec{R}_{A_2}) = \frac{1}{A}(A_1' \vec{R}_{S,A_1'} + A_2' \vec{R}_{S,A_2'}) . \tag{28}$$

We thus obtain the following relation between Eqs. (25) and (26):

$$I_0 = \left(\frac{2}{a_{A_1}/a_{A_1'} + a_{A_1'}/a_{A_1}} \right)^{3/2} \left(\frac{2}{a_{A_2}/a_{A_2'} + a_{A_2'}/a_{A_2}} \right)^{3/2} (\sqrt{\pi}\lambda)^{-3} \int I(\underline{\vec{r}}_{A_1A_2} + \vec{r}) \exp(-r^2/\lambda^2) d^3r , \tag{29}$$

with the width λ given by

$$\lambda^2 = 2(1/a_{A_1}^2 + 1/a_{A_1'}^2)^{-1} + 2(1/a_{A_2}^2 + 1/a_{A_2'}^2)^{-1} , \tag{30}$$

and the relative distance between the position parameters $\underline{\vec{r}}_{A_1A_2} = \underline{\vec{R}}_{A_1} - \underline{\vec{R}}_{A_2}$. By using the shell-model wave functions (23), instead of the exact intrinsic function given in Eq. (8), one averages the matrix elements over a sphere of radius of about λ, which is proportional to $A^{-1/3}$ and thus becomes smaller for heavier nuclei. All structures with widths smaller than λ are smeared out in the approximative matrix elements of Eq. (29). In the special case when one investigates antisymmetrization effects between identical nuclei, the two prefactors in Eq. (29) become unity and we have $\lambda = \sqrt{2}\, a_{A/2}$ since $A_1 = A_2 = A_1' = A_2' = A/2$.

Apart from the prefactors which arise from the integration over the center-of-mass coordinate $\vec{R}$ of (28), the integral I_0 given by (29) is the first term in an expansion of the exact integral $I(\vec{r}_{A_1A_2})$, of Eq. (25), namely,

$$I(\vec{r}_{A_1A_2}) = \sum_{k=0}^{\infty} \frac{\Psi_k(0)}{\Psi_0(0)} \int \Psi_k^*(\vec{r}) I(\vec{r}_{A_1A_2} + \vec{r}) \Psi_0(\vec{r}) d^3r , \tag{31}$$

with the S-wave functions Ψ_k of the three-dimensional harmonic oscillator given by

$$\begin{aligned} \Psi_0 &= (\sqrt{\pi}\lambda)^{-3/2} \exp[-r^2/(2\lambda^2)] , \\ \Psi_1 &= (\sqrt{\pi}\lambda)^{-3/2} (\tfrac{2}{3})^{1/2} \left(\frac{3}{2} - \frac{r^2}{\lambda^2} \right) \exp[-r^2/(2\lambda^2)], \ldots . \end{aligned} \tag{32}$$

Relation (31) is immediately understood by realizing the identity

$$\delta(\vec{r}) = \sum_{k=0}^{\infty} \Psi_k^*(\vec{r}) \Psi_k(0) .$$

The expansion (31) converges more rapidly than the similar one

$$I(\vec{r}_{A_1A_2}) = \sum_{k=0}^{\infty} \Psi_k(0) \int \Psi_k^*(\vec{r}) I(\vec{r}_{A_1A_2} + \vec{r}) d^3r .$$

This can be seen for $I(\vec{r}) = \text{constant}$, in which case Eq. (31) reduces to one term, while all higher moments contribute in the latter expansion.

E. Local Approximation of the Nonlocal Potentials

The potentials on the right-hand side of Eq. (15) are nonlocal. This nonlocality can be expressed in terms of a local differential expression by expanding the relative coordinate $\vec{r}_{S,A_1'A_2'}$ around the coordinates

$\pm\vec{r}_{A_1A_2}$. We obtain, from (13) and (12b),

$$0=\int \Phi^*_{n_{A1}}(\alpha_{A_1})\Phi^*_{n_{A2}}(\alpha_{A_2})(H-E-T_{\text{c.m.}})\Psi\, d\alpha_{A_1}d\alpha_{A_2}$$

$$=\sum_{m=0}^{\infty}\frac{1}{m!}\sum_{A_1' n_{A1'} n_{A2'}}\sum_{S}(-1)^{I_S}\Big\{\int \Phi^*_{n_{A1}}(\alpha_{A_1})\Phi^*_{n_{A2}}(\alpha_{A_2})(H-E-T_{\text{c.m.}})$$
$$\times\Phi_{n_{A1'}}(\alpha_{S,A_1'})\Phi_{n_{A2'}}(\alpha_{S,A_2'})[(\vec{r}_{S,A_1'A_2'}\mp\vec{r}_{A_1A_2})\cdot\vec{\nabla}_{r_{A1A2}}]^m d\alpha_{A_1}d\alpha_{A_2}\Big\}\varphi_{n_{A1'}n_{A2'}}(\pm\vec{r}_{A_1A_2})\,. \tag{33}$$

The differential operator $\vec{\nabla}$ should only act on the function $\varphi_{n_{A1'}n_{A2'}}$. The upper sign is useful for particle partitions differing little from the basic partition (3) while the lower sign should be applied for partitions differing not much from the partitions in which all particles are exchanged. Thus, one minimizes the difference $\vec{r}_{S,A_1'A_2'}-\vec{r}_{A_1A_1}$.

Since $\vec{P}_{r_{A1A2}}=(\hbar/i)\vec{\nabla}_{r_{A1A2}}$, Eq. (33) shows that the nonlocalities of Eq. (21) are transformed into a velocity dependence of the potentials. Both forms are equivalent. The velocity dependence (or nonlocality) is due to the Pauli principle and the transfer of particles. The effects due to the Pauli principle and due to the transfer processes (e.g., recoil effects,[20] *Mitbewegungs* effects) can obviously not be separated and are simultaneously described in Eq. (33).

When the colliding nuclei come into contact, the partitions in which a small number of particles or all particles are exchanged play a dominant role, as will be shown in Sec. III. In these partitions the differences between the relative distances $\vec{r}_{S,A_1'A_2'}\mp\vec{r}_{A_1A_2}$ are small so that in the first approximation the expansion (33) can be restricted to the term with $m=0$:

$$0=\int \Phi^*_{n_{A1}}(\alpha_{A_1})\Phi^*_{n_{A2}}(\alpha_{A_2})(H-E-T_{\text{c.m.}})\sum_{A_1' n_{A1'} n_{A2'}}\sum_{S}(-1)^{I_S}\Phi_{n_{A1'}}(\alpha_{S,A_1'})\Phi_{n_{A2'}}(\alpha_{S,A_2'})d\alpha_{A_1}d\alpha_{A_2}\varphi_{n_{A1'}n_{A2'}}(\vec{r}_{A_1A_2})\,. \tag{34}$$

Thus, one neglects all recoil effects and all nonlocalities arising from the antisymmetrization. Combining Eq. (34) with Eq. (26), we finally obtain an approximate system of coupled equations for the case of scattering of nuclei with $A_1\approx A_2\approx A/2$:

$$\sum_{\lambda'}[(T_{A_1A_2}+\epsilon_{n_{A1}}+\epsilon_{n_{A2}}-E)F_{\lambda\lambda'}(\vec{r}_{A_1A_2})+V_{\lambda\lambda'}(\vec{r}_{A_1A_2})]\varphi_{\lambda'}(\vec{r}_{A_1A_2})=0\,, \tag{35}$$

with

$$\left.\begin{matrix}F_{\lambda\lambda'}(\vec{r}_{A_1A_2})\\ V_{\lambda\lambda'}(\vec{r}_{A_1A_2})\end{matrix}\right\}=\int \chi^*_{n_{A1}}(\vec{r}_1-\underline{\vec{R}}_{A_1},\ldots)\chi^*_{n_{A2}}(\vec{r}_{A_1+1}-\underline{\vec{R}}_{A_2},\ldots)\left\{\begin{matrix}1\\ \sum_{i\le A_1<j}V_{ij}\end{matrix}\right\}$$
$$\times\sum_{S}(-)^{I_S}\chi_{n_{A1'}}(\vec{r}_{S,1}-\underline{\vec{R}}_{A_1},\ldots)\chi_{n_{A2'}}(\vec{r}_{S,A_1'+1}-\underline{\vec{R}}_{A_2},\ldots)\prod_{\nu=1}^{A}d\tau_\nu, \tag{36}$$

where $\lambda=(n_{A_1},n_{A_2})$, $\lambda'=(n_{A_1'},n_{A_2'})$, and $\vec{r}_{A_1A_2}=\underline{\vec{R}}_{A_1}-\underline{\vec{R}}_{A_2}$. If the many-body functions $\chi_{n_{A1}}$, $\chi_{n_{A2}}$ are constructed from single-particle functions which are mutually orthogonal with respect to both centers at $\underline{\vec{R}}_{A_1}$ and $\underline{\vec{R}}_{A_2}$, then we have $F_{\lambda\lambda'}=\delta_{\lambda\lambda'}$. This is the case in the two-center shell model, as we shall see in Sec. III B.

III. PARTICLE-CORE MODEL

In the study of antisymmetrization effects in heavy-ion scattering, it is convenient to describe each nucleus in terms of a core and extracore particles.[11] The core is defined as the assembly of deep-shell nucleons in the potentials of the two fragments. It is not treated explicitly but described by collective coordinates. Only the extracore particles are treated microscopically. The relative motion of the nuclei is represented by the relative coordinate $\vec{r}$ between the centers of mass of both nuclei. When the number of core particles is large compared to the number of the extracore particles, the distance between the cores is approximately equal to the distance between the mass centers of the two nuclei. Therefore, in the particle-core model the distance between the mass centers of the cores serves very naturally as the relative coordinate for the scattering problem (see Fig. 2).

Within the spirit of the particle-core model only the antisymmetrization of the wave functions of the extracore particles is considered. For identical

cores, the intrinsic wave functions of the cores should be symmetrized. This corresponds to the change of the relative coordinate $\vec{r}$ of the cores to $-\vec{r}$. A physical justification for the antisymmetrization of the extracore part only is that for heavy-ion scattering the region of the contact of two colliding nuclei is the most important area where the overlap of the cores is much smaller than that of the extracore particles. Furthermore, the extracore particles are loosely bound and their exchange leads to antisymmetrization effects in the scattering which are expected to be much more important than those of the core particles. In addition the imaginary part of the ion-ion potential which increases for decreasing ion-ion distance reduces more the exchange contribution of the cores than that of the extracore particles.

An important advantage of the particle-core model is that the interchange of the extracore particles leaves the relative coordinate of the scattering problem unchanged. Moreover, the model simplifies the antisymmetrization problem greatly in many practical cases by reducing the number of nucleons whose interchange need to be considered.

For example, the scattering of ^{18}O on ^{18}O may be studied within the model by considering the ^{18}O nucleus as a ^{16}O core (a closed-shell nucleus) plus two loosely bound neutrons. Another example of the particle-core model is the study of the ^{12}C-(^{16}O, ^{16}O)^{12}C reaction by von Oertzen,[21] who considered the ^{16}O nucleus as a ^{12}C core plus an α cluster and investigated the exchange effects of the α cluster between the two identical ^{12}C cores (for more examples see Ref. 10).

If A_1 and A_2 denote the number of nucleons in the two colliding nuclei 1 and 2, respectively, and N_1 and N_2 corresponding numbers of extracore nucleons, the total nucleon number A of the system is given by

$$\begin{aligned} A &= A_1 + A_2 \\ &= [(A_1 - N_1) + N_1] + [(A_2 - N_2) + N_2] \\ &= (A - N) + N , \end{aligned} \tag{37}$$

where $N = N_1 + N_2$ is the total number of the extracore nucleons in the system. For the scattering of identical nuclei, $A_1 = A_2 = A/2$ and $N_1 = N_2 = N/2$.

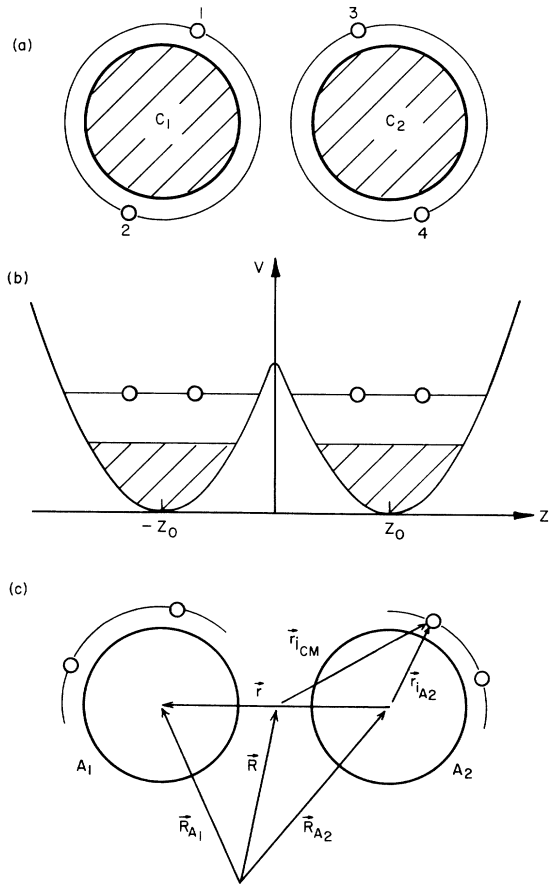

FIG. 2. The particle-core model. (a) Schematic sketch of the model. (b) The two-center oscillator potential. The deep shells which are not explicitly treated (cores) are dashed. The centers are concentrated at $z = \pm z_0$. (c) Definition of the various coordinates.

A. Hamiltonian

In the particle-core model the Hamiltonian of the system may be written in the form (see also Ref. 11)

$$H = T_{C_1} + T_{C_2} + W(\vec{r}_{C_1 C_2}) + \sum_{i=1}^{N} h(i) + \sum_{i<j}^{N} V_{ij} - T_{\text{c.m.}} , \tag{38}$$

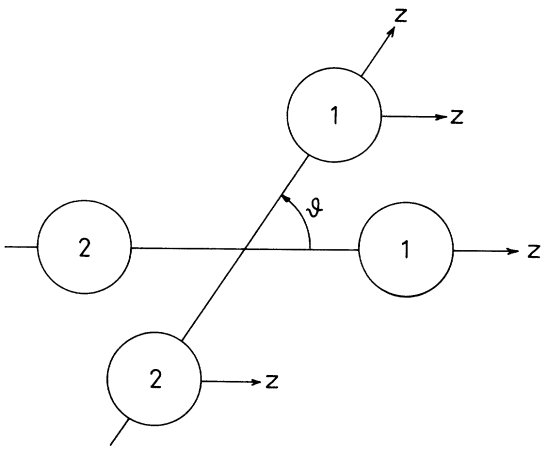

FIG. 3. Rotating coordinate system. The arrows give the direction of the laboratory z axis and the intrinsic z' axis. The angle θ between them is the scattering angle.

with

$$h(i) = t_i + U(\vec{r}_i, \vec{r}_{C_1C_2}) .$$

The Hamiltonian contains the kinetic energies T_{C_1} and T_{C_2} of the cores 1 and 2 and the intrinsic energy and their mutual interaction $W(\vec{r}_{C_1C_2})$ which depends on the relative distance $\vec{r}_{C_1C_2}$ between the cores (see Fig. 2). The one-body operators $h(i)$ describe the motion of the extracore particles within an effective shell-model potential $U(\vec{r}_i, \vec{r}_{C_1C_2})$ generated by the cores. This may be the potential of the two-center shell model. The two-body operators V_{ij} represent the interaction between the extracore particles. An extension of this ansatz may include the dependence of the Hamiltonian on the intrinsic core coordinates. The approximation of the particle-core model consists of the neglect of the internal degrees of freedom of the cores. A further improvement may be obtained by allowing collective modes, such as surface vibrations, rotations, and giant-resonance oscillations for the cores. We shall not, however, pursue here this extension, which is rather straightforward.

It is convenient to describe the scattering of the two nuclei by the relative distance between the nuclear centers and by the coordinates of the extracore particles. The relative coordinate $\vec{r}$ depends on the partition of the extracore particles, as explained in Eqs. (2)–(4). When the numbers of the extracore particles are much smaller than those of the core particles, i.e., $N_i/(A_i - N_i) \ll 1$, the relative coordinate can be approximated by the distance between the cores, i.e., $\vec{r} \approx \vec{r}_{C_1C_2}$. In this approximation the distance $\vec{r}_{C_1C_2}$ in the potentials W and U in (38) may be replaced by $\vec{r}$.

The relative coordinate $\vec{r}$ includes already the relative motion of the centers of mass of the extracore particles against each other. Therefore, one choice of the coordinates of the extracore particles is to measure the particle positions from the centers of mass of the nuclei to which each particle belongs. Another possibility is to measure the coordinates of the particles from the center of mass of the total system. Both cases are studied in the Appendix A. For $N_i/A_i \ll 1$ the kinetic energy in the particle-core model can be written, according to Eqs. (A7) and (A8) of Appendix A, as

$$T = \frac{1}{2\mu} P_r^{\,2} + \frac{1}{2M} \sum_{i=1}^{N_1} P_{i_{A1}}^{\,2} + \frac{1}{2M} \sum_{i=N_1+1}^{N} P_{i_{A2}}^{\,2} \qquad (39)$$

or

$$T = \frac{1}{2\mu} P_r^{\,2} + \frac{1}{2M} \sum_{i=1}^{N} P_{i_{\text{c.m.}}}^{\,2} ,$$

where μ is the reduced mass, $\mu = [A_1A_2/(A_1 + A_2)]M$, and $\vec{P}_r$ denotes the momentum of the relative motion. The particle momenta $\vec{P}_{i_{A_1}}$ and $\vec{P}_{i_{A_2}}$ are referred to the individual centers of mass at $\vec{R}_{A_1}$ and $\vec{R}_{A_2}$ (see Fig. 1). Here, we assumed that particles with $i \leq N_1$ belong to the nucleus A_1 and particles with $i > N_1$ to the nucleus A_2. The momenta $\vec{P}_{i_{\text{c.m.}}}$ are referred to the center of mass of the total system at $\vec{R}$. Thus, the Hamiltonian (38) can be approximated, when $N_i/A_i \ll 1$, by

$$H = H_0 + H_1 + H_2 , \qquad (40)$$

with

$$H_0 = \frac{1}{2\mu} P_r^{\,2} + W(r) , \qquad (40a)$$

$$H_1 = \sum_{i=1}^{N} h(i) , \qquad (40b)$$

and

$$H_2 = \sum_{i<j}^{N} V_{ij} , \qquad (40c)$$

where H_1 can be written as

$$\sum_{i=1}^{N_1} \frac{1}{2M} P_{i_{A1}}^{\,2} + U\left(\vec{r}_{i_{A1}} + \frac{A_2}{A}\vec{r}, \vec{r}\right) + \sum_{i=N_1+1}^{N} \frac{1}{2M} P_{i_{A2}}^{\,2} + U\left(\vec{r}_{i_{A2}} - \frac{A_1}{A}\vec{r}, \vec{r}\right) \qquad (41)$$

or

$$\sum_{i=1}^{N} \frac{1}{2M} P_{i_{\text{c.m.}}}^{\,2} + U(\vec{r}_{i_{\text{c.m.}}}, \vec{r}) .$$

The Hamiltonian has been divided into operators which are ordered according to the number of extracore particles involved in the operators. The particle coordinates $\vec{r}_{i_{A1}}$ and $\vec{r}_{i_{A2}}$ are measured from the nuclear centers at $\vec{R}_{A_1}$ and $\vec{R}_{A_2}$, respectively, and the coordinates $\vec{r}_{i_{\text{c.m.}}}$ from the center of mass at $\vec{R}$. They are defined in the Appendix A (see Fig. 2).

B. Wave Function

1. *Angular Momentum Coupling in the Framework of the Two-Center Shell Model*

For scattering involving two heavy ions the total, not yet antisymmetrized, wave function of the system can usually be written as

$$\Psi = \sum_{\lambda LJI} R_{\lambda LJI}(r)[i^L Y_L(\theta, \phi) \otimes \Phi_{\lambda J}]_{IM} , \qquad (42)$$

where $R_{\lambda LJI}(r)$ represents the wave function describing the relative motion of the colliding nuclei with the orbital angular momentum L when the channel spin is J and the total angular momentum

of the system is I. The function $\Phi_{\lambda J}$ is the intrinsic wave function for the total system describing all degrees of freedom except the center of mass and the relative motion. Here, λ denotes a set of intrinsic quantum numbers. The structure of the wave function (42) is convenient in the asymptotic region ($r \geq R_1 + R_2$, where R_i are the nuclear radii). We will show in the following that the wave function (42) can be brought to a strong-coupling form, which is more advantageous for the internal region (strong-coupling region, i.e., for $r < R_1 + R_2$) than the representation (42). In the internal region the orbital angular momentum L and the channel spin J are strongly coupled and hence they are no good quantum numbers.

In scattering experiments, scattered nuclei are usually detected at some angles $\hat{r}'$ with the incident direction $\hat{r}$. The total angular momentum I and its projection M along a fixed quantization axis (z axis) remain good quantum numbers during the scattering process (see Fig. 3). On the other hand, if the scattering is described in terms of the two-center shell model,[16] the quantization axis is always taken along the direction connecting the two centers (z' axis in Fig. 3). This means that the quantization axis rotates with the scattering angles and is not fixed in space.

Since the projection of the total angular momentum M on a space-fixed axis is a good quantum number during the scattering, we construct wave functions from the two-center single-particle wave function and rotate them to a space-fixed axis (say, z axis).

In the simplest case the two-center potential is symmetric. For large separation distance of the two centers the wave functions approach asymptotically the one-center wave functions bound in general to both individual centers. Since the two-center potential approaches to spherically symmetric potentials around each center, one can construct new two-center wave functions which are bound asymptotically only to one center and have good angular momentum quantum number with respect to this center (see Appendix B and Fig. 4). Such wave functions are automatically obtained in the case of the asymmetric two-center shell model (asymmetric break-up).[17,18] We denote the single-particle wave functions by $\varphi^{\pm}_{n(j)m}$, where

$$\lim_{z_0 \to \infty} \varphi^{\pm}_{n(j)m} = \varphi_{njm}(x', y', z' \mp z_0) . \tag{43}$$

Here, we note that j is only asymptotically a good quantum number. Therefore, j is placed inside parentheses.

The plus and minus signs indicate that the wave functions are asymptotically concentrated around the right or left side in the two-center potential, respectively. The distance between the two centers is $r = 2z_0$ (see Fig. 2). The set of all other quantum numbers is denoted by n, and the coordinates x', y', z' are related to a rotating system (see Fig. 3). For later convenience we require the following phase convention between the two wave functions (symmetric two-center shell model):

$$\varphi^{+}_{n(j)m}(x', -y', -z') = (-1)^{j-2m} \varphi^{-}_{n(j)-m}(x', y', z') . \tag{44}$$

This symmetry is identical with the R_2 symmetry (rotation around the x' axis) of the rotation-vibration model.[15]

According to the usual shell-model procedure we construct many-body wave functions $\chi^{\pm}_{(I)M}$ from these single-particle wave functions which describe asymptotically nuclei with definite angular momenta I and M concentrated at the right or left center indicated by the $\pm$ sign. The intrinsic wave function of the total system is then given in the rotating system by

$$\begin{aligned} \tilde{\Phi}_{\lambda(J)M}(1', 2', r) &= [\chi^{+}_{(I_1)}(1') \otimes \chi^{-}_{(I_2)}(2')]_{(J)M} \\ &= \sum_{M_1 M_2} (I_1 I_2 M_1 M_2 | JM) \chi^{+}_{(I_1)M_1}(1') \chi^{-}_{(I_2)M_2}(2') . \end{aligned} \tag{45}$$

Here, the sets of the particle coordinates are abbreviated by $1'$ and $2'$. The coordinates are referred to a rotating coordinate system in which the z' axis is defined by the direction connecting the two centers. This z' axis serves also as quantization axis. The wave function $\tilde{\Phi}_{\lambda(J)M}(1', 2', r)$ has good angular momentum only at large separation distance of the two nuclei, and hence J is denoted by parentheses.

The rotated coordinate system is specified with respect to the laboratory system by the two angles ϕ and θ of the relative coordinate and a third angle Ψ which describes a rotation around the z' axis (see Appendix A). We assume that the Hamiltonian of the system is expressed to depend on the relative coordinate and the intrinsic particle coordinates of the rotating frame. For example, the two-center shell-model Hamiltonian can be used for the intrinsic Hamiltonian H_1. As in the rotator model with extracore particles, the three angles describe the rotation of the whole system so that their canonically conjugate momenta are related with the total angular momentum operator. Hence,

$$\Phi_{\lambda(J)M} = \sum_{M'} D^{J*}_{MM'}(\phi, \theta, \Psi) \tilde{\Phi}_{\lambda(J)M'}(1', 2', r) . \tag{46}$$

This superposition of the two-center wave function has asymptotically the intrinsic angular momentum J and the projection M on the space-fixed axis.

If we insert the wave function $\Phi_{\lambda(J)M}$ into the ansatz (42), we obtain a wave function which has asymptotically the orbital angular momentum L and the intrinsic angular momentum J of the nuclei:

$$R_{\lambda LJI}(r)\left[i^L Y_L(\theta,\phi)\otimes\sum_{M'} D^{J*}_{MM'}(\phi,\theta,\Psi)\tilde{\Phi}_{\lambda(J)M'}(1',2',r)\right]_{IM}$$
$$= R_{\lambda LJI}(r)\sum_{M'} i^L\left(\frac{2L+1}{4\pi}\right)^{1/2}(LJ0M'|IM')D^{I*}_{MM'}(\phi,\theta,\Psi)\tilde{\Phi}_{\lambda(J)M'}(1',2',r)\,. \tag{47}$$

Here, we used the identity[22]

$$\sum_m (L\,J\,m\,M-m|IM)Y_{Lm}D^{J*}_{M-m\,M'} = \left(\frac{2L+1}{4\pi}\right)^{1/2}(LJ0M'|IM')D^{I*}_{MM'}\,. \tag{48}$$

In Eq. (47) L and J are asymptotic quantum numbers just like the asymptotic quantum numbers of the Nilsson model. If we write the most general solution in the form

$$\Psi = \sum_{\lambda JIM'} \tilde{R}_{\lambda(J)IM'}(r)D^{I*}_{MM'}(\phi,\theta,\Psi)\tilde{\Phi}_{\lambda(J)M'}(1',2',r)\,, \tag{49}$$

then the analogy with the strong-coupling wave functions of the rotation-vibration model and the unified model becomes evident.[15] In this connection it is worthwhile to comment on the symmetries of the wave functions. In the rotation-vibration model two very essential symmetries are required, namely, the invariance of the wave function under rotations through π around the intrinsic z' axis and the x' (or y') axis. The last symmetry is connected with the exchange symmetry of identical nuclei [see Eq. (51)]. The first symmetry usually leads to the condition $K-\Omega=2\nu$ ($\nu=0,1,2,\ldots$) for the wave function $D^{I*}_{MK}\tilde{\Phi}_{\lambda(J)\Omega}$. In our case there results $\nu=0$ only, which simply means that rotations described by the angle Ψ are redundant, i.e., they are already described by the wave function $\tilde{\Phi}_{\lambda(J)M}$ in its dependence on the particle coordinates. (See the later discussion of $\tilde{\Phi}_{\lambda(J)M}$ in connection with the particle-core model.) The wave function (49) becomes asymptotically (i.e., for $r\to\infty$) a superposition of eigenstates of L^2 and J^2, in addition to I^2, provided that

$$\tilde{R}_{\lambda(J)IM'}(r)\xrightarrow[r\to\infty]{}\sum_L R_{\lambda LJI}(r)\,i^L\left(\frac{2L+1}{4\pi}\right)^{1/2}\times(LJ0M'|IM')\,.$$

This condition expresses the dependence of the radial wave function R on the substates M' in the asymptotic region. Since the total angular momentum operator has to be expressed in terms of the differential operators acting on the angles, one immediately verifies that the wave function (47) has good total angular momentum I and good projection M on the space-fixed z axis. One can easily show that the wave function has also a good angular momentum asymptotically, by writing the orbital angular momentum operator $\vec{L}$ in the rotating coordinate system:

$$\vec{L}=\vec{I}-\vec{J}'\,, \tag{50}$$

where $\vec{I}$ is the total angular momentum operator of the system, and $\vec{J}'=\vec{I}_1'+\vec{I}_2'$ is the sum of the intrinsic angular momentum operators of the nuclei with respect to their centers [see Eq. (A13)]. Asymptotically it yields

$$\vec{J}'^2\tilde{\Phi}_{\lambda(J)M}(1',2',r)\xrightarrow[r\to\infty]{}J(J+1)\hbar^2\tilde{\Phi}_{\lambda(J)M}\,.$$

The fact that the operator $\vec{I}$ acts on the Euler angles of the wave function (47) only, together with the above equation, indeed proves that the orbital angular momentum becomes asymptotically a good quantum number. Therefore, the wave function (47) can be used to solve the scattering problem since, as in ansatz (42), asymptotically the angular momentum splits into the orbital and the intrinsic angular momenta.

For the case of identical nuclei, the wave functions are usually symmetrized for the exchange of all particles between the two nuclei. With the aid of Eq. (44) it turns out that the intrinsic wave function which is written in the rotating coordinate system has to be symmetrized as the intrinsic wave function in the laboratory system:

$$\tilde{\Phi}_{\lambda(J)M}\sim[\chi^+_{(I_1)}(1')\otimes\chi^-_{(I_2)}(2') + (-)^L\chi^-_{(I_1)}(2')\otimes\chi^+_{(I_2)}(1')]_{JM}\,. \tag{51}$$

2. *Intrinsic Wave Function*

The intrinsic wave function can be chosen in two different ways. In the first case one chooses the product of the individual shell-model configurations of the two fragments as a basis. These configurations are not mutually orthogonal. In the second case the antisymmetrized orthogonal two-center shell-model wave functions are chosen as basis states which are prediagonalized states.

For simplicity of the discussion the two cores are assumed to be composed of the same even-even nucleus which can in general be in different states. The numbers of extra-core particles in both nuclei, however, need not to be the same. Since the number of extracore nucleons is smaller than the number of core nucleons, the relative coordinate $\vec{r}$ is approximately equal to the distance between the cores. When all nucleons are exchanged between two nuclei having the same number of nucleons, the relative coordinate $\vec{r}$ transforms to $-\vec{r}$. Even for two nuclei with different numbers of nucleons, $\vec{r}$ transforms to $-\vec{r}$ approximately when the cores as well as a maximum number of extra-core particles are exchanged.

The intrinsic wave function $\Phi_{\lambda J}$ is assumed to be separable into wave functions for the cores and extracore particles. In the present treatment the antisymmetrization between the cores and extra core particles is neglected. It is useful to express the wave function as a sum of two terms, the first representing the usual product of the intrinsic wave functions of the cores and extracore particles, the second corresponding to the similar product with exchange of all core particles between the two nuclei. In the second case, the z' axis of the rotating coordinate system is reversed to the $-z'$ axis. When the states of the cores are the same, the second term gives the largest overlap with the first term. Other wave functions corresponding to exchange of only a part of the core particles all give smaller overlaps with the first term. Thus, we write

$$\Phi_{\lambda JM} \sim \mathcal{A}(1,\ldots,N)\{[\chi_{I_{C1}}(\mathrm{I},+z_0)\otimes\Phi_{I_{N1}}(1,2,\ldots,N_1,+z_0)]_{I_1}\otimes[\chi_{I_{C2}}(\mathrm{II},-z_0)\otimes\Phi_{I_{N2}}(N_1+1,\ldots,N,-z_0)]_{I_2} + (-)^L[\chi_{I_{C1}}(\mathrm{II},-z_0)\otimes\Phi_{I_{N1}}(1,2,\ldots,N_1,-z_0)]_{I_1}\otimes[\chi_{I_{C2}}(\mathrm{I},+z_0)\otimes\Phi_{I_{N2}}(N_1+1,\ldots,N,+z_0)]_{I_2}\}_{JM}. \tag{52}$$

Here, L is the orbital angular momentum. The antisymmetrization operator $\mathcal{A}$ acts on the coordinates of the extracore particles described by the wave functions $\Phi_{I_{N1}}$ and $\Phi_{I_{N2}}$ concentrated around the center at $z' = \pm z_0$ (see Fig. 2). They are already antisymmetrized, e.g.,

$$\Phi^{\pm}_{I_{N1}} = \Phi_{I_{N1}}(1,\ldots,N_1,\pm z_0) = (N_1!)^{-1/2}\mathcal{A}\{\varphi^{\pm}_{A_1 n_1}(1)\otimes\varphi^{\pm}_{A_1 n_2}(2)\otimes\cdots\}_{I_{N1}}, \tag{53}$$

with the single-particle wave functions $\varphi^{\pm}_{A_i n_j}$ corresponding to the nucleus A_i and discussed in connection with Eqs. (43) and (44). Both sets of single-particle wave functions $\varphi^{\pm}_{A_i n_j}$ are orthonormalized, but they are not necessarily mutually orthogonal.

In Eq. (52) the intrinsic wave functions of the cores are denoted by $\chi_{I_{C1}}$ and $\chi_{I_{C2}}$. The intrinsic coordinates of the cores are abbreviated by I and II. In most cases of application both cores are in the ground state with zero spin. Therefore, we restrict further discussion to this case, namely, $\chi_{I_{C1}} = \chi_{I_{C2}} = \chi_0$. One possible extension of the present work is to describe the cores by the vibrational wave functions $\chi(\alpha_{2\mu})$ of the collective model.[23] The symmetries discussed in the last section apply again for the total intrinsic wave function, which is then constructed of products of particle and collective wave functions. In the case when $I_{C_1} = I_{C_2} = 0$, the spin of the nuclei is due to the angular momentum of the extracore particles, i.e., $I_1 = I_{N_1}$ and $I_2 = I_{N_2}$. The wave functions $\Phi_{\lambda JM}$ may be simply written as

$$\Phi_{\lambda JM} \sim \chi_0(\mathrm{I})\chi_0(\mathrm{II})\mathcal{A}\varphi_d(1,2,\ldots,N_1;N_1+1,\ldots,N), \tag{54}$$

where

$$\varphi_d = [\Phi_{I_1}(1,2,\ldots,N_1,+z_0)\otimes\Phi_{I_2}(N_1+1,\ldots,N,-z_0) + (-1)^L\Phi_{I_1}(1,2,\ldots,N_1,-z_0)\otimes\Phi_{I_2}(N_1+1,\ldots,N,+z_0)]_{JM}. \tag{55}$$

It proves useful to expand the wave function $\Phi_{\lambda JM}$ according to the number of nucleons exchanged between the two nuclei. For this purpose, we define the normalized direct, nonexchange wave function Φ_d as the product of the wave functions of the two nuclei:

$$\Phi_d(1,\ldots,N_1;N_1+1,\ldots,N) = [\langle\varphi_d|\varphi_d\rangle]^{-1/2}\chi_0(\mathrm{I})\chi_0(\mathrm{II})\,\varphi_d(1,\ldots,N_1;N_1+1,\ldots,N). \tag{56}$$

The exchange wave function $\Phi^{(i)}_{\mathrm{ex},l}$ corresponding to the exchange of l nucleons can be similarly expressed, as shown in Eq. (11). For example,

$$\Phi^{(i)}_{\mathrm{ex},1} = \Phi_d(1,N_1+1,3,\ldots,N_1;2,N_1+2,\ldots,N).$$

Here, the superscript i specifies a particular partition for an exchange of l particles. For an l-particle

exchange there are $\binom{N_1}{l}\binom{N_2}{l}$ possible combinations. The completely antisymmetrized and normalized intrinsic wave function $\Phi^A_{\rm int}$ can now be expanded according to the number of nucleons exchanged[8]:

$$\Phi^A_{\rm int} \equiv \Phi_{\lambda JM} = \left(\frac{N_1!N_2!}{N!f}\right)^{1/2}\left[\Phi_d + \sum_{l=1}^{N_1}(-1)^l \sum_{i=1}^{\binom{N_1}{l}\binom{N_2}{l}} \Phi^{(i)}_{{\rm ex},l}\right]. \tag{57}$$

Here, we assumed $N_1 < N_2$. As will be shown in Sec. IV A, the normalization constant f is given by

$$f = 1 + \sum_{l=1}^{N_1}(-1)^l \binom{N_1}{l}\binom{N_2}{l}\langle\Phi_d|\Phi_{{\rm ex},l}\rangle . \tag{58}$$

C. System of Coupled Equations

The same method on which the approximation given in Eq. (35) is based is used to derive a system of coupled equations which describes the relative motion of the nuclei in the particle-core model. For this we integrate the Hamiltonian (40), over the extracore particle and intrinsic core coordinates and over the angle coordinates of the relative motion using the wave functions constructed in the preceding section, III B. The Schrödinger equation with the model Hamiltonian (40) is given by

$$H\Psi = E\Psi . \tag{59}$$

The wave function Ψ can be expanded according to Eq. (42) or Eq. (47), which are rewritten here for convenience:

$$\Psi = \sum_{\lambda LJI} R_{\lambda LJI}(r)[i^L Y_L \otimes \Phi_{\lambda J}]_{IM} , \tag{60a}$$

or

$$\Psi = \sum_{\lambda LJI}\left(\frac{2L+1}{4\pi}\right)^{1/2} i^L R_{\lambda(LJ)I}(r)\sum_{M'}(LJ0M'|IM')D^{I*}_{MM'}\tilde{\Phi}_{\lambda(J)M'} . \tag{60b}$$

Only when J is a good quantum number, Eqs. (60a) and (60b) are identical expansions. Both types of wave functions are useful, depending on the choice of the single-particle states from which Φ is constructed.

(a) First we consider the case when the wave functions Φ in Eq. (60a) are constructed in terms of asymptotic single-particle states which are bound to individual centers, e.g., one-center oscillator states. These states have good angular momentum j, so that the single-particle states can be coupled to the angular momentum J of the extracore particles. Then the angular momentum J in Eq. (60a) is a good quantum number which is independent of the relative distance of the nuclear centers. In addition to the intrinsic motion, the wave functions $\Phi_{\lambda J}$ describe physically irrelevant spurious oscillations of the centers of mass. To be consistent we have to omit the coupling terms between the spurious and relative motions, as was done in Eq. (39). Since the one-body Hamiltonian H_1 is usually given in the coordinates of the rotating system, it is convenient to transform the intrinsic functions $\Phi_{\lambda J}$, according to Eq. (46), to the rotating system. Thereby, Eq. (60a) transforms to Eq. (60b), and then by applying (60b), we obtain from Eq. (59), the following system of coupled equations:

$$\begin{aligned}\left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}+\frac{L(L+1)\hbar^2}{2\mu r^2}+W(r)-E+\sum_M (JIM-M|L0)^2\langle\tilde{\Phi}_{\lambda JM}|H_1+H_2|\tilde{\Phi}_{\lambda JM}\rangle\right]R_{\lambda LJI}(r)\\ = -\sum_{\lambda'L'J'\neq(\lambda LJ),M} i^{L-L'}(JIM-M|L0)(J'IM-M|L'0)\left[\left(-\frac{\hbar^2}{2\mu r^2}\frac{d}{dr}r^2\frac{d}{dr}+\frac{L(L+1)\hbar^2}{2\mu r^2}+W(r)-E\right)\langle\tilde{\Phi}_{\lambda JM}|\tilde{\Phi}_{\lambda'J'M}\rangle\right.\\ \left.+\langle\tilde{\Phi}_{\lambda JM}|H_1+H_2|\tilde{\Phi}_{\lambda'J'M}\rangle\right]R_{\lambda'L'J'I}(r) ,\end{aligned} \tag{61}$$

where H_1 and H_2 are defined by (40b) and (40c).

In Eq. (61) we assume that the one-body Hamiltonian H_1 is invariant under rotations around the z' axis in the rotating coordinate frame (see Fig. 3) so that no states with different angular momentum M are mixed by H_1. The right-hand side of Eq. (61) contains all the coupling terms to the inelastic channels.

(b) Next we study the case when the single-particle states in $\tilde{\Phi}$ of Eq. (60b) are solutions of the Hamiltonian H_1 of the two-center shell model. Then the particle-core interaction is already prediagonalized. An

advantage of this method is that the single-particle functions are mutually orthogonal with respect to different nuclear centers and hence the calculation of the potentials is considerably simplified, as will be shown in Sec. IV. The wave functions $\tilde{\Phi}$ do not fulfill the requirement of true intrinsic wave functions, i.e., they are not independent of the relative motion of the nuclear centers besides the spurious oscillations of the centers of mass of the extracore particles. We consider the dependence of the two-center wave functions on the relative coordinate $\vec{r}$ as physically relevant. They describe already an important coupling of the relative and the intrinsic motions, contained in H_1. Therefore, the angular momentum operator $\vec{J}$ has a good quantum number J only in the asymptotic region where the nuclear centers are well separated. Then the orbital angular momentum appearing in the Hamiltonian is r-dependent, and has to be calculated according to Eq. (50) using the coordinates of the rotating frame [see also Eq. (A12)]. We obtain from Eqs. (59) and (60b)

$$\left[T_{\lambda(LJ)I}(r)+W(r)-E+\sum_M (JIM-M\,|\,L0)^2\langle\tilde{\Phi}_{\lambda(J)M}|H_1+H_2|\tilde{\Phi}_{\lambda(J)M}\rangle\right]R_{\lambda(LJ)I}(r)$$

$$=-\sum_{M'M'',\lambda'J'L'\neq(\lambda JL)} i^{L-L'}(-)^{M''-M'}(JIM''-M''\,|\,L0)(J'IM'-M'\,|\,L'0)$$

$$\times\frac{2I+1}{8\pi^2}\langle D^{I*}_{MM''}\tilde{\Phi}_{\lambda(J)M''}|H-E|D^{I*}_{MM'}\tilde{\Phi}_{\lambda'(J')M'}\rangle R_{\lambda'(L'J')I}(r)\,. \tag{62}$$

Since the intrinsic functions $\tilde{\Phi}$ now have a physically relevant dependence on the relative coordinate $\vec{r}$, the operator $\vec{p}_r$ of the relative motion in the kinetic energy of Eq. (40a) has to act also on the intrinsic function $\tilde{\Phi}$. Therefore, the operator $T_{\lambda(LJ)I}(r)$ of the kinetic energy on the left-hand side of Eq. (62) is given by

$$T_{\lambda(LJ)I}=-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}+\sum_M (JIM-M\,|\,L0)^2\right.$$

$$\left.\times\left(2\left\langle\tilde{\Phi}_{\lambda(J)M}\left|\frac{\partial}{\partial r}\right|\tilde{\Phi}_{\lambda(J)M}\right\rangle\frac{d}{dr}+\left\langle\tilde{\Phi}_{\lambda(J)M}\left|\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\right|\tilde{\Phi}_{\lambda(J)M}\right\rangle\right)\right]$$

$$+\frac{1}{2\mu r^2}\sum_{M'M''}(-)^{M''-M'}(JIM'-M'\,|\,L0)(JIM''-M''\,|\,L0)\frac{2I+1}{8\pi^2}\langle D^{I*}_{MM'}\tilde{\Phi}_{\lambda(J)M'}|(\vec{I}-\vec{J}')^2|D^{I*}_{MM''}\tilde{\Phi}_{\lambda(J)M''}\rangle\,. \tag{63}$$

The coupling term $\langle\tilde{\Phi}\,|\,\partial/\partial r\,|\,\tilde{\Phi}\rangle$ is imaginary and vanishes for the usual two-center shell-model wave functions. The nondiagonal matrix elements $\langle\tilde{\Phi}_\lambda\,|\,\partial/\partial r\,|\,\tilde{\Phi}_{\lambda'}\rangle$ are different from zero and contribute on the right-hand side of Eq. (62). They, together with the other nondiagonal terms of the kinetic-energy operator, describe the nonadiabaticity of the scattering process (Zener effect[24]). The term

$$\left\langle\tilde{\Phi}\left|\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}\right|\tilde{\Phi}\right\rangle$$

acts as an r-dependent additional potential. Such a potential must occur if one uses a relative coordinate which leads to the reduced mass for all distances r in the relative motion.[25] The additional potential vanishes outside of the overlap region of the two nuclei. The operator $\vec{J}'$ is the angular momentum operator of the extracore particles referred to the origin of the coordinates of the rotating frame [see Eq. (A14)]. The total angular momentum operator $\vec{I}$, expressed in Euler angles, acts on the rotator functions $D^{I*}_{MM'}$. The Coriolis term which is proportional to $\vec{I}\cdot\vec{J}'$ is the only operator which mixes states with different intrinsic angular momentum projection M'. If axially asymmetric deformations are introduced in the two-center shell-model potential, of course, additional M'-mixing terms will occur. Except for a small r-independent contribution which can be neglected for small ratios $N_i/A_i\ll 1$, as discussed in Appendix A [Eq. (A10)], Eq. (63) has the same asymptotic behavior as Eq. (61),

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}+\frac{L(L+1)\hbar^2}{2\mu r^2}+W(r)-E+\langle\tilde{\Phi}_{\lambda(J)M}|H_1+H_2|\tilde{\Phi}_{\lambda(J)M}\rangle\right]R_{\lambda(LJ)I}(r)=0\quad\text{for } r\to\infty\,.$$

Which of the two types of wave functions, constructed from one- or two-center shell-model functions, is the most convenient one depends on the problem under consideration, especially on the relation between the strength of the particle-core and the core-core interactions.

IV. DIRECT AND EXCHANGE POTENTIALS

In addition to the core-core interaction $W(r)$, the extracore particles contribute an effective potential in Eq. (61) or Eq. (62) which is the sum of the expectation values of the one- and two-body Hamiltonians H_1 and H_2 with the intrinsic wave functions. That is,

$$V(r)=\sum_M (JIM\ -M|\ L0)^2\langle\tilde{\Phi}_{\lambda(J)M}|H_1+H_2|\tilde{\Phi}_{\lambda(J)M}\rangle\,. \tag{64}$$

This equation represents an average over the matrix elements with different M values. In this section we calculate the matrix elements occurring in (64). The matrix elements are the same in the space fixed and rotating systems for $\vec{r}=r\hat{z}$, i.e., if both coordinate systems coincide. Therefore, we are allowed to use the functions $\Phi_{\lambda(J)M}$ which are identical to $\Phi^A_{\rm int}$ [see Eq. (57)] with the subsidiary condition $\vec{r}=r\hat{z}$:

$$V_n=\langle\tilde{\Phi}_{\lambda(J)M}|H_n|\tilde{\Phi}_{\lambda(J)M}\rangle=\langle\Phi^A_{\rm int}|H_n|\Phi^A_{\rm int}\rangle \quad \text{if } \vec{r}=r\hat{z}\,. \tag{65}$$

In the following, we study in detail all contributions which arise from the antisymmetrization in (65).

A. General Case

The additional contribution to the effective potential V_n of Eq. (65), due to antisymmetrization effects, is calculated from the difference

$$\Delta V_n(r)=\langle\Phi^A_{\rm int}|H_n|\Phi^A_{\rm int}\rangle-\langle\Phi_d|H_n|\Phi_d\rangle\,.$$

The operator H_n can be a one- or two-body operator, H_1 or H_2. The last term may be called the direct potential, since it is the contribution of H_n to V_n when no antisymmetrization between the nuclei is applied. It will now be shown that the correction term ΔV_n can be expanded according to the number of exchanged particles. Namely, using Eq. (57), we have

$$\int\Phi^{*A}_{\rm int}H_n\Phi^A_{\rm int}\,d\tau=\left(\frac{N!}{N_1!\,N_2!\,f}\right)^{1/2}\int\Phi^*_dH_n\Phi^A_{\rm int}\,d\tau=\frac{1}{f}\int\Phi^*_dH_n\left[\Phi_d+\sum_l(-1)^l\sum_{i=1}^{\binom{N_1}{l}\binom{N_2}{l}}\Phi^{(i)}_{{\rm ex},l}\right]d\tau\,.$$

Since the wave functions are antisymmetrized within one nucleus, the matrix elements $\langle\Phi_d|H_n|\Phi^{(i)}_{{\rm ex},l}\rangle$ are independent of i for all l values. Hence, we obtain the expectation value of H_n which is expanded according to the number of nucleons exchanged:

$$\langle\Phi^A_{\rm int}|H_n|\Phi^A_{\rm int}\rangle=\frac{1}{f}\left[\langle\Phi_d|H_n|\Phi_d\rangle+\sum_l(-1)^l\binom{N_1}{l}\binom{N_2}{l}\langle\Phi_d|H_n|\Phi_{{\rm ex},l}\rangle\right]. \tag{66}$$

This result is in agreement with a similar expansion for the scattering amplitude given by Goldberger and Watson.[8] Since both $\Phi^A_{\rm int}$ and Φ_d are normalized to unity, setting $H_n=1$ in (66) immediately yields the expression for the normalization constant f given in (58). Thus, the additional contribution to the effective potential due to antisymmetrization is given by

$$\Delta V_n=\left(\frac{1}{f}-1\right)\langle\Phi_d|H_n|\Phi_d\rangle+\frac{1}{f}\sum_l(-1)^l\binom{N_1}{l}\binom{N_2}{l}\langle\Phi_d|H_n|\Phi_{{\rm ex},l}\rangle\,. \tag{67}$$

B. Case of Identical Nuclei

Since we are primarily concerned in the scattering of two identical nuclei, such as the $^{14}N+{}^{14}N$ scattering, we now consider an important special case in which the extracore particles in both nuclei are in the same state, i.e., $I_1=I_2=I$. Furthermore, if, as in this case, $N_1=N_2=N/2$, the wave function (54) simplifies to

$$\Phi_{\lambda JM}\sim\chi_0({\rm I})\chi_0({\rm II})\,\mathcal{A}\,\varphi_d(1,2,\ldots,N/2;\,N/2+1,\ldots,N)\,, \tag{68}$$

with

$$\varphi_d=\tfrac{1}{2}[1+(-1)^{L+J+N/2}][\Phi_I(1,\ldots,N/2,+z_0)\otimes\Phi_I(N/2+1,\ldots,N,-z_0)]_{JM}\,. \tag{68a}$$

We note in (68a) that φ_d vanishes unless

$$L+J+N/2=\text{even}\,.$$

This means that the sum of the angular momentum quantum numbers L and J has to be even or odd for the scattering of identical nuclei depending whether the mass number A is even or odd. Indeed, for a nucleus with even number of core nucleons the number $N/2$ of extracore particles is even (odd) when A is even (odd). The direct wave function Φ_d can be constructed by inserting φ_d, given by (68a), into Eq. (56).

1. *Orthogonal Single-Particle Wave Functions*

The single-particle wave functions, which are the same in both nuclei when the nuclei are identical, are already orthonormal around each center. The formalism developed simplifies considerably when the single-particle wave functions of both centers are also mutually orthogonal, e.g.,

$$\langle \varphi_m^+ | \varphi_n^- \rangle = 0$$

for all m and n. Such wave functions are, for example, obtained from the two-center shell model. In this case all overlap integrals between the direct and exchange parts vanish, i.e.,

$$\langle \Phi_d | \Phi_{\mathrm{ex},l} \rangle = 0$$

for all l. It follows immediately from Eq. (58) that for orthogonal wave functions, we have $f = 1$.

We investigate now the structure of the various possible matrix elements. The Hamiltonian can be expressed as a sum of n-body operators H_n in the coordinates of the extracore particles [see Eq. (40)]. All matrix elements of the n-body operator H_n between the direct and l-nucleon exchange states vanish for l larger than $n/2$, i.e.,

$$\langle \Phi_d | H_n | \Phi_{\mathrm{ex},l} \rangle = 0 \quad \text{for } l > n/2 . \tag{69}$$

This is because, for example, an exchange of two nucleons necessarily involves a two-body force and a one-body force cannot exchange particles. For a one-body operator H_1, Eq. (69) implies

$$\langle \Phi_{\mathrm{int}}^A | H_1 | \Phi_{\mathrm{int}}^A \rangle = \langle \Phi_d | H_1 | \Phi_d \rangle = \langle \Phi | H_1 | \Phi \rangle , \tag{70}$$

where Φ is the wave function which is not antisymmetrized, namely

$$\Phi = \chi_0(I)\chi_0(II)\left[\prod_{k=1}^{N/2} \varphi_{n_k}^+(k) \otimes \varphi_{n_{N/2+k}}^-(N/2+k)\right]_{JM} . \tag{70a}$$

Thus, we obtain the following well-known result: When the Hamiltonian consists of one-body operators, which is symmetric in all particle coordinates, the Pauli principle is already fulfilled when simple product wave functions are used, such as Φ given in Eq. (70a), in which each particle occupies a different single-particle state.

For a two-body operator H_2 only one transition matrix element does not vanish, namely $\langle \Phi_d | H_2 | \Phi_{\mathrm{ex},1} \rangle$.

2. *Non-Orthogonal Single-Particle Wave Functions*

In general two sets of single particle functions φ_m^+ and φ_n^- are used which are orthonormalized with respect to each center at $z' = \pm z_0$ but which are not mutually orthogonal with respect to different centers (we call such wave functions *one-center functions*). That is,

$$\langle \varphi_m^+ | \varphi_n^- \rangle \neq 0 . \tag{71}$$

In the following we consider the consequences of Eq. (71). To simplify the further discussion we restrict us to the case of two identical nuclei with only two extracore particles bound to each center. Then, in the framework of the particle-core model, the wave function which is antisymmetrized between the extracore particles only may be written as follows:

$$\Phi^A = \frac{1+(-1)^{L+J}}{2} \frac{1}{\sqrt{f}} \chi_0(I)\chi_0(II) \sum_{m_1 m_2 m_3 m_4} C_{m_1 m_2 m_3 m_4} \frac{1}{\sqrt{4!}} \mathfrak{A}(\varphi_{m_1}(1)\varphi_{m_2}(2)\varphi_{m_3}(3)\varphi_{m_4}(4)) . \tag{72}$$

Here, the constant coefficients $C_{m_1 \ldots m_4}$ describe the coupling of the various angular momenta and are given by

$$C_{m_1 m_2 m_3 m_4} = [1-(-1)^{2j_1-I}\delta_{n_1 n_2}\delta_{j_1 j_2}](1+\delta_{n_1 n_2}\delta_{j_1 j_2})^{-2} \times (j_1 j_2 m_1 m_2 | I\, m_1+m_2)(j_1 j_2 m_3 m_4 | I\, m_3+m_4)(I\, I\, m_1+m_2\; m_3+m_4 | JM) . \tag{72a}$$

For convenience, the single-particle wave functions are abbreviated by

$$\varphi_{m_1}=\varphi^{+}_{n_1 j_1 m_1}, \quad \varphi_{m_2}=\varphi^{+}_{n_2 j_2 m_2}$$
$$\varphi_{m_3}=\varphi^{-}_{n_1 j_1 m_3}, \quad \varphi_{m_4}=\varphi^{-}_{n_2 j_2 m_4}. \tag{72b}$$

The single-particle states have angular momentum j with the projection m on the z axis of the laboratory system. By n we denote all additional quantum numbers including the isospin quantum number. The symbol m_i indicates not only the projection of the angular momentum on the z axis, but also to which center the wave function belongs; $i=1, 2$ means φ^{+} and $i=3, 4$ means φ^{-}. Introducing the matrix elements g_{ij} defined by the overlap integrals as

$$g_{ij}=\langle\varphi_{m_i}|\varphi_{m_j'}\rangle \quad (i,j=1,2,3,4), \tag{73}$$

the normalization constant f can be expressed in terms of the determinant, $\det(g)$ which is constructed with the matrix-elements g_{ij}, namely,

$$f=\sum_{m_1\cdots m_4}\sum_{m_1'\cdots m_4'} C_{m_1\cdots m_4}C_{m_1'\cdots m_4'}\det(g). \tag{74}$$

The expectation values of the one- and two-body operators H_1 and H_2 [see Eqs. (40b) and (40c)] are obtained using the matrix elements $g^{-1}{}_{ij}$ of the inverse matrix g^{-1}. Namely,

$$\left\langle\Phi^A\left|\begin{Bmatrix}H_1\\H_2\end{Bmatrix}\right|\Phi^A\right\rangle=\frac{1}{f}\sum_{m_1\cdots m_4}\sum_{m_1'\cdots m_4'}C_{m_1\cdots m_4}C_{m_1'\cdots m_4'}\det(g)$$
$$\times\begin{cases}\sum_{i,j=1}^{4}\langle\varphi_{m_i}|h|\varphi_{m_j'}\rangle g^{-1}{}_{ji}\\ \sum_{i,j,k,l=1}^{4}\langle\varphi_{m_i}\varphi_{m_j}|V|\varphi_{m_k'}\varphi_{m_l'}\rangle\frac{1}{2}(g^{-1}{}_{ki}g^{-1}{}_{lj}-g^{-1}{}_{kj}g^{-1}{}_{li}).\end{cases} \tag{75}$$

It is evident that this formalism is not restricted only to four extracore particles. In the general case one has only to replace the number 4 by the number N of the extracore particles.

In order to express the matrix elements in Eq. (75) in the form of the expansion similar to Eq. (66), we note that the direct function Φ_d in the expansion is given by

$$\Phi_d=\frac{1+(-1)^{L+J}}{2}\chi_0(\mathrm{I})\chi_0(\mathrm{II})\sum_{m_1\cdots m_4}C_{m_1\cdots m_4}\frac{1}{\sqrt{2}}\mathfrak{A}(\varphi^{+}_{m_1}(1)\varphi^{+}_{m_2}(2))\frac{1}{\sqrt{2}}\mathfrak{A}(\varphi^{-}_{m_3}(3)\varphi^{-}_{m_4}(4)). \tag{76}$$

The antisymmetrization operator $\mathfrak{A}$ acts only on the two-particle functions. The function Φ_d is normalized. The normalization constant f is obtained by setting $N_1=N_2=2$ in Eq. (58):

$$f=1-4\langle\Phi_d|\Phi_{\mathrm{ex},1}\rangle+\langle\Phi_d|\Phi_{\mathrm{ex},2}\rangle. \tag{77}$$

In particular, we find

$$\left.\begin{matrix}4\langle\Phi_d|\Phi_{\mathrm{ex},1}\rangle\\ \langle\Phi_d|\Phi_{\mathrm{ex},2}\rangle\end{matrix}\right\}=\sum_{m_1\cdots m_4}\sum_{m_1'\cdots m_4'}C_{m_1\cdots m_4}C_{m_1'\cdots m_4'}\begin{cases}\sum_{i\neq j=1}^{2}\sum_{k\neq l=3}^{4}(g_{ii}g_{lj}-g_{ij}g_{li})(g_{kk}g_{jl}-g_{kl}g_{jk})\\ (g_{13}g_{24}-g_{14}g_{23})(g_{31}g_{42}-g_{41}g_{32}).\end{cases} \tag{77a}$$

Summing up the terms in Eq. (77) one obtains again the result given in Eq. (74). Equation (77) is an expansion of (74) according to the number of overlap integrals $\langle\varphi^{+}_{m}|\varphi^{-}_{n}\rangle$ between different centers appearing in each term of the sum (77). The matrix element $\langle\Phi_d|\Phi_{\mathrm{ex},1}\rangle$ contains terms with only two factors of these overlap integrals, while the matrix element $\langle\Phi_d|\Phi_{\mathrm{ex},2}\rangle$ includes only terms which are products of four such overlap integrals. Therefore, the expansion converges rapidly with increasing number of exchanged nucleons and with increasing separation distance between the nuclear centers. Without going into details we

give the following integral expressions from which the various matrix elements can be easily derived:

$$\langle\Phi_d|H_n\begin{Bmatrix}|\Phi_d\rangle\\|\Phi_{ex,1}\rangle\\|\Phi_{ex,2}\rangle\end{Bmatrix}=\frac{1}{4}\sum_{m_1\cdots m_4}\sum_{m_1'\cdots m_4'}C_{m_1\cdots m_4}C_{m_1'\cdots m_4'}$$
$$\times\sum_{i\neq j=1}^{2}\sum_{k\neq l=3}^{4}\int\varphi^{+*}_{m_i}(1)\varphi^{+*}_{m_j}(2)\varphi^{-*}_{m_k}(3)\varphi^{-*}_{m_l}(4)H_n\begin{Bmatrix}\mathcal{A}(\varphi^{+}_{m_i'}(1)\varphi^{+}_{m_j'}(2))\mathcal{A}(\varphi^{-}_{m_k'}(3)\varphi^{-}_{m_l'}(4))\\ \mathcal{A}(\varphi^{+}_{m_i'}(3)\varphi^{+}_{m_j'}(2))\mathcal{A}(\varphi^{-}_{m_k'}(1)\varphi^{-}_{m_l'}(4))\\ \mathcal{A}(\varphi^{+}_{m_i'}(3)\varphi^{+}_{m_j'}(4))\mathcal{A}(\varphi^{-}_{m_k'}(1)\varphi^{-}_{m_l'}(2))\end{Bmatrix}\times d\tau_1\cdots d\tau_4. \tag{78}$$

As an example, we give here the explicit expressions for the expectation values $\langle\Phi_d|H_n|\Phi_d\rangle$ for the one- and two-body operators. For the one-body operator H_1 we obtain

$$\langle\Phi_d|H_1|\Phi_d\rangle=\sum_{m_1\cdots m_4}\sum_{m_1'\cdots m_4'}C_{m_1\cdots m_4}C_{m_1'\cdots m_4'}(1+\delta_{n_1n_2}\delta_{j_1j_2})^2$$
$$\times\left\{\delta_{m_1m_1'}\delta_{m_2m_2'}\sum_{i\neq j=3}^{4}\langle\varphi^{-}_{m_i}|h|\varphi^{-}_{m_i'}\rangle\delta_{m_jm_j'}+\delta_{m_3m_3'}\delta_{m_4m_4'}\sum_{i\neq j=1}^{2}\langle\varphi^{+}_{m_i}|h|\varphi^{+}_{m_i'}\rangle\delta_{m_jm_j'}\right\}, \tag{79}$$

and for the two-body operator H_2 we have

$$\langle\Phi_d|H_2|\Phi_d\rangle=\sum_{m_1\cdots m_4}\sum_{m_1'\cdots m_4'}C_{m_1\cdots m_4}C_{m_1'\cdots m_4'}(1+\delta_{n_1n_2}\delta_{j_1j_2})$$
$$\times\Big\{\delta_{m_1m_1'}\delta_{m_2m_2'}(\langle\varphi^{-}_{m_3}\varphi^{-}_{m_4}|V|\varphi^{-}_{m_3'}\varphi^{-}_{m_4'}\rangle-\langle\varphi^{-}_{m_3}\varphi^{-}_{m_4}|V|\varphi^{-}_{m_4'}\varphi^{-}_{m_3'}\rangle)$$
$$+\delta_{m_3m_3'}\delta_{m_4m_4'}(\langle\varphi^{+}_{m_1}\varphi^{+}_{m_2}|V|\varphi^{+}_{m_1'}\varphi^{+}_{m_2'}\rangle-\langle\varphi^{+}_{m_1}\varphi^{+}_{m_2}|V|\varphi^{+}_{m_2'}\varphi^{+}_{m_1'}\rangle)$$
$$+(1+\delta_{n_1n_2}\delta_{j_1j_2})\sum_{i\neq j=1}^{2}\sum_{k\neq l=3}^{4}\langle\varphi^{+}_{m_i}\varphi^{-}_{m_k}|V|\varphi^{+}_{m_i'}\varphi^{-}_{m_k'}\rangle\delta_{m_jm_j'}\delta_{m_lm_l'}\Big\}. \tag{80}$$

In Eq. (80) the last term contains the interaction between nucleons belonging to different centers. As one can easily prove, the equations of this section can be reduced to the Eqs. (69) and (70) of the last section in the case where the wave functions at different centers are orthogonal, i.e., $\langle\varphi^{+}_{m}|\varphi^{-}_{n}\rangle=0$. For this case it yields $g_{ik}=g_{ki}=0$ with $i\leq 2<k$.

C. Application of the Formalism to the Scattering of ^{14}N on ^{14}N

To illustrate the application of the formalism developed, we consider the elastic scattering of ^{14}N on ^{14}N. The problem of antisymmetrization can be studied explicitly in this case using the particle-core model. The spin $I=1$ of the ground state of ^{14}N enables us to examine the effects of spin on the elastic scattering.

Within the framework of the particle-core model we assume that each ^{14}N nucleus is composed of a ^{12}C core and two extracore nucleons, i.e., one $1p_{1/2}$ proton and one $1p_{1/2}$ neutron. Since the ground state of ^{12}C has zero spin, these two extracore nucleons couple to give spin $I=1$ for the ground state of the ^{14}N nucleus.

In this section we calculate some special matrix elements using an attractive two-body force of Gaussian type

$$V_{ij}=V_0e^{-\gamma r_{ij}^2}. \tag{81}$$

1. Direct Potential with a Two-Body Force

First, the direct potential, given by Eq. (80) is calculated with the two-body force (81). For this purpose, we define the direct wave function of the extracore particles in analogy to Eq. (76), but without coupling the angular momenta of the nuclei to a total channel spin J:

$$\varphi_{d,M_1M_2}(1,2,3,4)=\sum_{m_1m_2m_3m_4}(\tfrac{1}{2}\tfrac{1}{2}m_1m_2|1M_1)(\tfrac{1}{2}\tfrac{1}{2}m_3m_4|1M_2)$$
$$\times\frac{1}{\sqrt{2}}\mathcal{A}(\Psi^{+}_{\frac{1}{2},m_1}(1)\pi(1)\Psi^{+}_{\frac{1}{2},m_2}(2)\nu(2))\frac{1}{\sqrt{2}}\mathcal{A}(\Psi^{-}_{\frac{1}{2},m_3}(3)\pi(3)\Psi^{-}_{\frac{1}{2},m_4}(4)\nu(4)). \tag{82}$$

In the wave function (82) it is assumed that a $1p_{1/2}$ proton and a $1p_{1/2}$ neutron are bound to each nuclear center at $z=\pm z_0=\pm r/2$ with the angular momenta coupled to $I=1$. The proton and neutron states are denoted by π and ν, respectively. Since we calculate matrix elements using an isospin-independent force, the antisymmetrization in (82) is, in fact, superfluous, but for the sake of completeness we retain it there. The single-particle wave functions $\Psi^{\dagger}_{\frac{1}{2}m}$ are defined in terms of the $1p$ oscillator function $\varphi^{\pm}_{m_l}$, Eq. (A19), and the spin functions S_{m_s}:

$$\Psi^{\pm}_{\frac{1}{2},m}=\sum_{m_l,m_s}(1\tfrac{1}{2}m_l m_s\,|\,\tfrac{1}{2}m)\varphi^{\pm}_{m_l}S_{m_s}. \tag{83}$$

From Eq. (80) and Appendix C we find

$$\left\langle\varphi_{d,M_1M_2}\left|\sum_{i<j}^{4}V_{ij}\right|\varphi_{d,M_1'M_2'}\right\rangle=\delta_{M_1M_1'}\delta_{M_2M_2'}[4I_d(r)+2I_d(r=0)], \tag{84}$$

with $I_d(r)$ given by (see Table III in Appendix C)

$$\begin{aligned}I_d(r)&=I_d(M,m,m)\\&=V_0(1+2\zeta)^{-7/2}\exp\left(-\frac{\zeta}{1+2\zeta}\xi^2\right)\left[1+2\zeta+\frac{5}{3}\zeta^2+\frac{4}{9}\frac{3+\zeta}{1+2\zeta}\zeta^2\xi^2+\frac{4}{9}\frac{\zeta^4}{(1+2\zeta)^2}\xi^4\right],\end{aligned} \tag{85}$$

where $\xi=\sqrt{\mu}\,r$, $\zeta=\gamma/\mu$, and $\mu=M\omega/\hbar$. The r-independent term of Eq. (84) represents the interaction between the proton and neutron in the $1p_{1/2}$ shell within each ^{14}N nucleus. The matrix elements (84) are diagonal and do not depend on the angular momentum projections M_1 and M_2. These results arise for two reasons, namely, that the space distribution of the extracore nucleons is spherically symmetric for the wave functions (82) around the two nuclear centers and that the two-body force used is independent of spin and isospin.

Next the direct part of the intrinsic wave function of the $^{14}\mathrm{N}+^{14}\mathrm{N}$ system is defined according to Eq. (76), by

$$\Phi_{d,JM}=\tfrac{1}{2}[1+(-)^{J+L}]\,\chi_{12_C}(\mathrm{I})\chi_{12_C}(\mathrm{II})\sum_{M_1M_2}(1\,1M_1M_2\,|\,JM)\varphi_{d,M_1M_2}. \tag{86}$$

It is noted that all terms in Eq. (86) with $M_1=M_2$ do not contribute to odd orbital angular momenta L; i.e., only even orbital angular momenta L are allowed when colliding ^{14}N nuclei are in the same magnetic substate. For different magnetic substates ($M_1\neq M_2$), there is no restriction on the L values. The direct part in the effective potential, Eq. (64), which arises from the two-body forces between the extracore particles, is easily obtained using the wave function (86) and Eq. (84). The result is independent of the angular momenta L, J, and I:

$$V_d=\sum_M(JIM-M\,|\,L0)^2\left\langle\Phi_{d,JM}\left|\sum_{i<j}^{4}V_{ij}\right|\Phi_{d,JM}\right\rangle=4I_d(r)+2I_d(r=0). \tag{87}$$

The potential V_d shown in Fig. 5 is calculated with the realistic parameters $V_0=-67.8$ MeV, $\gamma=0.4217/\mathrm{F}^2$, which fit the low-energy nucleon-nucleon scattering data.[26]

2. *One-Exchange Matrix Elements*

We calculate a special one-exchange matrix element defined by

$$V_{\mathrm{ex},1}(M_1,M_2)=-4\langle\varphi_{d,M_1M_2}(1,2,3,4)\,|\,V_{13}\,|\,\varphi_{d,M_1M_2}(3,2,1,4)\rangle. \tag{88}$$

The minus sign and the factor 4 are inserted here because of the factor $(-)^l\binom{N}{l}^2$ with $l=1$ and $N_1=2$ which appear in Eq. (66). The matrix element (88) is representative of the one-exchange contribution. It would be the only nonvanishing matrix element in $\langle\varphi_d|H_2|\varphi_{\mathrm{ex},1}\rangle$ [see Eq. (78)] if the single-particle wave functions $\varphi^{+}_{m_l}$ and $\varphi^{-}_{m_l}$ are mutually orthogonal. However, this is not the case in Eq. (82). The matrix element (88) satisfies the following symmetry relation:

$$V_{\mathrm{ex},1}(M_1,M_2)=V_{\mathrm{ex},1}(M_2,M_1)=V_{\mathrm{ex},1}(-M_1,-M_2). \tag{89}$$

Therefore, only four cases with $M_1=0$, $M_2=0$ or 1 and $M_1=1$, $M_2=+1$ or -1 need to be calculated. The matrix elements are obtained with the help of Table III in Appendix C and are listed in Table I. Their values and the ratios $V_{\mathrm{ex},1}(M_1,M_2)/4|I_d|$, with I_d of Eq. (85), are shown in Figs. 6 and 7.

In the surface region where the ^{14}N surfaces first come into contact, that is, between $r=5$ and 7 F, the

direct processes occur, generating the main structures in the various cross sections. In this region the one-exchange term in the expansion of Eq. (66) contributes an additional effective potential which is of the order of 10% compared to the direct term, as shown in Fig. 7. The small ratio of the one-exchange potential to the direct potential indicates that the effects arising from the antisymmetrization can be well treated in the surface region by expanding the wave function according to the number of exchanged nucleons [see Eq. (12a) or Eq. (57)]. With increasing overlap of the nuclei, higher-exchange terms become larger and, therefore, have to be taken into account. This leads to a soft-core potential in heavy-ion collisions.[1,13] It is clear from the discussion that our treatment of antisymmetrization may be considered as an expansion of the wave function from the asymptotic to the interior region of scattering.

V. SUMMARY AND CONCLUSIONS

A microscopic theory is developed to describe the direct part of heavy-ion reactions, namely noncompound reactions. In the region where the nuclei come in contact, the direct reactions play a dominant role. All processes occurring in this region can be classified according to the number of nucleons transferred and exchanged between the nuclei. A particular exchange of nucleons is connected with the antisymmetrization of the wave function. Therefore, transfer processes and the Pauli principle produce equivalent effects and are treated on the same footing in the present work.

The wave functions, and hence the matrix elements are expanded according to the number of transferred and exchanged nucleons. This is obviously an asymptotic expansion in the sense that one starts with the asymptotic partition of nucleons and adds the one-, two-, etc. nucleon exchange parts to the wave function as it becomes necessary for shorter distances of the nuclei. Therefore, the method is convenient to apply for all surface reactions which, in fact, can be adequately described in a particle-core model. In this model, only a few nucleons are treated microscopically. In principle, reactions which take place at smaller relative distances of the nuclei can also be studied in the present formalism. However, in this case, an increasing number of extracore particles should be taken into consideration to ensure the convergence of the method.[27]

As a first test of the procedure we have examined how the antisymmetrization between the nuclei influences the real part of the heavy-ion potential. For the contact region of two ^{14}N nuclei we find the expected result: The contributions from the antisymmetrization decrease strongly with the number of exchanged nucleons.

In the particle-core model the single-particle

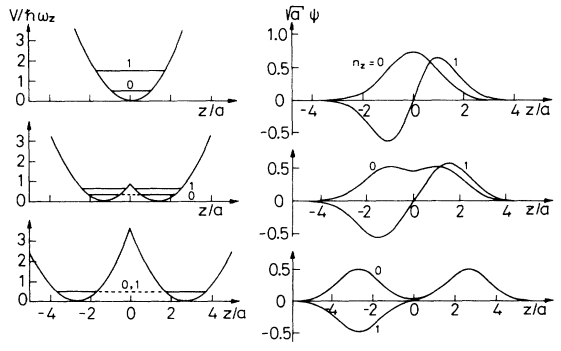

FIG. 4. Potential and wave functions of the one-dimensional two-center oscillator. For the distances $z_0/a = 0$, 1.3 and 2.7 the energies and wave functions of the two lowest states are shown on the left and right side, respectively. The oscillator constant is $a = (\hbar/M\omega_z)^{1/2}$. The energies of the two states are given by $(n_z + 1/2)\hbar\omega_z$ with $n_z = 0$, 1 for $z_0 = 0$ and by $\frac{1}{2}\hbar\omega_z$ for $z_0 \to \infty$. The wave functions have good parity with respect to $z = 0$.

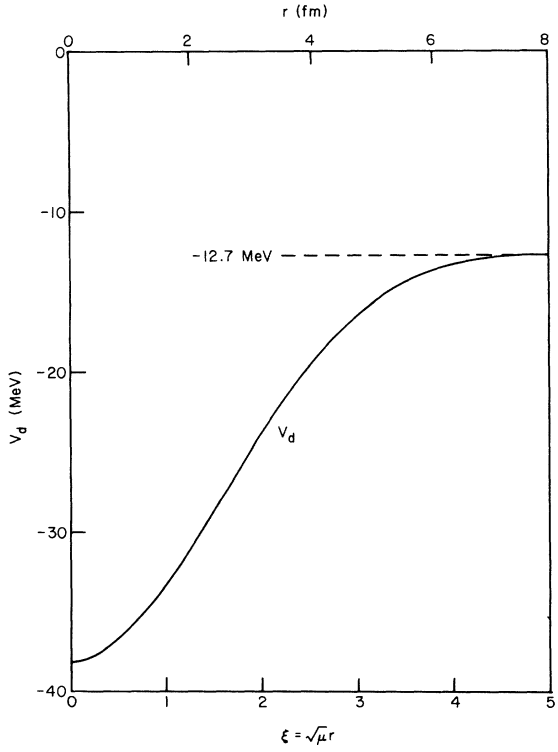

FIG. 5. The direct effective potential V_d of the $^{14}N + ^{14}N$ scattering calculated from Eq. (87) for an attractive two-body force of Gaussian type. The same paramters, $V_0 = -67.8$ MeV and $\gamma = 0.4217/F^2$ are used in Figs. 5–11.

TABLE I. One-exchange matrix elements $V_{ex,1}(M_1, M_2)$ for two-body force ($\xi = \sqrt{\mu}\, r$, $\zeta = \gamma/\mu$).

M_1	M_2	$\frac{V_{ex,1}(M_1 M_2)}{V_0(1+2\zeta)^{-7/2}\exp(-\frac{1}{2}\xi^2)\times}$
0	0	$[1+2\zeta+\frac{5}{3}\zeta^2+\frac{1}{9}(-3+\zeta)(1+2\zeta)\xi^2+\frac{1}{36}(1+2\zeta)^2\xi^4]$
0	1	
1	1	$2[1+2\zeta+\frac{5}{3}\zeta^2-\frac{1}{3}(1+\zeta)(1+2\zeta)\xi^2+\frac{1}{36}(1+2\zeta)^2\xi^4]$
1	−1	$\frac{8}{9}\zeta(1+2\zeta)\xi^2$

motion can be described by one- or two-center wave functions. Both types of functions are equivalently used in heavy-ion theories.[14, 28-30] With one-center wave functions most of the matrix elements can be calculated analytically and without difficulties. Many-body functions built from one-center oscillator functions show a well-understood and simple dependence on the spurious center-of-mass motion. On the other hand two-center wave functions are single-particle solutions in an effective potential generated by the two nuclei. Therefore, they include the influence of the nucleus-nucleus interaction already (at least to an essential extent) and describe the single-particle motion rather realistically. Because two-center functions form an orthonormalized set of functions the number of matrix elements needed is appreciably reduced and the formalism of the second quantization can be applied. Both sets of single-particle functions are advantageous in microscopical scattering theories and which one is to be preferred depends on the special problem concerned.

The present work can be extended in two directions: namely, to study the nonlocality effects of the potentials (which are equivalent to a velocity dependence) and to derive a theory for transfer reactions.

In fact, two possibilities leading to energy-dependent real potentials have been considered up to now. Fliessbach[28] obtains an energy-dependent potential by calculating the expectation value of the Hamiltonian using antisymmetrized, velocity-dependent wave functions (see also Ref. 29). Müller[31] investigates the extent to which nuclear matter is compressed in the overlap region of the nuclei as the bombarding energy increases. He obtains a strongly energy-dependent potential by eliminating the compression channel from the

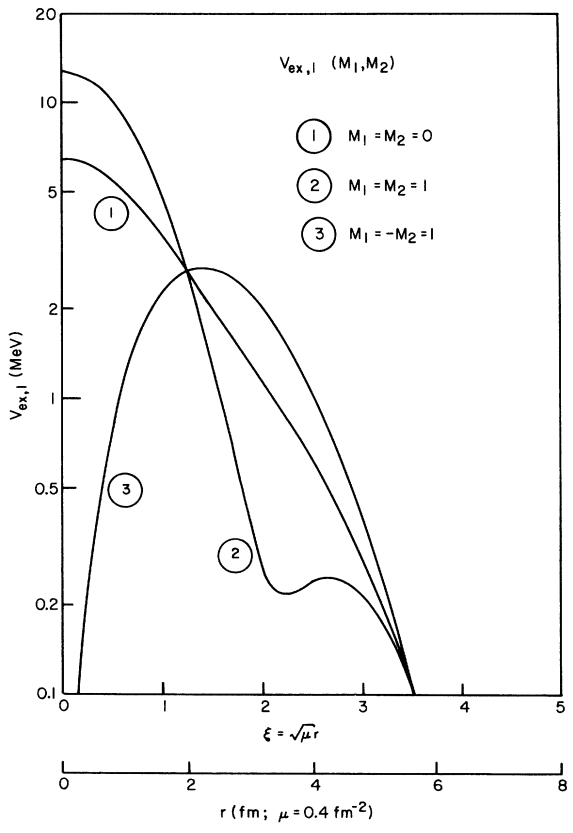

FIG. 6. The one-nucleon exchange matrix elements $V_{ex,1}$ for the $^{14}N+^{14}N$ scattering defined by Eq. (88) and listed in Table I. The curves correspond to the various values of the angular momentum projection M of the colliding ^{14}N nuclei.

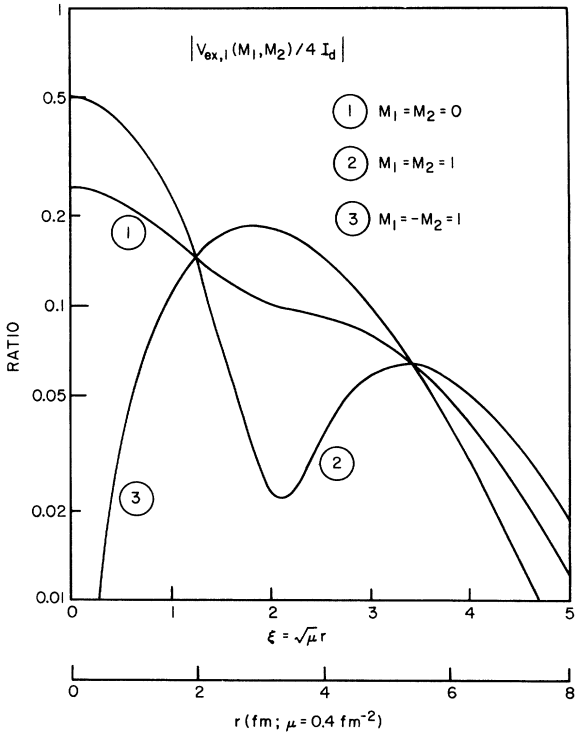

FIG. 7. The ratios of the one-nucleon exchange matrix elements $V_{ex,1}$ to the direct matrix element for various M values.

dynamical treatment. The energy dependence of the potentials is caused by the nonlocality of the nucleus-nucleus interaction. The equations derived in Sec. II allow one to study the nonlocal effects systematically and to transform them into effective masses (which are coordinate-dependent) and effective energy-dependent local potentials.

Recently semiclassical theories for transfer reactions with heavy ions were proposed by Toepffer[32] and by Broglia and Winther.[33] The theory for transfer reactions between light nuclei in the framework of a coupled-channel Born approximation has been studied by Tamura *et al.*[34] An extension of the coupled-channel method can be made starting from the system of equations shown in Sec. II. In this theory recoil effects should also be included since they cannot be neglected in the scattering of light nuclei. As a first possible application we mention the study of the ^{12}C-^{20}Ne channel occurring in the ^{16}O-^{16}O scattering. This channel is most strongly coupled to the elastic ^{16}O-^{16}O entrance channel besides the inelastic excitation of the ^{16}O nuclei, as it has been shown in recent experiments.[35] Theoretical studies on these coupled molecular channels are in progress.

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APPENDIX A: KINETIC ENERGY IN THE PARTICLE-CORE MODEL

The degrees of freedom in the particle-core model are described by the coordinates of the two cores, $\vec{R}_{C_1}$ and $\vec{R}_{C_2}$, and the coordinates $\vec{r}_1, \ldots, \vec{r}_N$ of the N extracore particles which are all measured from an arbitrary coordinate origin. If we denote the momenta canonically conjugate to these coordinates by $\vec{P}_{C_1}$, $\vec{P}_{C_2}$, and $\vec{P}_i$, the kinetic energy in the particle-core model can be expressed according to Eq. (38) as

$$T=\frac{P_{C_1}^2}{2C_1M}+\frac{P_{C_2}^2}{2C_2M}+\sum_{i=1}^{N}\frac{P_i^2}{2M}. \tag{A1}$$

The cores contain $C_i=A_i-N_i$ nucleons ($i=1,2$) where A_i is the atomic number and N_i the number of extracore particles of each nucleus. Since we wish to describe the scattering of two nuclei with the particle-core model we need to introduce the relative coordinate $\vec{r}$ between the nuclei. But the relative coordinate is not symmetrical in the particle coordinates [see Eq. (2)]. Therefore, all coordinate transformations using the relative coordinate $\vec{r}$ lead to expressions for the kinetic energy which are not symmetric in the coordinates of the extracore particles.

In the following discussion we consider the basic partition of extracore particles which is defined by assigning all particles with numbers $i\leq N_1$ to nucleus A_1 and all particles with numbers $i>N_1$ to nucleus A_2. For such a partition the relative coordinate $\vec{r}$ is given by

$$\begin{aligned}\vec{r}&=\frac{1}{A_1}\left(C_1\vec{R}_{C_1}+\sum_{i=1}^{N_1}\vec{r}_i\right)-\frac{1}{A_2}\left(C_2\vec{R}_{C_2}+\sum_{i=N_1+1}^{N}\vec{r}_i\right)\\&=\vec{R}_{C_1}-\vec{R}_{C_2}+\frac{1}{A_1}\sum_{i=1}^{N_1}(\vec{r}_i-\vec{R}_{C1})-\frac{1}{A_2}\sum_{i=N_1+1}^{N}(\vec{r}_i-\vec{R}_{C_2}).\end{aligned} \tag{A2}$$

For small numbers of extracore particles ($N_i/A_i\ll 1$) the relative coordinate can be approximated by the distance between the cores, i.e., $\vec{r}\approx\vec{R}_{C_1}-\vec{R}_{C_2}$, which is independent of the coordinates of the extracore particles.

In the following we transform the coordinates $\vec{R}_{C_1}$, $\vec{R}_{C_2}$, and $\vec{r}_i$ to the center-of-mass coordinate

$$\vec{R}=\frac{1}{A}\left(C_1\vec{R}_{C_1}+C_2\vec{R}_{C_2}+\sum_{i=1}^{N}\vec{r}_i\right),$$

with $A=A_1+A_2$, to the relative coordinate $\vec{r}$, Eq. (A2) and n independent particle coordinates. Depending from which point we measure the particle coordinates we distinguish the following two cases.

(a) In the first case the coordinates of the extracore particles are measured from the centers of the individual nuclei at $\vec{R}_{A_1}$ and $\vec{R}_{A_2}$ (Fig. 2):

$$\begin{aligned}\vec{r}_{i_{A1}}&=\vec{r}_i-\vec{R}_{A_1}\\&=\vec{r}_i-\frac{1}{A_1}\left(\sum_{i=1}^{N_1}\vec{r}_i+C_1\vec{R}_{C_1}\right)\quad\text{for } i\leq N_1,\\ \vec{r}_{i_{A2}}&=\vec{r}_i-\vec{R}_{A_2}\\&=\vec{r}_i-\frac{1}{A_2}\left(\sum_{i=N_1+1}^{N}\vec{r}_i+C_2\vec{R}_{C_2}\right)\quad\text{for } i>N_1.\end{aligned} \tag{A3}$$

The transformation (A3) is useful if one describes the motion of the extracore particles by one-center shell-model states concentrated around each center at $\vec{R}_{A_1}$ and $\vec{R}_{A_2}$. In this case the shell-model functions depend on the distances $\vec{r}_{iA_1}$ and $\vec{r}_{iA_2}$, respectively. Introducing the momenta $\vec{P}$, $\vec{P}_r$, $\vec{P}_{iA_1}$, $\vec{P}_{iA_2}$, which are canonically conjugate to $\vec{R}$, $\vec{r}$, $\vec{r}_{iA_1}$, and $\vec{r}_{iA_2}$, respectively, the kinetic energy in the particle-core model, Eq. (A1), becomes

$$\begin{aligned}T=&\frac{1}{2AM}P^2+\frac{1}{2\mu}P_r^2+\frac{1}{2M}\sum_{i=1}^{N_1}P_{i_{A_1}}^2+\frac{1}{2M}\sum_{i=N_1+1}^{N}P_{i_{A2}}^2\\&-\frac{1}{2A_1M}\left(\sum_{i=1}^{N_1}\vec{P}_{i_{A1}}\right)^2-\frac{1}{2A_2M}\left(\sum_{i=N_1+1}^{N}\vec{P}_{i_{A2}}\right)^2,\end{aligned} \tag{A4}$$

where μ is the reduced mass of the relative motion.

(b) In the second case the coordinates of the extracore particles are measured from the center of mass at $\vec{R}$ (Fig. 2).

$$\vec{r}_{i_{\text{c.m.}}}=\vec{r}_i-\vec{R}=\vec{r}_i-\frac{1}{A}\left(\sum_{i=1}^{N}\vec{r}_i+C_1\vec{R}_{C_1}+C_2\vec{R}_{C_2}\right). \quad \text{(A5)}$$

The coordinates (A5) are applicable if the motion of the extracore particles is described by the wave functions of the two-center shell model. In this model all particle coordinates are measured in the same coordinate system in which the origin is assumed to coincide with the center of mass. If the momenta canonically conjugate to $\vec{r}_{i_{\text{c.m}}}$ are denoted by $\vec{P}_{i_{\text{c.m.}}}$, the kinetic energy is given by

$$T=\frac{1}{2AM}P^2+\frac{1}{2\mu}P_r^2+\frac{1}{2M}\sum_{i=1}^{N}P_{i_{\text{c.m.}}}^2+\left(\frac{1}{A_1M}\sum_{i=1}^{N_1}\vec{P}_{i_{\text{c.m.}}}-\frac{1}{A_2M}\sum_{i=N_1+1}^{N}\vec{P}_{i_{\text{c.m}}}\right)\cdot\vec{P}_r-\frac{1}{2AM}\left(\sum_{i=1}^{N}\vec{P}_{i_{\text{c.m.}}}\right)^2. \quad \text{(A6)}$$

If the numbers of the extracore particles are small compared to those of the core particles (N_1/C_1, $N_2/C_2 \ll 1$), the expression (A4) and (A6) can be approximated by

$$T=\frac{1}{2AM}P^2+\frac{1}{2\mu}P_r^2+\frac{1}{2M}\left(\sum_{i=1}^{N_1}P_{i_{A1}}^2+\sum_{i=N_1+1}^{N}P_{i_{A2}}^2\right) \quad \text{(A7)}$$

and

$$T=\frac{1}{2AM}P^2+\frac{1}{2\mu}P_r^2+\frac{1}{2M}\sum_{i=1}^{N}P_{i_{\text{c.m.}}}^2. \quad \text{(A8)}$$

To prove that both expressions (A7) and (A8) are the same in the above approximation we consider the transformation between the coordinates defined in (A3) and (A5). In transforming Eq. (A4) into (A6) we need to substitute

$$\vec{P}_{i_{A1}} \text{ and } \vec{P}_{i_{A2}} \to \vec{P}_{i_{\text{c.m.}}}$$

and

$$\vec{P}_r \to \vec{P}_r+\frac{1}{A}\left(A_2\sum_{i=1}^{N_1}\vec{P}_{i_{\text{c.m.}}}-A_1\sum_{i=N_1+1}^{N}\vec{P}_{i_{\text{c.m.}}}\right). \quad \text{(A9)}$$

If we insert (A9) into Eq. (A7) and subtract Eq. (A8) we obtain the difference term

$$\frac{1}{2\mu}\left\{\left[\vec{P}_r+\frac{1}{A}\left(A_2\sum_{i=1}^{N_1}\vec{P}_{i_{\text{c.m.}}}-A_1\sum_{i=N_1+1}^{N}\vec{P}_{i_{\text{c.m.}}}\right)\right]^2-P_r^2\right\}. \quad \text{(A10)}$$

This energy difference is small when $N_i/C_i \ll 1$, and should be neglected in accordance with the approximation $\vec{r} \approx \vec{r}_{C_1}-\vec{r}_{C_2}$.

As discussed in Sec. III B, it is convenient to introduce a rotating coordinate system with the z' axis coinciding with the direction of $\vec{r}$. The rotating coordinate system is fixed by three Euler angles which are the two polar angles defining the direction of $\vec{r}$ and an arbitrary angle describing rotation around the z' axis (see Fig. 3). The particle coordinates in the rotating frame are denoted by $\vec{r}'_{iA_1}$, $\vec{r}'_{iA_2}$, and $\vec{r}'_{i_{\text{c.m.}}}$, where the coordinates $\vec{r}'_{iA_1}$ and $\vec{r}'_{iA_2}$ are measured from the nuclear centers and $\vec{r}'_{i_{\text{c.m.}}}$ from the center of the total mass. The transformation from the space-fixed system to the rotating system can be carried out by replacing the momenta $\vec{P}_{iA_1}$, $\vec{P}_{iA_2}$, and $\vec{P}_{i_{\text{c.m.}}}$ by the corresponding momenta $\vec{P}'_{iA_1}$, $\vec{P}'_{iA_2}$, and $\vec{P}'_{i_{\text{c.m.}}}$ in the intrinsic rotating frame, i.e.,

$$\vec{P}_{i_{A1}} \to \vec{P}'_{i_{A1}}, \quad \vec{P}_{i_{A2}} \to \vec{P}'_{i_{A2}}, \quad \vec{P}_{i_{\text{c.m.}}} \to \vec{P}'_{i_{\text{c.m.}}}. \quad \text{(A11)}$$

The momentum of the relative motion transforms as follows:

$$\vec{P}_r \to \hat{r}P_r-\left[\frac{\hat{r}}{r}\times(\vec{I}-\vec{J}')\right]$$

$$=\hat{z}'\frac{\hbar}{i}\frac{\partial}{\partial r}+\frac{1}{r}[\hat{x}'(I_{y'}-J'_{y'})-\hat{y}'(I_{x'}-J'_{x'})] \quad \text{(A12)}$$

since $\hat{r}=\hat{z}'$. The angular momentum $\vec{I}$ of the total system is the well-known differential operator expressed in Euler angles.[15] The intrinsic angular momentum $\vec{J}'$ depends on the coordinates of the core particles used. If the coordinates $\vec{r}'_{iA_1}$ and $\vec{r}'_{iA_2}$ are used, $\vec{J}'$ is the sum of the angular momenta of the particles with respect to the two nuclear centers:

$$\vec{J}'=\vec{I}'_{A_1}+\vec{I}'_{A_2}=\sum_{i=1}^{N_1}(\vec{r}'_{iA_1}\times\vec{P}'_{iA_1})+\sum_{i=N_1+1}^{N}(\vec{r}'_{iA_2}\times\vec{P}'_{iA_2}). \quad \text{(A13)}$$

If the coordinates $\vec{r}_{i_{\text{c.m.}}}$ are used, $\vec{J}'$ is the total angular momentum of the extracore particles with respect to the center of mass in the rotating frame,

$$\vec{J}'=\sum_{i=1}^{N}(\vec{r}'_{i_{\text{c.m.}}}\times\vec{P}'_{i_{\text{c.m.}}}). \quad \text{(A14)}$$

APPENDIX B: CONSTRUCTION OF ORTHOGONAL TWO-CENTER WAVE FUNCTIONS WITH ASYMPTOTIC BEHAVIOR OF OSCILLATOR FUNCTIONS

In this Appendix we discuss two methods for constructing an orthonormal set of two-center

wave functions with the same asymptotic behavior: namely, when the centers are separated far enough, these wave functions approach oscillator functions which are bound to only one of the two centers.

1. Double Oscillator Model

The two-center oscillator model developed for the description of nuclear fission[16-18] provides a very convenient basis for a microscopic formulation of heavy-ion scattering.[14] The model combines the shell-model potentials of the nuclei into a common potential for all the nucleons (see Fig. 4)

The Hamiltonian for the model in the symmetric case without $\vec{l}\cdot\vec{s}$ and l^2 terms may be written as[16]

$$H = T + \tfrac{1}{2}M\omega_0^2[x^2 + y^2 + (|z| - z_0)^2]. \tag{A15}$$

The single-particle solutions of the Hamiltonian (A15) which form an orthogonal set are given by Holzer *et al.*[16] (see also Merzbacher[36]). These solutions can be grouped into wave functions which are symmetric or antisymmetric with respect to the z coordinate. For large separations of the two centers the wave functions asymptotically approach the usual oscillator functions. There exists a pair of symmetric and antisymmetric solutions, φ_S and φ_A, which are asymptotically degenerate in energy. This pair can be combined to give wave functions, φ^+ and φ^-, which are concentrated asymptotically only on the right and left center at $z = \pm z_0$, respectively (see Fig. 4):

$$\varphi^+ = \frac{1}{\sqrt{2}}(\varphi_S \pm \varphi_A), \qquad \varphi^- = \frac{1}{\sqrt{2}}(\varphi_S \mp \varphi_A). \tag{A16}$$

Here, the upper sign should be taken if the wave functions behave as follows for positive z and for large separation z_0 of the two centers:

$$\lim_{z_0\to\infty}\varphi_S = \lim_{z_0\to\infty}\varphi_A \quad \text{for } z>0. \tag{A17}$$

Otherwise, the lower sign is used. Thus, by a combination of the symmetric and antisymmetric wave functions, we obtain a new orthonormal set of single-particle wave functions with asymptotic behavior as described above. We remark that these functions φ^+ and φ^- are no longer eigenfunctions of the Hamiltonian (A15) for finite separations of the two centers. In the case of the asymmetric two-center shell model which has been recently developed by Maruhn *et al.*,[17,18] the wave functions are automatically orthonormal one-center functions asymptotically; i.e., there is no need to construct the functions $\varphi^\pm$ as in the symmetric case.

In general, the eigenfunctions of the Hamiltonian (A15) do not have good angular momentum around each center for large separation distances. For such large distances the eigenfunctions are a superposition of oscillator functions which have different angular momenta and are degenerate in energy. This degeneracy is removed when the l^2 and $\vec{l}\cdot\vec{s}$ terms are included in the Hamiltonian.[16]

TABLE II. Direct and exchange matrix elements with $1p$ oscillator wave functions ($\xi = \sqrt{\mu}\,r$, $\zeta = \gamma/\mu$).

M,	m_l,	m_l'	$\dfrac{K_d(M, m_l, m_l')}{V_0(1+2\zeta)^{-7/2}\exp\left(-\dfrac{\zeta}{1+2\zeta}\xi^2\right)\times}$	$\dfrac{K_{ex}(M, m_l, m_l')}{V_0(1+2\zeta)^{-7/2}\exp(-\frac{1}{2}\xi^2)\times}$
0	0	0	$\left[1+2\zeta+3\zeta^2+\dfrac{4(1-\zeta)}{1+2\zeta}\zeta^2\xi^2+\dfrac{4\zeta^4}{(1+2\zeta)^2}\xi^4\right]$,	$\left[1+2\zeta+3\zeta^2-(1+\zeta)(1+2\zeta)\xi^2+\dfrac{(1+2\zeta)^2}{4}\xi^4\right]$
0	0	1	$\zeta\left(-\zeta+\dfrac{2\zeta^2}{1+2\zeta}\xi^2\right)$	$\zeta\left(-\zeta+\dfrac{1+2\zeta}{2}\xi^2\right)$
0	1	1	$(1+2\zeta+2\zeta^2)$	$2\zeta^2$
0	1	−1	$2\zeta^2$	$(1+2\zeta+2\zeta^2)$
1	0	0	$(1+\zeta)\left(1+\zeta+\dfrac{2\zeta^2}{1+2\zeta}\xi^2\right)$	$\zeta\left(\zeta+\dfrac{1+2\zeta}{2}\xi^2\right)$
1	0	1	$\zeta\left(\zeta-\dfrac{2\zeta^2}{1+2\zeta}\xi^2\right)$	$(1+\zeta)\left(1+\zeta-\dfrac{1+2\zeta}{2}\xi^2\right)$
2	1	1	$1+2\zeta+2\zeta^2$	$1+2\zeta+2\zeta^2$

Therefore, if the eigenfunctions of the generalized Hamiltonian with l^2 and $\vec{l}\cdot\vec{s}$ terms are used in Eq. (A16), the wave functions, φ^+ and φ^-, have good angular momenta j asymptotically.

2. Two-Center Wave Functions Deduced from One-Center Functions by Schmidt Orthogonalization Procedure

Orthogonal two-center wave functions can be also obtained from usual one-center wave functions bound to different centers by the Schmidt orthogonalization procedure. In order to generalize the method, we construct single-particle wave functions which describe the states of different nuclei.

Oscillator wave functions which are bound at the centers 1 and 2 located at $z=\pm z_0$, respectively, with different oscillator strength are taken as the basis states in the Schmidt orthogonalization procedure:

$$\varphi_n^+ = \varphi_{1,Nlm}(x, y, z - z_0)\,. \qquad \varphi_n^- = \varphi_{2,Nlm}(x, y, z + z_0)\,. \tag{A18}$$

Here, N denotes the principal quantum numoer of the oscillator state. All oscillator functions φ_n^+ or φ_n^- belonging to the same center are already orthonormal and complete. Wave functions with different magnetic quantum numbers m around different centers are also orthogonal. Therefore, it is only necessary to orthonormalize the wave functions φ_n^+ and φ_n^- in the subsets of the same magnetic quantum number m.

Such orthogonalization can be accomplished straightforwardly using the Schmidt orthogonalization procedure. The only quantities needed in this method are the overlap integrals:

$$\int \varphi_k^{+*}\varphi_n^- d\tau$$

and

$$\int \varphi_k^{-*}\varphi_n^+ d\tau\,.$$

Calculations along these lines are done by Ong and Fliessbach.[28]

As an example, we consider the set of p-wave functions with equal oscillator strength on both

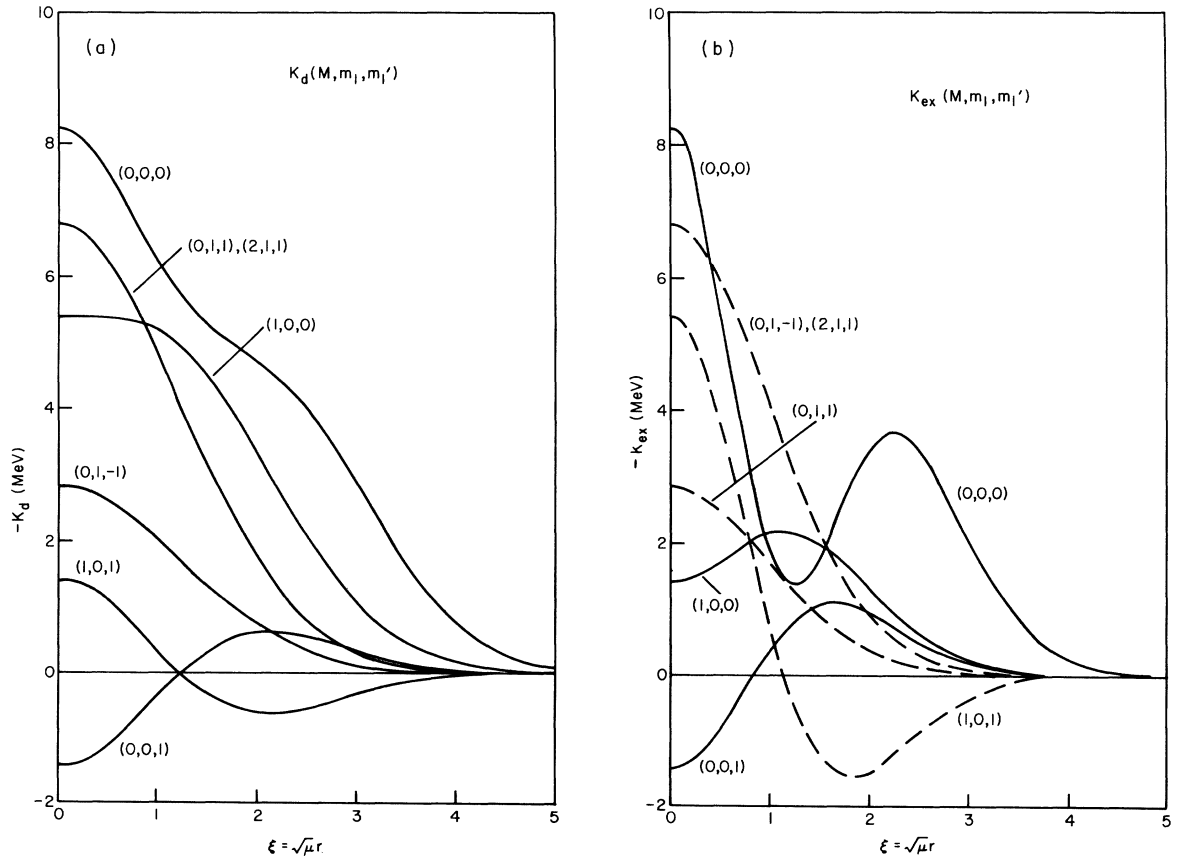

FIG. 8. (a) The direct matrix elements K_d with $1p$ oscillator functions. (b) The one-nucleon exchange matrix elements K_{ex} defined by Eq. (A27) and summarized in Table II.

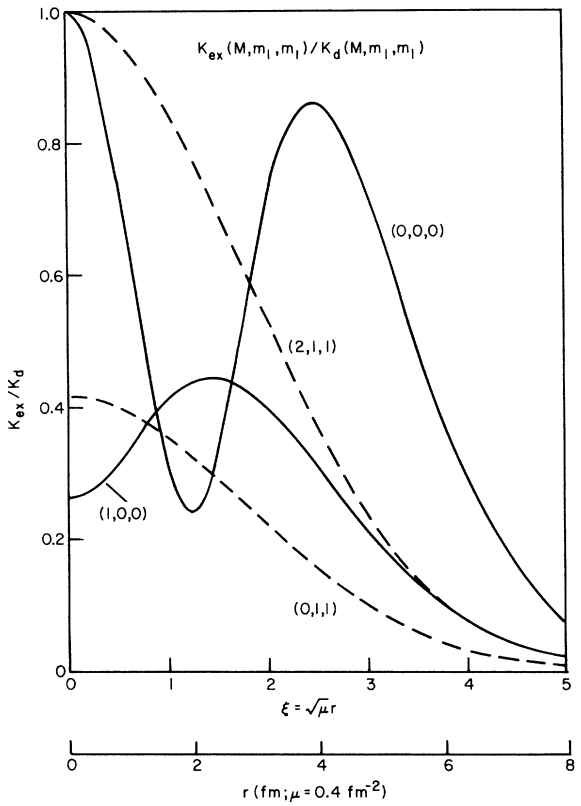

FIG. 9 The ratio of the one-nucleon exchange matrix elements to direct matrix elements, K_{ex}/K_d.

centers:

$$\varphi_m^{\pm}=\left(\frac{4\mu^5}{\pi^3}\right)^{1/4}\exp\{-\tfrac{1}{2}\mu[x^2+y^2+(z\mp z_0)^2]\}$$

$$\times\begin{cases}-(1/\sqrt{2})(x+iy) & (m=1)\\ z\mp z_0 & (m=0)\\ (1/\sqrt{2})(x-iy) & (m=-1)\end{cases}, \qquad \text{(A19)}$$

where $\mu=M\omega/\hbar$. With these functions $\varphi_m^{\pm}$, we construct a set of symmetric and antisymmetric functions with respect to the z coordinate which form an orthonormal set, namely,

$$\left.\begin{matrix}\varphi_{S,m}\\ \varphi_{A,m}\end{matrix}\right\}=[2(1\mp(-1)^m K_m)]^{-1/2}[\varphi_m^{+}\mp(-1)^m\varphi_m^{-}], \qquad \text{(A20)}$$

where K_m denotes the overlap integral

$$K_m=\int\varphi_m^{+}\varphi_m^{-}d\tau=e^{-\mu z_0^2}(1-2\mu z_0^2\delta_{m,0}). \qquad \text{(A21)}$$

In the limit $z_0\to 0$, $K_m\to 1$, and the normalization constants for the wave functions $\varphi_{S,m=0}$ and $\varphi_{A,m=\pm1}$ become zero. In these cases a Taylor expansion in the two-center distance z_0 yields the following limiting expressions:

$$\lim_{z_0\to 0}\varphi_{S,m=0}=\left(\frac{16\mu^3}{9\pi^3}\right)^{1/4}(1-\mu z^2)\times\exp[-\tfrac{1}{2}\mu(x^2+y^2+z^2)],$$
$$\lim_{z_0\to 0}\varphi_{A,m=\pm1}=2\sqrt{\mu}\,z\varphi_{m=\pm1}(z_0=0). \qquad \text{(A22)}$$

The other wave functions $\varphi_{S,m=\pm1}$ and $\varphi_{A,m=0}$ do not pose any difficulty in the limit, $z_0\to 0$, i.e.,

$$\varphi_{S,m=\pm1}\to\varphi_{m=\pm1}(z_0=0),$$
$$\varphi_{A,m=0}\to\varphi_{m=0}(z_0=0).$$

Now we construct orthonormal wave functions $\Psi_m^{\pm}$ which approach asymptotically to the functions φ_m^{+} and φ_m^{-}. According to Eq. (A16) one obtains

$$\Psi_m^{+}=\frac{1}{\sqrt{2}}(\varphi_{S,m}+\varphi_{A,m}),$$
$$\Psi_m^{-}=(-1)^{m+1}\frac{1}{\sqrt{2}}(\varphi_{S,m}-\varphi_{A,m}), \qquad \text{(A23)}$$

or in terms of the basis functions $\varphi_m^{\pm}$,

$$\Psi_m^{\pm}=C_m^{+}\varphi_m^{\pm}+(-)^{m+1}C_m^{-}\varphi_m^{\mp}, \qquad \text{(A24)}$$

where

$$C_m^{\pm}=\tfrac{1}{2}\{[1-(-1)^m K_m]^{-1/2}\pm[1+(-1)^m K_m]^{-1/2}\}.$$

Orthonormal two-center wave functions constructed

TABLE III. Direct and exchange matrix elements $I(M, m, m')$ with $1p_{1/2}$ wave functions ($\xi=\sqrt{\mu}\,r$, $\zeta=\gamma/\mu$).

$I_d(0,\frac{1}{2},-\frac{1}{2})$	0	
$I_d(0,\frac{1}{2},\frac{1}{2})$ $I_d(1,\frac{1}{2},\frac{1}{2})$	$V_0(1+2\zeta)^{-7/2}\exp\left(-\frac{\zeta}{1+2\zeta}\xi^2\right)\times$	$\left[1+2\zeta+\frac{5}{3}\zeta^2+\frac{4}{9}\frac{3+\zeta}{1+2\zeta}\zeta^2\xi^2+\frac{4}{9}\frac{\xi^4}{(1+2\zeta)^2}\xi^4\right]$
$I_{ex}(0,\frac{1}{2},\frac{1}{2})$	$V_0(1+2\zeta)^{-7/2}\exp(-\frac{1}{2}\xi^2)\times$	$[\frac{4}{3}\zeta(1+2\zeta)\xi^2]$
$I_{ex}(0,\frac{1}{2},-\frac{1}{2})$ $I_{ex}(1,\frac{1}{2},\frac{1}{2})$	$V_0(1+2\zeta)^{-7/2}\exp(-\frac{1}{2}\xi^2)\times$	$[1+2\zeta+\frac{5}{3}\zeta^2-\frac{1}{3}(1+\zeta)(1+2\zeta)\xi^2+\frac{1}{36}(1+2\zeta)^2\xi^4]$

from one-center oscillator functions are advantageous in practical calculations. Because of their simplicity and of the convenience of the oscillator wave functions, matrix elements between the basis functions (A18) can be analytically given for ordinary central forces. As shown in the above example, a disadvantage of these functions lies in their behavior at $z_0 = 0$. However, since the scattering of heavy ions is dominated by surface reactions, this behavior causes no real problems in actual calculations.

APPENDIX C: MATRIX ELEMENTS OF THE TWO-BODY FORCES

We summarize here the matrix elements of the two-body force in two bases. Specifically, we consider a Gaussian two-body central force,

$$V_{ij} = V_0 e^{-\gamma r_{ij}^2}, \tag{A25}$$

and give explicit expressions for the $1p$ oscillator and $1p_{1/2}$ functions in the particle-core model. The results are used in the study of the $^{14}N + ^{14}N$ elastic scattering as discussed in Sec. IV C. The following dimensionless quantities are used:

$$\xi = \sqrt{\mu}\, r, \quad \zeta = \gamma/\mu, \tag{A26}$$

where $\mu = M\omega/\hbar$ is the oscillator constant.

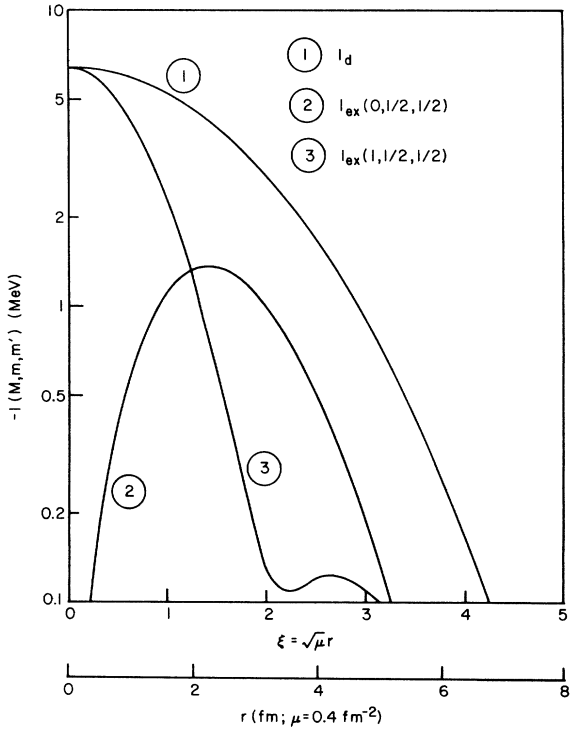

FIG. 10. The direct and one-nucleon exchange matrix elements, I_d and I_{ex}, with $1p_{\frac{1}{2}}$ wave functions, as defined by Eq. (A31) and summarized in Table III.

1. $1p$-Oscillator Functions

First, we calculate matrix elements with $1p$-oscillator wave functions concentrated at different centers for the two-body force. We use the following notation for the direct and exchange matrix elements:

$$K_d(M, m_1, m_1') = \langle \varphi^-_{m_1}(1)\varphi^+_{M-m_1}(2) \,|\, V_{12} \,|\, \varphi^-_{m_1'}(1)\varphi^+_{M-m_1'}(2) \rangle, \tag{A27}$$

$$K_{ex}(M, m_1, m_1') = \langle \varphi^-_{m_1}(1)\varphi^+_{M-m_1}(2) \,|\, V_{12} \,|\, \varphi^-_{m_1'}(2)\varphi^+_{M-m_1'}(1) \rangle.$$

The $1p$-wave functions $\varphi^\pm_m$ are those given in Eq. (A19).

The matrix elements K_d and K_{ex} both satisfy the following symmetry relations:

$$K(M, m_1, m_1') = K(M, m_1', m_1) = K(-M, -m_1, -m_1'), \tag{A28}$$

and with respect to the r dependence,

$$K(M, m_1, m_1', r) = K(M, M - m_1, M - m_1', -r). \tag{A29}$$

Thus, only seven different matrix elements need to be calculated for $1p$-oscillator wave functions. The results are summarized in Table II. Direct and exchange matrix elements with $V_0 = -67.8$ MeV and $\zeta = 1.054$, which corresponds to $\mu = 0.4/\text{F}^2$ and

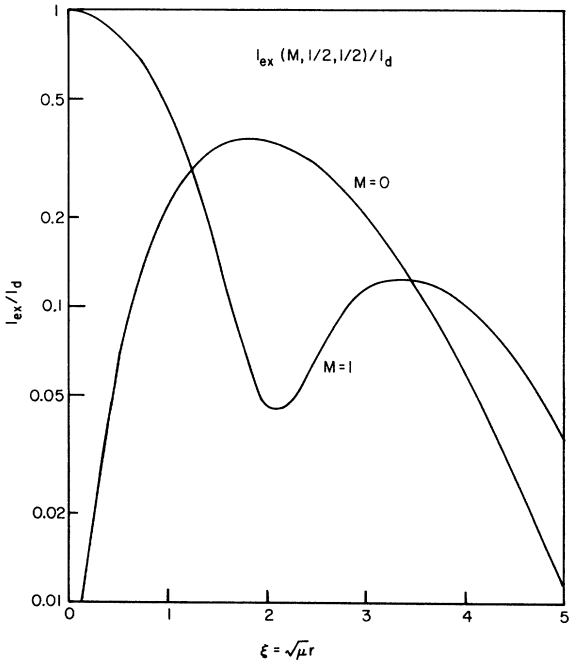

FIG. 11. The ratios of the one-nucleon exchange matrix elements to the direct matrix element I_{ex}/I_d.

$\gamma = 0.4217/F^2$, are plotted in Fig. 8. The ratios of the exchange and direct matrix elements are shown in Fig. 9, illustrating the dependence of the exchange contribution on the separation distance of two colliding nuclei.

2. $1p_{1/2}$ Wave Functions

Next, we calculate special matrix elements with $1p_{1/2}$ wave functions given by (83),

$$\Psi^{\pm}_{\frac{1}{2},m} = \sum_{m_l,m_s} (1\tfrac{1}{2} m_l m_s | \tfrac{1}{2} m) \varphi^{\pm}_{m_l} S_{m_s} . \tag{A30}$$

Here, the functions $\varphi^{\pm}_{m_l}$ are the $1p$ wave functions defined in (A19) and used in (A27). The spin functions are denoted by S_{m_s}. In Sec. IV C, we use the following matrix elements, defined by

$$I_d(M,m,m') = \langle \Psi^{-}_{\frac{1}{2},m}(1) \Psi^{+}_{\frac{1}{2},M-m}(2) | V_{12} | \Psi^{-}_{\frac{1}{2},m'}(1) \Psi^{+}_{\frac{1}{2},M-m'}(2) \rangle , \tag{A31}$$

$$I_{ex}(M,m,m') = \langle \Psi^{-}_{\frac{1}{2},m}(1) \Psi^{+}_{\frac{1}{2},M-m}(2) | V_{12} | \Psi^{-}_{\frac{1}{2},m'}(2) \Psi^{+}_{\frac{1}{2},M-m'}(1) \rangle . \tag{A31'}$$

The matrix elements I_d and I_{ex} both fulfill symmetry relations which have the same form as given by Eqs. (A28) and (A29), namely

$$I(M,m,m') = I(M,m',m) = I(-M,-m,-m') , \tag{A32}$$
$$I(M,m,m',r) = I(M,M-m,M-m',-r) .$$

Therefore, only three different matrix elements need to be calculated using the results of Table II. These are listed in Table III. The matrix elements and the ratios of the exchange and direct terms with $V_0 = -67.8$ MeV and $\zeta = 1.054$ are shown in Figs. 10 and 11. It is interesting to note that in the case of $1p_{1/2}$ wave functions the transition matrix elements of I_d vanish and the expectation values are independent of M and m. That is,

$$I_d(M,m,m') = \delta_{m,m'} I_d(M,m,m) = \delta_{m,m'} I_d(r) . \tag{A33}$$

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Angular Distributions and Absolute Cross Sections for the T(p, n)^{3}He Neutron Source Reaction*

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The T(p, n)^{3}He neutron source reaction has been reinvestigated utilizing the time-of-flight technique. This study was motivated by the lack of cross-section data above 13 MeV, by large uncertainties in the zero-degree absolute cross sections, and by the need to improve the accuracy of both the absolute and relative cross-section data. Angular distributions were measured from 0°–140° at proton energies of 6, 7, 10, 11, 12, 13, 14, 15, and 16 MeV with a neutron detector whose relative efficiency was established to ±1.5%. Absolute cross sections at zero degrees were obtained by normalization of the zero-degree yields measured with the neutron detector to precise charged-particle cross sections obtained for the reaction T(p,^{3}He)n. These results were compared to data obtained with a proton-recoil counter telescope.

I. INTRODUCTION

The reaction T(p, n)^{3}He is widely used as a source of monoenergetic neutrons. While the reaction threshold occurs at 1.019-MeV incident proton energy, the spectrum is complicated by kinematic effects due to center-of-mass motion up to 1.148 MeV. Above this energy, only monoenergetic neutrons are produced up to at least 8.34 MeV, the threshold for the T(p, pn)D tritium breakup. The breakup process seems to have a very low cross section, however, at least up to 11.9 MeV.[1] An accurate knowledge of the T(p, n)^{3}He cross section is increasingly important as nuclear reaction measurements become more precise and demanding. Also, the total $n+^3$He cross section, which is the sum of the elastic scattering of neutrons by ^{3}He and the charge-exchange reactions ^{3}He(n, p)T and ^{3}He(n, d)D, is poorly known at higher energies. These charge-exchange cross sections can be calculated from detailed balance once the inverse cross sections are known. Finally, data from the reaction T(p, n)^{3}He give qualitative information concerning the intermediate excited nucleus ^{4}He. For example, the broad peak in the total cross section for this reaction centered near 3 MeV can be interpreted as indicating a 2^- (T = 0) excited state of ^{4}He near 22.4 MeV.[2,3]

Numerous angular distribution measurements for this reaction between threshold and 5 MeV were made with a long counter.[2,4] The variation in sensitivity of the long counter with energy was investigated in detail by a group at Los Alamos[5] who repeated the angular distribution measurements and extended the zero-degree differential cross section measurements up to 7.5 MeV, using a proton-recoil counter telescope.[6] Before 1960, measurements above 7.5 MeV were considerably less extensive and precise[7] than the data at lower energies. In 1961, Wilson *et al.* at Wisconsin published relative angular distributions and the zero-degree differential cross section at about