Molecular particle-core model and its application to ^{13}C-^{13}C scattering*

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On the basis of the two-center shell model a theory is developed for the excitation of loosely bound nucleons in heavy ion collisions. These nucleons move in the two-center shell model potential generated by all the nucleons and are described by molecular wave functions. The model is applied to calculate the cross sections for the elastic and inelastic ^{13}C-^{13}C scattering. The cross sections show intermediate structures caused by the excitation of quasibound resonances in the molecular nucleus-nucleus potential.

[NUCLEAR REACTIONS $^{13}C(^{13}C,^{13}C)$ molecular wave functions, dynamical two-center shell model, quasimolecular resonances, radial and Coriolis coupling, coupled channel calculations for $\sigma(\theta)$.]

I. INTRODUCTION

In this paper we study the dynamics of loosely bound nucleons in heavy ion collisions. We assume that the loosely bound nucleons move in molecular orbits during the reaction. Collective molecular effects in nucleus-nucleus collisions are observed in systems such as ^{12}C-^{12}C and ^{12}C-^{16}O in resonances which have been interpreted as arising from nuclear molecules.[1-3] Molecular single-particle effects are not yet well established in heavy ion collisions. Recently molecular wave functions were used to describe polarization effects in proton transfer reactions.[4]

The theory of molecular orbits in nucleus-nucleus collisions began with the introduction of the two-center shell model (TCSM) by Holzer *et al.*[5] Up to now the two-center shell model was mainly applied for static calculations of nucleus-nucleus potentials.[6,7] Dynamic treatments of molecular orbits in nucleus-nucleus collisions were investigated by Park *et al.*,[8] von Oertzen and Nörenberg,[9] and Becker *et al.*[10] In this paper we extend the theory of Park *et al.*[8] to a state of practical applicability. The theory is based on the idea that the loosely bound nucleons move in a two-center shell model potential generated by all nucleons. The nuclear surface defines a rotating body-fixed system with its z' axis fixed in the direction of the relative coordinate. In complete analogy to the Nilsson model we assume a strong coupling between the loosely bound nucleons and their shell model potential.

The quantum mechanical treatment of molecular orbits in rotating coordinate systems is extensively studied in atomic physics. In contrast to atomic physics we treat the relative motion also quantum mechanically. Therefore, in our formulation all asymptotic transition matrices vanish. This causes problems in atomic physics where special asymptotic translation factors have to be introduced to correct the asymptotic transition matrices.[11]

In Sec. II we formulate the theory of the particle-core model in the framework of the symmetric TCSM. The formulation of the theory does not depend on the special type of molecular wave functions. The formalism is applied to the ^{13}C-^{13}C collision in the framework of the harmonic two-center shell model.[12,13] The ^{13}C nuclei can be described by a ^{12}C core and a neutron. The two neutrons move in the symmetric TCSM potential generated by the ^{13}C nuclei. We study the excitations of the neutrons leading to excited ^{13}C states after the reaction. Transfer reactions are easily included in the theory, but have been left out of the discussion. Finally, in Sec. III we compare the coupled channel calculations for the elastic ^{13}C-^{13}C cross section with the experimental data of Helb *et al.*,[14] which have measured the elastic 90° excitation function up to $E_{c.m.} = 13.75$ MeV. The predicted inelastic ^{13}C-^{13}C cross sections show similar intermediate structures as the experimental inelastic ^{12}C-^{12}C cross sections.[1,3]

II. THE PARTICLE-CORE MODEL IN NUCLEUS-NUCLEUS SCATTERING

The scattering of ^{13}C on ^{13}C is studied in the frame of the particle-core model. The ^{13}C nuclei are thought to be built up of ^{12}C cores and neutrons [Fig. 1(a)]. For simplicity we have restricted the theory to the elastic and inelastic scattering of ^{13}C on ^{13}C without the neutron transfer.

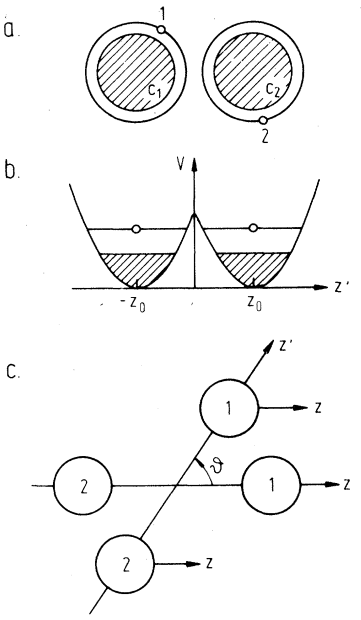


FIG. 1. (a) Schematic sketch of the particle-core model. (b) The two-center potential (cut along the z' axis). The hatched area indicates the levels occupied by the nucleons of the cores. (c) The definition of the laboratory z axis and the intrinsic z' axis fixed by the direction of the relative coordinate.

A. The particle-core model

The model describes the nucleus-nucleus scattering with two cores and N extra particles.[8] The Hamiltonian of the system is given by

$$H = T_{C_1} + T_{C_2} + W_{C_1C_2}(\vec{r}_{C_1C_2}) + \sum_{i=1}^{N} h(i) + \sum_{i<j=1}^{N} V_{ij} - T_{\text{c.m.}} . \quad (1)$$

The first three terms of H are the kinetic energies of the cores C_1 and C_2 and their interaction $W_{C_1C_2}$ which depends on the relative distance $\vec{r}_{C_1C_2} = \vec{R}_{C_1} - \vec{R}_{C_2}$ of the cores (Fig. 2). The kinetic energy of the center of mass is subtracted. The extra particles are described by the coordinates $\vec{r}_i$. They move in a time-dependent, average field generated by the cores. Their dynamics is described by the sum of single-particle Hamiltonians and by two-body interactions acting between the extra particles. The single-particle Hamiltonians are taken in the form of the two-center shell model[5]:

$$h(i) = \frac{p_i^2}{2M} + U(\vec{r}_i, \vec{r}_{C_1C_2}, \vec{p}_i, \vec{s}_i) . \quad (2)$$

The formulation of the following theory does not depend on the exact form of the two-center potential U. It can be taken as realistic Woods-Saxon wells as used by Pruess and Lichtner[4] or in the form resulting from self-consistent Hartree Fock calculations done by Flocard[26] or Zint and Mosel.[27] For reasons of simplicity we assume a two-center oscillator [Fig. 1(b)]. In that case U contains also a l^2 term in addition to the spin-orbit interaction. The harmonic two-center oscillator for identical nuclei is discussed in Appendix B.

The two-body interactions in Eq. (1) are partly included in the two-center potential if we assume that the single-particle potential U represents the average interaction between all nucleons and not only the average interaction between an extra particle and the core nucleons. Assuming that U is the average potential generated by all nucleons, we have to replace the two-body terms in Eq. (1) by the residual interaction. The residual interaction becomes important for the neutron transfer process in the ^{13}C-^{13}C scattering where asymptotically the ^{14}C nucleus consists of a ^{12}C core and two neutrons. To reproduce the ^{14}C states a residual interaction between the extra neutrons has necessarily to be taken into account.

Since we assume in Eq. (2) a two-center potential for the extra nucleons, we anticipate that the extra particles move on molecular orbits during the collision of the nuclei. A molecular picture for the scattering process is justified if the relative velocity of the centers is smaller than the orbiting velocities of the extra nucleons. At relative velocities much higher than the orbiting velocities of the nucleons the nuclear matter becomes compressed during the interpenetration of the nuclei.[15] At that energy the first stage of interpenetration may be described in terms of atomic states (one-center states) centered around the two moving nuclear centers.

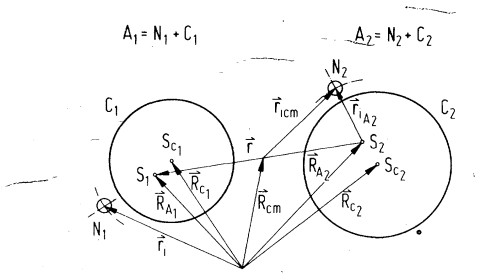


FIG. 2. The definition of the various coordinates of the particle-core model. $\vec{R}_{\text{c.m.}}$ = center of mass coordinate, $\vec{r}$ = relative coordinate, S_1, S_2 = center of mass of nucleus with A_1, A_2 nucleons, S_{C1}, S_{C2} = center of mass of the cores with C_1, C_2 nucleons, $\vec{r}_{iA\,1,\,2}$ = nucleon coordinates measured from S_1, S_2, $\vec{r}_{i\text{cm}}$ = nucleon coordinates measured from the center of mass.

However, in the ^{13}C-^{13}C system at energies slightly above the Coulomb barrier, the reaction and orbiting times are of the same magnitude of order, so that the molecular picture has to be applied. Transitions of the extra nucleons occurring outside the interpenetration region are sufficiently well described in terms of atomic states. However, for reactions happening in the interpenetration region, molecular states have necessarily to be taken into account. Although the atomic states centered at the nuclear centers form a complete set of states for the extra particles, they do not possess the unique advantage of the molecular states to include the average interaction of the extra nucleons with *all* the nucleons.

In the Hamiltonian (1) we have assumed that the cores remain unexcited. It is straightforward to include in Eq. (1) the core excitation according to the method outlined in Ref. 16. For that we have to introduce the collective kinetic energy $T_{c_1c_2}(\alpha_{lm}^{(1)}, \alpha_{lm}^{(2)}, \vec{r}_{c_1c_2})$ depending on the multipole deformation parameters α_{lm} of the nuclear surfaces and the core-core distance. The mass parameters in the collective kinetic energy can be calculated with the cranking model as shown in Ref. 25. Also the core-core potential and the two-center potential will depend on the intrinsic core coordinates, e.g. $W_{c_1c_2}(\vec{r}_{c_1c_2}, \alpha_{lm}^{(1)}, \alpha_{lm}^{(2)})$, and include all the potential terms needed to describe the collective rotations and vibrations. For reasons of simplicity and clarity we have omitted the core excitation in the present work.

B. The kinetic energy in molecular coordinates

In Eqs. (1) and (2) the single-particle coordinates are measured from the coordinate origin of the laboratory system. Since we want to describe the extra particle motion in the framework of the two-center shell model, we introduce molecular single-particle coordinates measured from the center of mass of the total system (see Fig. 2):

$$\vec{r}_{i_{\text{c.m.}}} = \vec{r}_i - \vec{R}_{\text{c.m.}} \tag{3}$$

with

$$\vec{R}_{\text{c.m.}} = \frac{1}{A}\left(C_1\vec{R}_{C_1} + C_2\vec{R}_{C_2} + \sum_{i=1}^{N}\vec{r}_i\right). \tag{3a}$$

The system consists of C_1 and C_2 core nucleons and N extra nucleons. The total number of nucleons is A. The relative coordinate is given for the partition of the extra particles $i \leq N_1$ to nucleus A_1 and $N_1+1 \leq i \leq N$ to nucleus A_2 by

$$\vec{r} = \frac{1}{A_1}\left(C_1\vec{R}_{C_1} + \sum_{i=1}^{N_1}\vec{r}_i\right) - \frac{1}{A_2}\left(C_2\vec{R}_{C_2} + \sum_{i=N_1+1}^{N}\vec{r}_i\right). \tag{4}$$

As shown in Appendix A the total kinetic energy of the system can be transformed into the coordinates $\vec{R}_{\text{c.m.}}$, $\vec{r}$, and $\vec{r}_{i\text{c.m.}}$ and their canonically conjugate momenta $\vec{P}_{\text{c.m.}}$, $\vec{p}_r$, and $\vec{p}_{i\text{c.m.}}$ and results in

$$T = \frac{\vec{P}_{\text{c.m.}}^{\,2}}{2AM} + \frac{1}{2\mu}\vec{p}_r^{\,2} + \frac{1}{2M}\sum_{i=1}^{N}\vec{p}_{i\text{c.m.}}^{\,2} + \left(\frac{1}{A_1M}\sum_{i=1}^{N_1}\vec{p}_{i\text{c.m.}} - \frac{1}{A_2M}\sum_{i=N_1+1}^{N}\vec{p}_{i\text{c.m.}}\right)\cdot\vec{p}_r - \frac{1}{2AM}\left(\sum_{i=1}^{N}\vec{p}_{i\text{c.m.}}\right)^2. \tag{5}$$

Here, $\mu = A_1A_2M/A$ is the reduced mass. The first term in Eq. (5) is the kinetic energy $T_{\text{c.m.}}$ of the center of mass which is subtracted out in Eq. (1). The second term is the kinetic energy of the relative motion, the third term the kinetic energy of the extra nucleons in the center of mass system. The last term in (5) can be neglected for $N_i/A_i \ll 1$, whereas the fourth term has to be taken into account which can be recognized if $\vec{p}_r$ is replaced by $\mu\vec{v}_r$:

$$\left(\frac{A_2}{A}\sum_{i=1}^{N_1}\vec{p}_{i\text{c.m.}} - \frac{A_1}{A}\sum_{i=N_1+1}^{N}\vec{p}_{i\text{c.m.}}\right)\cdot\vec{v}_r. \tag{5a}$$

This term regards the effect of the relative velocity of the nuclear centers on the motion of the extra nucleons. The term vanishes only in the limit of small relative velocities $\vec{v}_r$. For very small relative velocities the orbits of the extra particles change adiabatically from the one-center orbits to the molecular one. The neglect of the term leads to unphysical excitations of the extra nucleons in the asymptotic region.[11] The progress of this work lies in the consistent treatment of the kinetic energy, so that no difficulties with unphysical asymptotic transitions occur.

C. The rotating coordinate system

Since the two-center shell model is conveniently written in a coordinate system in which the centers lie on the z axis, it is advantageous to introduce a rotating coordinate system with a z' axis along the direction of $\vec{r}$ [Fig. 1(c)]. The rotating coordinate system is fixed with respect to the laboratory system by the Euler angles φ, θ which are the spherical polar angles of the relative coordinate $\vec{r}$. The third Euler angle ψ, describing a rotation about the z' axis of the rotated system, is irrelevant and has no physical significance.

The canonical transformation to the relative coordinates r, θ, φ, the particle coordinates $\vec{r}_{i\text{c.m.}}$ in the rotating frame and their canonically conjugate momenta, yields the following expression

for the kinetic energy, which is derived in Eq. (A15) of Appendix A:

$$T=\frac{\vec{P}_{\text{c.m.}}^{\,2}}{2AM}-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\left(\frac{\partial}{\partial r}+D\right)r^2\left(\frac{\partial}{\partial r}+D\right)+\frac{(\vec{I}-\vec{J}_a)^2}{2\mu r^2}+\frac{1}{2M}\sum_{i=1}^{N}\vec{p}_{i\text{c.m.}}^{\,\prime 2}-\frac{1}{2A_1M}\left(\sum_{i=1}^{N_1}\vec{p}_{i\text{c.m.}}^{\,\prime}\right)^2-\frac{1}{2A_2M}\left(\sum_{i=N_1+1}^{N}\vec{p}_{i\text{c.m.}}^{\,\prime}\right)^2 \tag{6}$$

with the abbreviations

$$D=\frac{1}{A}\left(A_2\sum_{i=1}^{N_1}\frac{\partial}{\partial z_{i\text{c.m.}}^{\prime}}-A_1\sum_{i=N_1+1}^{N}\frac{\partial}{\partial z_{i\text{c.m.}}^{\prime}}\right), \tag{6a}$$

$$\vec{J}_a=\sum_{i=1}^{N_1}\vec{r}_{iA_1}^{\,\prime}\times\vec{p}_{i\text{c.m.}}^{\,\prime}+\sum_{i=N_1+1}^{N}\vec{r}_{iA_2}^{\,\prime}\times\vec{p}_{i\text{c.m.}}^{\,\prime}+\sum_{i=1}^{N}\vec{s}_i^{\,\prime}, \tag{6b}$$

$$\vec{r}_{iA_1}^{\,\prime}=\vec{r}_{i\text{c.m.}}^{\,\prime}-\frac{A_2}{A}\vec{r},\quad \vec{r}_{iA_2}^{\,\prime}=\vec{r}_{i\text{c.m.}}^{\,\prime}+\frac{A_1}{A}\vec{r}. \tag{6c}$$

The atomic coordinates $\vec{r}_{iA_1}^{\,\prime}$, $\vec{r}_{iA_2}^{\,\prime}$ are defined in Appendix A and depicted in Fig. 2. The operator $\vec{I}$ is the total angular momentum operator of the system and operates on the Euler angles. The operator $(\vec{I}-\vec{J}_a)^2$ is the square of the angular momentum operator of the relative motion and has only asymptotically the eigenvalues $l(l+1)\hbar^2$. We note that the kinetic energy operator in the form (6) does not induce unphysical transitions for large separations of the nuclei.

With the kinetic energy in the form of Eq. (6) and assuming that the core-core potential $W_{C_1C_2}$ depends approximately on the relative coordinate instead of the core-core coordinate we rewrite the Hamiltonian [see Eq. (1)] as follows:

$$H=H_0+H_1 \tag{7}$$

with

$$H_0=-\frac{\hbar^2}{2\mu r^2}\left(\frac{\partial}{\partial r}+D\right)r^2\left(\frac{\partial}{\partial r}+D\right)+\frac{(\vec{I}-\vec{J}_a)^2}{2\mu r^2}+W_{C_1C_2}(r), \tag{7a}$$

$$H_1=\sum_{i=1}^{N}h(i)-E_\infty=\sum_{i=1}^{N}\frac{\vec{p}_{i\text{c.m.}}^{\,\prime 2}}{2M}+U(\vec{r}_{i\text{c.m.}}^{\,\prime},\vec{p}_{i\text{c.m.}}^{\,\prime},\vec{s}_i^{\,\prime},r)-E_\infty. \tag{7b}$$

In H we have neglected the last two kinetic energies in Eq. (6), which are small corrections for $N_i/A_i\ll 1$, and the two-body interactions between the extra nucleons. The Hamiltonian H_1 is the two-center shell model Hamiltonian of the extra nucleons, written in the rotating coordinate system. The centers of the cores lie on the z' axis. For equal cores as in the ^{13}C-^{13}C system the centers have the coordinates $z'=\pm z_0$ with $z_0=r/2$. The precise form of the single-particle Hamiltonian h is given in Appendix B. In H_1 we have subtracted the asymptotic energy E_∞ of the ground state of the extra particles.

D. The wave functions

For the elastic and inelastic scattering of the two ^{13}C nuclei we introduce the following ansatz[8] for the wave function with total angular momentum I:

$$\Psi_{IM}=A(1,2)\sum_{\alpha,l,J}R_{\alpha lJI}(r)[i^l Y_l(\theta,\varphi)\otimes\Phi_{\alpha J}]_M^{[I]}. \tag{8}$$

The radial function $R_{\alpha lJI}(r)$ depends on the orbital angular momentum l, the channel spin J, and the angular momentum I of the system. The function $\Phi_{\alpha JM}$ describes the intrinsic degrees of freedom of the nuclei. Since the ^{12}C cores are assumed to be unexcited, it is unnecessary to introduce intrinsic wave functions for the cores. Therefore, the function $\Phi_{\alpha J}$ depends only on the coordinates of the two neutrons and the relative coordinate $\vec{r}$. The operator $A(1,2)$ antisymmetrizes the wave function for the exchange of the two neutrons. In addition the wave function should be antisymmetric for the exchange of the ^{13}C nuclei.

The channel spin $\vec{J}$ is asymptotically fixed by the spins of the nuclei $\vec{J}=\vec{I}_1+\vec{I}_2$. For unexcited ^{12}C cores the channel spin of the ^{13}C nuclei is given by the sum of the angular momenta of the extra neutrons: $\vec{J}=\vec{j}_1+\vec{j}_2$.

1. Wave functions in the rotating coordinate system

The transformation of the wave function (8) on the rotating coordinate system is outlined in Ref. 8. The relation connecting the laboratory intrinsic function $\Phi_{\alpha JM}$ with the intrinsic function $\tilde{\Phi}_{\alpha(J)M}$ in the rotated system is given by

$$\Phi_{\alpha JM}=\sum_{M'}D_{MM'}^{J*}(\varphi,\theta,\psi)\tilde{\Phi}_{\alpha(J)M'}. \tag{9}$$

The parentheses around the quantun number J of the channel spin should indicate that J is a good quantum number only for large internuclear distances. We use Eq. (9) also in the reaction region where $\tilde{\Phi}_{\alpha(J)}$ is no longer an eigenfunction of the channel spin $\vec{J}$. Equation (9) is assumed as the definition of the intrinsic wave function for arbi-

trary internuclear distances.

Inserting Eq. (9) into Eq. (8) we obtain the following form:

$$\Psi_{IM}=A(1,2)\sum_{\alpha,l,J}\left(\frac{2l+1}{4\pi}\right)^{1/2} i^l R_{\alpha lJI}(r) \times\sum_{M'}(l0JM'|IM') \times D^{I*}_{MM'}(\varphi,\theta,\psi)\tilde{\Phi}_{\alpha(J)M'}. \quad (10)$$

Here we have used the identity

$$\sum_M (l\,mJM-m\,|\,IM)\,Y_{lm}D^{J*}_{M-m,M'} =\left(\frac{2l+1}{4\pi}\right)^{1/2}(l0JM'|IM')D^{I*}_{MM'}. \quad (10a)$$

Since the operator $\vec{I}$ of the total angular momentum operates on the Euler angles only, one verifies immediately that the wave function (10) has good angular momentum I and good projection M on the space-fixed z axis. Since the intrinsic wave function $\tilde{\Phi}_{\alpha(J)}$ has asymptotically the good quantum number J, the wave function (10) becomes asymptotically an antisymmetrized superposition of eigenstates of the orbital angular momentum $l^2=(\vec{I}-\vec{J}_a)^2$ in addition to $\vec{I}^2$. Since the effects of the antisymmetrization operator $A(1,2)$ on the $\vec{r}$ coordinate are small as long as transfer processes are disregarded we neglect these effects in Eq. (10) and commute $A(1,2)$ with the $\vec{r}$ dependent factors of the wave function. For convenience we introduce the following abbreviation for the antisymmetrized intrinsic wave functions:

$$\tilde{\Phi}^A_{\alpha(J)M}(1,2,r)=A(1,2)\tilde{\Phi}_{\alpha(J)M}(1,2,r). \quad (11)$$

2. *The intrinsic wave functions* $\tilde{\Phi}^A_{\alpha(J)M}$

The two neutrons are described by the single-particle functions $\varphi_{\lambda(j)m}(\vec{r}'_{i\,\mathrm{c.m.}},\pm r/2)$ in the rotated system. The angular momentum j is only asymptotically a good quantum number. For large separations the neutron functions are concentrated at the nuclear centers which lie at $z'=\pm r/2$ on the z' axis of the rotated frame:

$$\varphi_{\lambda(j)m}(\vec{r}'_{i\,\mathrm{c.m.}},\pm r/2)\xrightarrow[r\to\infty]{}\varphi_{\lambda jm}(x'_{i\,\mathrm{c.m.}},y'_{i\,\mathrm{c.m.}},z'_{i\,\mathrm{c.m.}}\mp r/2). \quad (12)$$

The single-particle functions will be specified in terms of two-center wave functions in Sec. II D 3. Using the functions $\varphi_{\lambda(j)m}$ we can write the intrinsic wave functions as

$$\tilde{\Phi}^A_{\alpha(J)M}(1,2,r)=\frac{1}{2(1+\delta_{\alpha_1\alpha_2})^{1/2}}A(1,2)[\varphi_{\alpha_1}(\vec{r}'_{1\,\mathrm{c.m.}},r/2)\otimes\varphi_{\alpha_2}(\vec{r}'_{2\,\mathrm{c.m.}},-r/2) -(-1)^I\varphi_{\alpha_1}(\vec{r}'_{2\,\mathrm{c.m.}},-r/2)\otimes\varphi_{\alpha_2}(\vec{r}'_{1\,\mathrm{c.m.}},r/2)]^{[J]}_M \quad (13)$$

with the abbreviations

$$\alpha_i=\{\lambda_i,(j_i)\},\quad \alpha=\{\alpha_1,\alpha_2\}. \quad (13a)$$

The wave functions (13) are antisymmetric for the exchange of the extra neutrons. It is straightforward to generalize these functions to describe the neutron transfer. When the ^{13}C nuclei are exchanged, the direction of the z' axis is reversed. The effect of this operation on the intrinsic wave function can be obtained by rotating the intrinsic coordinate system by the angle π around the x' axis. It results with the operator P_N for nucleus exchange:

$$P_N\tilde{\Phi}^A_{\alpha(J)M}(1,2,r)=-(-1)^{I+J-2M}\tilde{\Phi}^A_{\alpha(J)-M}(1,2,r). \quad (14)$$

Here we have used the following phase convention of the single-particle wave functions:

$$\varphi_{\lambda(j)m}(x',-y',-z'-r/2) =(-1)^{j-2m}\varphi_{\lambda(j)-m}(x',y',z'+r/2). \quad (15)$$

In carrying out the antisymmetrization operation in Eq. (13) we neglect the fact that also the relative coordinate $\vec{r}$ is affected by the exchange of the extra particles. Also the antisymmetrization of the extra nucleons with the core nucleons is neglected for simplicity. The wave functions $\tilde{\Phi}^A$ are normalized as follows:

$$\langle\tilde{\Phi}^A_{\alpha I(J)M}|\tilde{\Phi}^A_{\alpha' I'(J')M'}\rangle=\frac{1+(-1)^{I+I'}}{2(1+\delta_{\alpha_1\alpha_2})}[\delta_{\alpha_1\alpha'_1}\delta_{\alpha_2\alpha'_2}-(-1)^{I+j_1+j_2-J}\delta_{\alpha_1\alpha'_2}\delta_{\alpha_2\alpha'_1}]\delta_{JJ'}\delta_{MM'}. \quad (16)$$

For deriving this result we have used the normalization of the single-particle wave functions

$$\int \varphi^*_{\lambda_1(j_1)m_1}(\vec{x}, r/2)\varphi_{\lambda_2(j_2)m_2}(\vec{x}, \pm r/2)d\tau = \tfrac{1}{2}(1 \pm 1)\delta_{\lambda_1\lambda_2}\delta_{j_1j_2}\delta_{m_1m_2}. \tag{17}$$

As can be recognized from Eq. (16) the wave functions $\tilde{\Phi}^A$ are orthonormalized when we restrict the quantum number $\alpha = \{\alpha_1, \alpha_2\}$ on the subset with $\alpha_1 \leq \alpha_2$. The subset of wave functions with $\alpha_2 < \alpha_1$ is superfluous because of the relation

$$\tilde{\Phi}^A_{\alpha_1\alpha_2 I(J)M} = -(-1)^{I+j_1+j_2-J}\tilde{\Phi}^A_{\alpha_2\alpha_1 I(J)M}. \tag{18}$$

3. *The single-particle wave functions* $\varphi_{\lambda(j)m}$

The single-particle wave functions $\varphi_{\lambda(j)m}$ needed for the intrinsic wave functions (13) have to fulfill the asymptotic condition (12), the phase condition (15), and the orthonormalization (17). The wave functions $\varphi_{\lambda(j)m}$ are asymptotically concentrated at $z' = r/2$ or $z' = -r/2$. However, the eigenfunctions of the symmetric two-center model used for the ^{13}C-^{13}C system have good parity and, therefore, are concentrated asymptotically at both centers. To obtain the required asymptotic behavior we subtract and add the asymptotically degenerated eigenfunctions χ of the two-center Hamiltonian:

$$\varphi_{\lambda(j)m}(\vec{r}', z_0 = r/2) = \frac{1}{\sqrt{2}}(\chi^g_{\lambda(j)m}(\vec{r}', z_0) + \chi^u_{\lambda(j)m}(\vec{r}', z_0)),$$

$$\varphi_{\lambda(j)m}(\vec{r}', -z_0 = -r/2) = \frac{(-1)^{l\alpha}}{\sqrt{2}} \times (\chi^g_{\lambda(j)m}(\vec{r}', z_0) - \chi^u_{\lambda(j)m}(\vec{r}', z_0)). \tag{19}$$

The functions χ^g and χ^u are the eigensolutions of the symmetric two-center shell model for even and odd parity, respectively,

$$h(\vec{r}', z_0)\chi^{g,u}_{\lambda(j)m} = \epsilon^{g,u}_{\lambda(j)|m|}(z_0)\chi^{g,u}_{\lambda(j)m}. \tag{20}$$

The single-particle Hamiltonian of the symmetric two-center shell model is discussed in Appendix B. The phases of the wave functions χ^g and χ^u are chosen under the condition that χ^g and χ^u become equal for $z_0 \to \infty$ and $z > 0$. The phase factor $(-1)^{l\alpha}$ in Eq. (19) is the parity of the asymptotic single-particle wave function $\varphi_{\lambda(j)m}(\vec{r}', \pm z_0)$ with respect to the centers at $z' = \pm z_0$, where l_α denotes the asymptotic quantum number of the orbital angular momentum. The phase factor is obtained from the asymptotic properties of the two-center wave functions [see Eq. (B8) of Appendix B] and is needed in order to fulfill the relation (15) which connects the phases of the single-particle wave functions $\varphi_{\lambda(j)m}(\vec{r}', +z_0)$ and $\varphi_{\lambda(j)m}(\vec{r}', -z_0)$.

Inserting Eq. (19) into the wave function (13) we obtain finally

$$\tilde{\Phi}^A_{\alpha(J)M} = A(1,2)\tilde{\Phi}_{\alpha(J)M} \tag{21a}$$

with

$$\tilde{\Phi}_{\alpha(J)M}(1,2,r) = \frac{1}{4(1+\delta_{\alpha_1\alpha_2})^{1/2}}[(-1)^{l\alpha_2}(\chi^g_{\alpha_1}(1) + \chi^u_{\alpha_1}(1)) \otimes (\chi^g_{\alpha_2}(2) - \chi^u_{\alpha_2}(2)) - (-1)^{I+l\alpha_1}(\chi^g_{\alpha_1}(2) - \chi^u_{\alpha_1}(2)) \otimes (\chi^g_{\alpha_2}(1) + \chi^u_{\alpha_2}(1))]^{[J]}_M. \tag{21b}$$

In order to calculate the matrix elements with the wave functions $\tilde{\Phi}^A$ we expand the two-center wave functions $\chi^{g,u}$ in the eigenfunctions of the symmetric two-center harmonic oscillator as discussed in Appendix B:

$$\chi^{g,u}_{\lambda(j)m} = \sum_\beta a^{g,u}_{\lambda(j)m,\beta}(z_0)\psi_\beta(\rho, \varphi, z; z_0) \tag{22}$$

with $\beta = \{n_z, N_\rho, m', m_s = m - m'\}$.

The basis functions ψ_β can be expressed in terms of higher analytic functions.

E. The coupled equations

In this section we derive the system of coupled equations for the relative wave functions $R_{\alpha IJI}$ defined in Eq. (8). The scattering wave function has to fulfil the stationary Schrödinger equation: $H\Psi = E\Psi$. The coupled equations are obtained by projecting with the channel wave functions

$$\langle [i^l Y_l \otimes \Phi_{\alpha J}]^{[I]}_M | H - E | \Psi \rangle = 0. \tag{23}$$

Inserting the Hamiltonian given in Eq. (7) and substituting $R_{\alpha IJI}(r) = i^{-l}u^I_{\alpha IJ}(r)/r$ we find the following system of coupled equations:

$$0=\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+W(r,E,I)-E\right)u_k^I(r)+\sum_{k',M',M''}(-1)^{l-l'+M''-M'}(IM''J-M''\,|\,l0)(IM'J'-M'\,|\,l'0)$$
$$\times\Big\{-2\delta_{M'M''}\frac{\hbar^2}{2\mu}\Big[2\Big\langle\tilde{\Phi}_{kM'}\Big|\Big(\frac{\partial}{\partial r}+D\Big)\Big|\tilde{\Phi}_{k'M'}\Big\rangle\frac{d}{dr}$$
$$+\Big\langle\tilde{\Phi}_{kM'}\Big|\Big(\frac{\partial^2}{\partial r^2}+D^2\Big)\Big|\tilde{\Phi}^A_{k'M'}\Big\rangle$$
$$+2\Big\langle\tilde{\Phi}_{kM'}\Big|\frac{\partial}{\partial r}D\Big|\tilde{\Phi}_{k'M'}\Big\rangle\Big]+\frac{2I+1}{8\pi^2}\frac{1}{2\mu r^2}$$
$$\times[\langle D^{I*}_{MM''}\tilde{\Phi}_{kM''}\,|(\vec{I}-\vec{J}_a)^2\,|\,D^{I*}_{MM'}\tilde{\Phi}^A_{k'M'}\rangle+\text{H.c.}]$$
$$+\delta_{M'M''}\delta_{\alpha\alpha'}\langle\tilde{\Phi}^A_{kM''}\,|H_1\,|\tilde{\Phi}^A_{k'M'}\rangle\Big\}u^I_{k'}(r) \tag{24}$$

with $k=\{\alpha,l,J\}, k'=\{\alpha',l',J'\}$.

The complex potential $W(r,E,I)$ will be discussed in Sec. III. The intrinsic wave functions, given in Eq. (21), are used in their antisymmetric and nonantisymmetric versions in the matrix elements. In deriving this result we noticed that the Hamiltonian commutes with the antisymmetrization operator and took the antisymmetrization of the relative coordinate approximately into account in order to obtain Hermitian coupling potentials. In the ^{13}C-^{13}C case the operator D is given as

$$D=\frac{1}{2}\left(\frac{\partial}{\partial z_1'}-\frac{\partial}{\partial z_2'}\right). \tag{25}$$

The operator $\vec{J}_a$ is the sum of the angular momenta of the extra neutrons measured with respect to $z'=\pm r/2$,

$$\vec{J}_a=(\vec{r}_1'-r/2\vec{e}_{z'})\times\vec{p}_1'+\vec{s}_1'+(\vec{r}_2'+r/2\vec{e}_{z'})\times\vec{p}_2'+\vec{s}_2'. \tag{26}$$

It can be replaced by the difference $\vec{J}_a=\vec{J}'-\vec{J}_0$ according to Eq. (A12) of Appendix A. The operator $\vec{J}'$ is defined as the angular momentum of the extra neutrons measured with respect to $z'=0$:

$$\vec{J}'=\vec{j}_1'+\vec{j}_2', \tag{26a}$$

$$\vec{J}_0=r/2\vec{e}_{z'}\times(\vec{p}_1'-\vec{p}_2'). \tag{26b}$$

The system of equations (24) for the unknown functions u_k^I has to be solved numerically. From the asymptotic behavior of the radial functions u_k^I we obtain the S matrix and then the cross sections which are derived in Appendix C.

F. Matrix elements

The matrix elements in the coupled equations (24) are easily evaluated by reducing them to the matrix elements of the symmetric two-center oscillator. In this section we present only the important points in the calculation of the matrix elements. Further details can be found in Ref. 12.

1. The matrix elements of H_1

With H_1 defined in Eq. (7b) and the eigenvalues $\epsilon^{g,u}$ defined in Eq. (20) we obtain ($k=\{\alpha,l,J\}$)

$$\langle\tilde{\Phi}^A_{kM}\,|H_1\,|\tilde{\Phi}^A_{k'M'}\rangle=\delta_{MM'}\delta_{\alpha\alpha'}\tfrac{1}{2}(1+(-1)^{l+l'})\sum_{m_1,m_2}(j_1m_1j_2m_2\,|JM)(j_1m_1j_2m_2\,|J'M)[\tfrac{1}{2}(\epsilon^g_{\gamma_1}+\epsilon^u_{\gamma_1}+\epsilon^g_{\gamma_2}+\epsilon^u_{\gamma_2})-E_\infty] \tag{27}$$

with $\gamma=\{\lambda,(j),m\}$.

In the actual calculations we take only states with $j_1=j_2=\frac{1}{2}$ into account. For this special case the summation over m_1 and m_2 can be immediately carried out, since the two-center energies depend only on $|m|$:

$$\langle\tilde{\Phi}^A_{kM}\,|H_1\,|\tilde{\Phi}^A_{k'M'}\rangle=\delta_{MM'}\delta_{jj'}\delta_{\alpha\alpha'}\tfrac{1}{2}[1+(-1)^{l+l'}][\tfrac{1}{2}(\epsilon^g_{\gamma_1}+\epsilon^u_{\gamma_1}+\epsilon^g_{\gamma_2}+\epsilon^u_{\gamma_2})-E_\infty]. \tag{28}$$

Inserting this result into Eq. (24) we find that the matrix elements of H_1 in Eq. (24) are diagonal. Abbreviating these matrix elements by E_k we obtain for $j_1=j_2=\frac{1}{2}$

$$E_k=\tfrac{1}{2}(\epsilon^g_{\lambda_1(1/2)1/2}+\epsilon^u_{\lambda_1(1/2)1/2}+\epsilon^g_{\lambda_2(1/2)1/2}+\epsilon^u_{\lambda_2(1/2)1/2})-E_\infty. \tag{29}$$

2. The matrix elements of $\partial/\partial r+D$

The sum of the coupling terms with the operators $\partial/\partial r$ and D in Eq. (24) is Hermitian, but not so for the single terms. We rearrange these terms such that the resulting terms are individually Hermitian. It follows that

$$4\left\langle\tilde{\Phi}_{kM}\left|\left(\frac{\partial}{\partial r}+D\right)\right|\tilde{\Phi}_{k'M}\right\rangle\frac{d}{dr}+2\left\langle\tilde{\Phi}_{kM}\left|\left(\frac{\partial^2}{\partial r^2}+D^2\right)\right|\tilde{\Phi}^A_{k'M}\right\rangle+4\left\langle\tilde{\Phi}_{kM}\left|D\frac{\partial}{\partial r}\right|\tilde{\Phi}_{k'M}\right\rangle=A_{kk'M}+B_{kk'M}, \tag{30}$$

$$A_{kk'M}=2M_{kk'M}(r)\frac{d}{dr}+\frac{d}{dr}(M_{kk'M}(r)), \tag{30a}$$

$$M_{kk'M}=2\left\langle\tilde{\Phi}_{kM}\left|\left(\frac{\partial}{\partial r}+D\right)\right|\tilde{\Phi}_{k'M}\right\rangle, \tag{30b}$$

$$B_{kk'M}=-2\left\langle D\tilde{\Phi}^A_{kM}\left|\left(\frac{\partial}{\partial r}+D\right)\right|\tilde{\Phi}_{k'M}\right\rangle-2\left\langle\frac{\partial}{\partial r}\tilde{\Phi}_{kM}\left|\left(\frac{\partial}{\partial r}+D\right)\right|\tilde{\Phi}^A_{k'M}\right\rangle. \tag{30c}$$

The operators $A_{kk'M}$ depend on the transition potentials $M_{kk'M}$ and their first derivatives. These potentials are easily reduced to matrix elements of the two-center wave functions defined in Eq. (19):

$$\begin{aligned}M_{kk'M}(r)=&\frac{(-1)^{l\alpha_2+l\alpha_2'}(1+(-1)^{l+l'+l\alpha_1+l\alpha_1'+l\alpha_2+l\alpha_2'}}{2(1+\delta_{\alpha_1\alpha_2})^{1/2}(1+\delta_{\alpha_1'\alpha_2'})^{1/2}}\\&\times\sum_{m_1,m_1'}\sum_{i,j=1}^{2}(j_1m_1j_2M-m_1\,|\,JM)\\&\times(j_1'm_1'j_2'M-m_1'\,|\,J'M)(-1)^{(l+1+l\alpha_1+l\alpha_2)(i-j)}\delta_{\bar{\gamma}_i\bar{\gamma}_j'}\\&\times\left[\frac{1}{2}\left(\left\langle\chi^g_{\gamma i}\left|\frac{\partial}{\partial r}\right|\chi^g_{\gamma j'}\right\rangle+\left\langle\chi^u_{\gamma i}\left|\frac{\partial}{\partial r}\right|\chi^u_{\gamma j'}\right\rangle\right)\right.\\&\left.+\frac{1}{4}\left(\left\langle\chi^g_{\gamma i}\left|\frac{\partial}{\partial z'}\right|\chi^u_{\gamma j'}\right\rangle+\left\langle\chi^u_{\gamma i}\left|\frac{\partial}{\partial z'}\right|\chi^g_{\gamma j'}\right\rangle\right)\right]\end{aligned} \tag{31}$$

with $\bar{\gamma}_1=\gamma_2=\{\alpha_2,m_2\}$, $\bar{\gamma}_2=\gamma_1=\{\alpha_1,m_1\}$.

With the aid of the expansion (22) of the functions $\chi^{g,u}$ the matrix elements in (31) can be reduced to the matrix elements between the states of the symmetric two-center oscillator. The coupling potentials $M_{kk'M}$ vanish asymptotically because of the relation [$r=2z_0$, see Eq. (B8)]

$$\lim_{r\to\infty}\frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial r}+\frac{1}{2}\frac{\partial}{\partial z'}\right)(\chi^g_{\lambda jm}+\chi^u_{\lambda jm})=\left(\frac{\partial}{\partial r}+\frac{1}{2}\frac{\partial}{\partial z'}\right)\varphi_{\lambda ljm}(\vec{r}'-r/2\vec{e}_{z'})=0. \tag{32}$$

The same method can be applied to calculate the matrix elements of the potentials (30c).

3. *The matrix elements of* $(\vec{I}-\vec{J}_a)^2$

The angular momentum operator $(\vec{I}-\vec{J}_a)^2$ has to be written in components of the intrinsic coordinate system. With the properties of the D functions we obtain for the matrix elements needed in Eq. (24)

$$\begin{aligned}\frac{2I+1}{8\pi^2}[\langle D^{I*}_{\mu M}\tilde{\Phi}_{kM}\,|(\vec{I}-\vec{J}_a)^2\,|D^{I*}_{\mu M'}\tilde{\Phi}^A_{k'M'}\rangle+\text{H.c.}]=&\delta_{MM'}\delta_{JJ'}\frac{1+(-1)^{l+l'}}{2}\delta_{\alpha\alpha'}(I(I+1)-M^2)\hbar^2\\&-\hbar[I(I+1)-M(M+1)]^{1/2}\\&\times\delta_{M'M+1}2\langle\tilde{\Phi}_{kM}\,|J^-_a\,|\tilde{\Phi}_{k'M+1}\rangle-\hbar[I(I+1)-M(M-1)]^{1/2}\delta_{M'M-1}\\&\times2\langle\tilde{\Phi}_{kM}\,|J^+_a\,|\Phi_{k'M-1}\rangle+\tfrac{1}{2}\delta_{MM'}(\langle\tilde{\Phi}_{kM}\,|(J^+_aJ^-_a+J^-_aJ^+_a)\,|\tilde{\Phi}^A_{k'M}\rangle\\&+\text{H.c.}).\end{aligned} \tag{33}$$

Asymptotically the intrinsic wave functions $\tilde{\Phi}_{kM}$ are eigenfunctions of the square of the angular momentum operator $\vec{J}_a$:

$$\lim_{r\to\infty}\vec{J}_a^{\,2}\tilde{\Phi}_{kM}=J(J+1)\hbar^2\tilde{\Phi}_{kM}. \tag{34}$$

In that case the above matrix elements (33) can easily be evaluated. Inserting the asymptotic matrix elements into Eq. (24) we obtain the usual centrifugal potentials

$$\lim_{r\to\infty}\sum_{k',M',M''}=\frac{l(l+1)}{2\mu r^2}\hbar^2u^I_k. \tag{35}$$

In complete analogy to Eq. (31) we get the following expression for the matrix elements of $\vec{J}_a$:

$$\langle \tilde{\Phi}_{kM} | \vec{J}_a | \tilde{\Phi}_{k'M'} \rangle = \frac{(-1)^{l_{\alpha_2}+l_{\alpha_2}'}[1+(-1)^{l+l'+l_{\alpha_1}+l_{\alpha_2}+l_{\alpha_1}'+l_{\alpha_2}'}]}{2(1+\delta_{\alpha_1\alpha_2})^{1/2}(1+\delta_{\alpha_1'\alpha_2'})^{1/2}}$$
$$\times \sum_{m_1,m_1'} \sum_{i,j=1}^{2} (j_1 m_1 j_2 M - m_1 | JM)(j_1' m_1' j_2' M' - m_1' | J'M')(-1)^{(l+l_{\alpha_1}+l_{\alpha_2})(i-j)}$$
$$\times \delta_{\bar{\gamma}i\bar{\gamma}j'}(\tfrac{1}{2}(\langle \chi^g_{\gamma i} | \vec{j}' | \chi^g_{\gamma j'} \rangle + \langle \chi^u_{\gamma i} | \vec{j}' | \chi^u_{\gamma j'} \rangle)$$
$$-\tfrac{1}{4} r \vec{e}_{z'} \times (\langle \chi^g_{\gamma i} | \vec{p}' | \chi^u_{\gamma j'} \rangle + \langle \chi^u_{\gamma i} | \vec{p}' | \chi^g_{\gamma j'} \rangle)) . \quad (36)$$

Using Eqs. (26a) and (26b) we rewrite the matrix elements of $\vec{J}_a{}^2$ in a more explicit form:

$$\langle \tilde{\Phi}_{kM} | \vec{J}_a{}^2 | \tilde{\Phi}^A_{k'M} \rangle + \text{H.c.} = 2\langle \tilde{\Phi}_{kM} | (\vec{j}_1' + \vec{j}_2')^2 | \tilde{\Phi}^A_{k'M} \rangle + \frac{r^2}{2} \langle \tilde{\Phi}_{kM} | (\vec{e}_{z'} \times (\vec{p}_1' - \vec{p}_2'))^2 | \tilde{\Phi}^A_{k'M} \rangle$$
$$-r[\langle \tilde{\Phi}_{kM} | (\vec{j}_1' + \vec{j}_2')(\vec{e}_{z'} \times (\vec{p}_1' - \vec{p}_2')) | \tilde{\Phi}_{k'M} \rangle + \text{H.c.}] . \quad (37)$$

The reduction of these matrix elements to expressions with two-center wave functions is straightforward. In the actual calculations presented in Sec. III we have replaced the orbital angular momentum in $\vec{J}_a$ defined in Eq. (26) by an expression which is also used for the calculation of the $\vec{l}\cdot\vec{s}$ and l^2 potentials of the two-center shell model (see Appendix B):

$$\vec{J}_a \to \vec{J}_s = \sum_{i=1}^{2} \tfrac{1}{2} \vec{\nabla}_i [\rho_i'^2 + (|z_i'| - r/2)^2] \times \vec{p}_i' + \vec{s}_i'$$
$$= \vec{J}_a + r\vec{e}_{z'} \times [\theta(-z_1')\vec{p}_1' - \theta(z_2')\vec{p}_2'] . \quad (38)$$

The operator $\vec{J}_s$ has the advantage to be symmetric in the particle coordinates and gives the same matrix elements as $\vec{J}_a$ for large and small relative distances r.

III. APPLICATION TO THE ^{13}C-^{13}C SCATTERING

In this section we apply the theory to the ^{13}C-^{13}C scattering. Figure 3 presents the states of the ^{13}C nucleus and their explanation in terms of the excitation of the ^{12}C core and the valence neutron. The strongest transition from the ground state is of $E1$ type and connects the $\frac{1}{2}^-$ ground state (gs) with the first $\frac{1}{2}^+$ (3.09 MeV) state. As shown in Fig. 3 the transition is caused by the valence neutron going from the $1p\frac{1}{2}$ to the $2s\frac{1}{2}$ state. In the present calculation we have restricted the channels to the elastic one (gs, gs), to the single excitation of the $\frac{1}{2}^+$ state in one of the ^{13}C nuclei (gs, $\frac{1}{2}^+$) and the mutual excitation of the $\frac{1}{2}^+$ state in both ^{13}C nuclei ($\frac{1}{2}^+$, $\frac{1}{2}^+$). As already stated, we disregard the neutron transfer and core excitation channels.

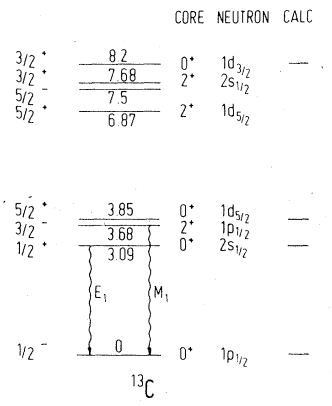


FIG. 3. Spectrum of ^{13}C from Ref. 17. On the right-hand side of the figure, the ^{13}C states are interpreted with the collective excitation of the ^{12}C core and the excitation of the loosely bound neutron. The last column presents the neutron states of ^{13}C calculated with the shell model parameters given in Eq. (42).

A. The complex potential

The complex potential $W(r,E,I)$ in Eq. (24) consists of the complex interaction between the ^{12}C cores and of an absorptive potential for the interaction of the extra particles with the cores:

$$W(r,E,I) = V(r) + iW_{cc}(r,E,I) + iW_{c\not p}(r) . \quad (39)$$

The real and imaginary potential between the cores is completely determined by the elastic and inelastic ^{12}C-^{12}C scattering. The additional imaginary potential $W_{c\not p}$ is caused by the neglected transfer and inelastic channels of the extra particles.

1. The real potential V(r)

The real ^{12}C-^{12}C potential is taken from Morović and Greiner,[7] who have calculated real potentials for the scattering of identical nuclei. They used the Strutinsky method with single-particle energies of the symmetric two-center shell model (TCSM). The potential of the symmetric TCSM is given in Appendix B and shown together with the corresponding nuclear shapes in Fig. 4. In the adiabatic approximation of Morović and Greiner[7] the resulting potential energy surface of the ^{12}C-^{12}C system depends on the distance between the centers ($r = 2z_0$) and on the inner barrier height h defined in Fig. 4. This potential energy surface (PES) is shown in

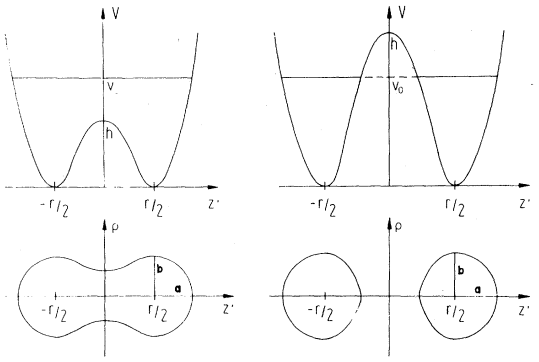


FIG. 4. The two-center shell model potential with the corresponding nuclear shapes for two different two-center distances. Left side: compound nucleus. Right side: separated nuclei (from Ref. 7).

Fig. 5. The main feature of the PES is that the Coulomb barrier is situated at $r \approx 5.4$ fm. The PES minimum at $r \approx 3$ fm and $h = 0$ reproduces the ^{24}Mg ground state. One estimates $r = 3.16$ fm for the measured quadrupole moment of ^{24}Mg in terms of the two-center distance of the TCSM. In the PES of Fig. 5 we have indicated the adiabatic path chosen for the ^{12}C-^{12}C collision. The resulting core-core potential is shown by the heavy line in Fig. 6.

2. *The imaginary potential W_{cc}*

As suggested by Helling *et al.*[18] and Fink *et al.*,[16] the imaginary potential for the elastic channels can be written

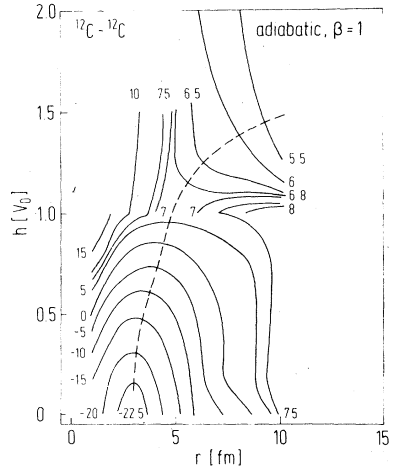
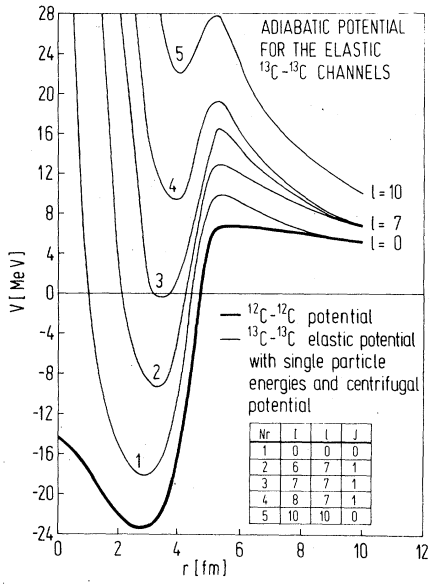


FIG. 5. The potential energy surface for the ^{12}C-^{12}C system in adiabatic approximation as function of the two-center distance r and the height h of the inner barrier of the potential defined in Fig. 4. The values of the equipotential lines are given in units of MeV. The dashed line is assumed as the path of the ^{12}C nuclei in an adiabatic collision (from Ref. 7).



Nr	I	L	J
1	0	0	0
2	6	7	1
3	7	7	1
4	8	7	1
5	10	10	0

FIG. 6. Selected potentials for the elastic ^{13}C-^{13}C channels. The adiabatic core-core potential (heavy line) is obtained from the PES of Fig. 5 (path along the dashed line in Fig. 5). The ^{13}C-^{13}C elastic potentials (light lines) are calculated by adding the r-dependent single-particle energies of Fig. 9 and the centrifugal potentials to the ^{12}C-^{12}C potential. Asymptotically the potentials are degenerated for fixed orbital angular momentum I.

$$W_{cc}(r,E,I) = \alpha N(r)\,\frac{2I+1}{\sigma^3} \times \exp\{2[a[E - V(r) - I(I+1)\hbar^2/2\theta(r)]]^{1/2}\} \quad (40)$$

with

$$N(r) = A(1 - r/d)^2(1 + r/2d)\,, \quad r \le d \quad (40a)$$

$$\sigma^2(r) = \frac{\theta(r)}{\hbar^2}\left(\frac{E - V(r)}{a}\right)^{1/2}\,, \quad (40b)$$

$$\theta(r) = \mu(\tfrac{8}{5}R^2 + r^2)\,, \quad (40c)$$

$$a = 0.035(A - 12)\ \text{MeV}^{-1} = 0.42\ \text{MeV}^{-1}\,. \quad (40d)$$

For θ we have assumed the moment of inertia of two equal rigid spheres with the ^{12}C radius $R = 3.11$ fm and relative distance r. The excitation energy $E^* = E - V(r)$ of the precompound nucleus is measured with respect to the adiabatic potential $V(r)$ shown in Fig. 6. The function $N(r)$ is the number of nucleons in the overlap region of two spheres with homogeneous densities. The touching distance d is chosen so that it agrees with the position of the Coulomb barrier, namely $d = 5.4$ fm (see Fig. 6). Finally we have fitted the only free parameter α to the experimental 90° cross sections for elastic ^{12}C-^{12}C scattering.

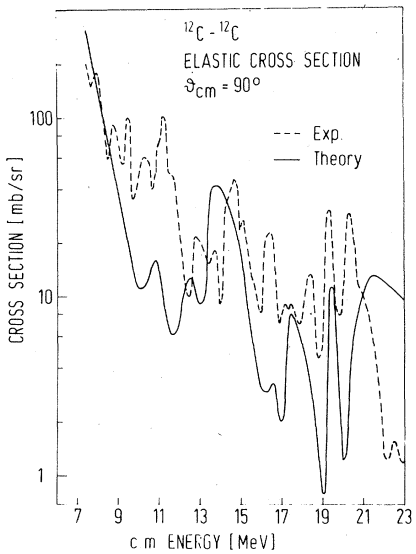


FIG. 7. The 90°-differential cross section for elastic ^{12}C-^{12}C scattering. The experimental data are taken from Ref. 24. The calculations are carried out with the real ^{12}C-^{12}C potential shown in Fig. 6 and the imaginary potential given in Fig. 8. Since we have coupled the single and mutual excitation of the first 2^+ state in ^{12}C to the elastic channel, the theoretical cross section reveals intermediate structures.

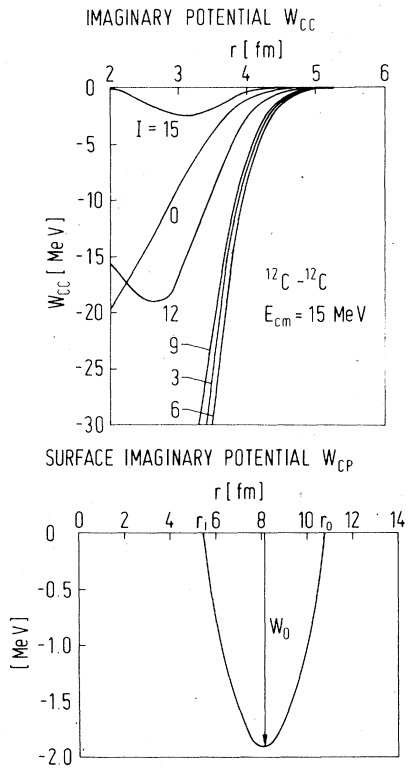


FIG. 8. (a) The imaginary ^{12}C-^{12}C potential for various total angular momenta at $E_{c.m.} = 15$ MeV. (b) The additional surface imaginary potential for ^{13}C-^{13}C.

Figure 7 shows the theoretical 90° cross section for elastic ^{12}C-^{12}C scattering obtained by fitting the free parameter α. It results in $\alpha = -0.1$ MeV. In the calculations we have coupled the single and mutual excitation of the first 2^+ state in ^{12}C according to the method described in Ref. 16. The imaginary potential used for the elastic channels is drawn in Fig. 8(a) for $E_{c.m.} = 15$ MeV.

3. The additional imaginary potential W_{cp}

Since we treat only a very restricted number of channels for the extra particles in our calculations, we have to approximate the disregarded single-particle channels by an extra absorptive potential in the elastic ^{13}C-^{13}C channels. This potential arises partly from the neglected neutron transfer channels. Therefore, we localize this potential in the touching zone by the following ansatz:

$$W_{cp}(r) = W_0 \frac{4(r - r_i)(r_0 - r)}{(r_0 - r_i)^2}, \quad r_i \leq r \leq r_0 \qquad (41)$$

$$= 0 \text{ otherwise.}$$

The parameters W_0, r_i, and r_0 are taken as the only free parameters to fit the experimental elastic cross section of ^{13}C-^{13}C. The resulting surface-absorptive potential is drawn in Fig. 8(b). It is assumed that this additional potential gets strongly reduced if the neutron transfer channel is explicitly included in the system of coupled equations (24).

B. The TCSM for the extra nucleons

The theory formulated in Sec. II is independent of the special type of the two-center shell model (TCSM). To simplify our calculations we assume an harmonic two-center oscillator for the potential of the extra neutrons. The simplification does not influence the gross structure of the radial and rotational coupling potentials, and is justified as long as we disregard polarization effects and the neutron transfer channels.

The parameters of the TCSM described in Appendix B have to be chosen such that the asymptotic single-particle states are reproduced. As shown in Fig. 3 the ^{13}C states have the peculiarity that the $2s\frac{1}{2}$ state lies lower than the $1d\frac{5}{2}$ state. Kurath and Lawson[17] have explained the spectrum assuming weak coupling between the deformed ^{12}C core and the neutron. Since for simplicity we do not take any core deformation into account, we have to adjust the asymptotic parameters $\hbar\omega(r \to \infty) = \hbar\omega_\infty$, μ_∞ and κ_∞ of the TCSM in order to reproduce the relative positions of the $1p\frac{1}{2}$, $2s\frac{1}{2}$, $1d\frac{5}{2}$, and $1d\frac{3}{2}$ states in the ^{13}C spectrum (see Fig. 3).

It results in

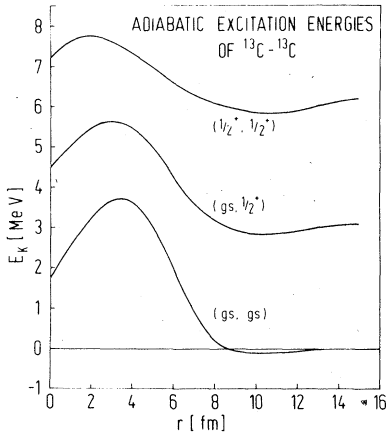


FIG. 9. The sum of the adiabatic single-particle energies for the channels (gs, gs), $(gs, \frac{1}{2}^+)$, and $(\frac{1}{2}^+, \frac{1}{2}^+)$ calculated according to Eq. (29).

$$\hbar\omega_\infty = 6.95 \text{ MeV}, \quad \kappa_\infty = 0.127, \quad \mu_\infty = -0.479. \quad (42)$$

The small value of the oscillator frequency indicates that the extra neutron is loosely bound to the ^{12}C core and simulates the effects of the deformation of the ^{12}C core. Figure 9 presents the excitation energy of the neutrons in the considered channels calculated with the single-particle energies of the adiabatic TCSM which are inserted into Eq. (29).

C. The coupling potentials

Using the TCSM wave functions for the neutrons we have calculated the various coupling potentials in Eqs. (24) by the methods outlined in Sec. II F.

Figure 10 shows the constituents of the radial coupling matrix element given in Eq. (31) for a special transition. As already mentioned the asymptotic radial coupling matrix elements vanish. In the present calculations we have taken only the radial matrix elements of Eq. (30a) into account and disregarded the higher order terms given by Eq. (30c). The radial coupling matrix elements of Eq. (30a) have no diagonal contributions.

The matrix elements of the angular momentum operators are calculated according to Eq. (33) where the angular momentum $\vec{J}_a$ of the extra neutrons is replaced by the symmetric operator $\vec{J}_s$ defined in Eq. (38). This replacement is done only for numerical simplification and will be revised in future calculations.

The matrix elements of $(\vec{I}-\vec{J}_s)^2$ have diagonal contributions since they approach the values $l(l+1)\hbar^2$ for $r \to \infty$. In Fig. 6 we have added the centrifugal potential and the single-particle excitation energy for the elastic channels (see Fig. 9) to the adiabatic core-core potential. Asymptotically the potentials are degenerated for fixed orbital angular momentum, whereas in the overlap region the potentials split for different total

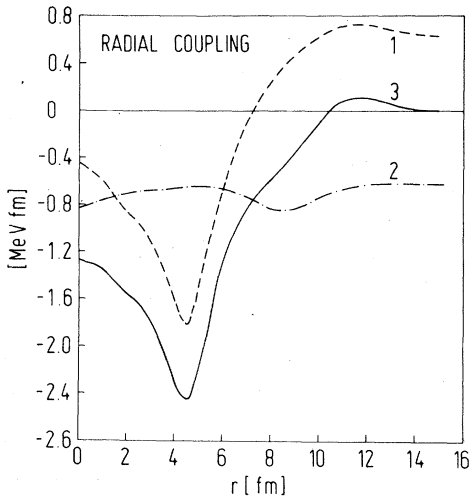


FIG. 10. The radial coupling potential for the special transition

$$\frac{\hbar^2}{2\mu}\langle \tilde{\Phi}^A(gs,gs),\ l=1,\ J=1,\ M=-1 | D_n | \tilde{\Phi}^A(gs,\tfrac{1}{2}^+),0,1,-1\rangle$$

with the following choices of D_n: Curve 1: $D_1 = 2\partial/\partial r$. Curve 2: $D_2 = \partial/\partial z_1' - \partial/\partial z_2'$. Curve 3: $D_3 = D_1 + D_2$.

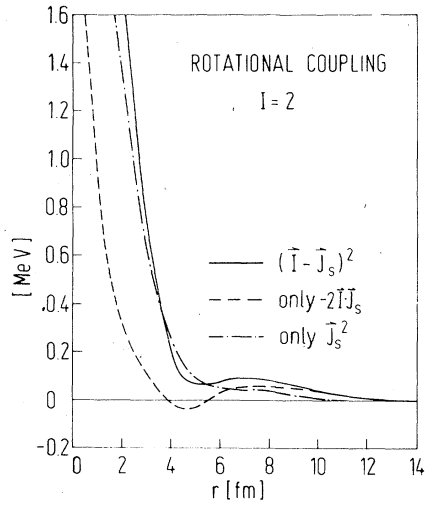


FIG. 11. Selected nondiagonal matrix elements of the rotational coupling;

$$\frac{1}{2\mu r^2}\langle [Y_l \otimes \Phi^A_{\alpha IJ}]^{[I]} | (\vec{I}-\vec{J}_S)^2 | [Y_{l'} \otimes \Phi^A_{\alpha' I' J'}]^{[I]}\rangle,$$

$k = \{\alpha, I, j\}$, $k = \{(gs,gs),1,1)\}$,

$k' = \{(gs, \tfrac{1}{2}^+), 2, 0\}$.

angular momenta I. This effect removes the degeneracy of the virtual and quasibound resonances. Therefore, the resonance states are spread over all energies and are not so well separated as the ^{12}C-^{12}C resonances (see Ref. 3). The richness of resonances in the potentials of Fig. 6 leads to an enhancement of the intermediate structure in the ^{13}C-^{13}C cross sections. Figure 11 shows nondiagonal matrix elements of the operator $(\vec{I}-\vec{J}_s)^2$ which increase rapidly at smaller relative distances because of the $1/r^2$ factor.

D. Results of coupled channel calculations

Coupled channel calculations have been carried out with the above selected ^{13}C-^{13}C channels (gs, gs), (gs, $\frac{1}{2}^+$), and ($\frac{1}{2}^+$, $\frac{1}{2}^+$).

In Fig. 12 we compare the calculated elastic 90° differential cross section with the experimental data of Helb *et al.*[14] In this calculation we have fitted the strength of the absorptive surface potential given in Eq. (41). As shown in Fig. 12 the 90°-excitation function can be reasonably reproduced in the measured energy range between 7 and 13.75 MeV. The angular distributions are compared with the experimental data in Fig. 13.

The inelastic ^{13}C-^{13}C cross sections for single and mutual excitation of the $\frac{1}{2}^+$ (3.09 MeV) state in ^{13}C are drawn in Fig. 14 (solid lines). As in the inelastic ^{12}C-^{12}C cross section the inelastic

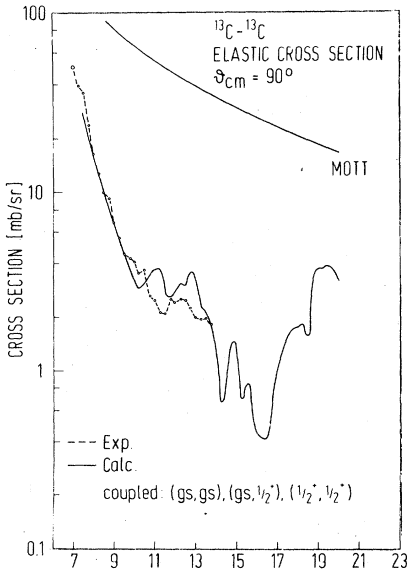


FIG. 12. The 90°-differential cross section for the elastic ^{13}C-^{13}C scattering. The experimental data are measured by Helb *et al.* [14] In the calculation we have coupled the channels (gs, gs), (gs, $\frac{1}{2}^+$), ($\frac{1}{2}^+$, $\frac{1}{2}^+$).

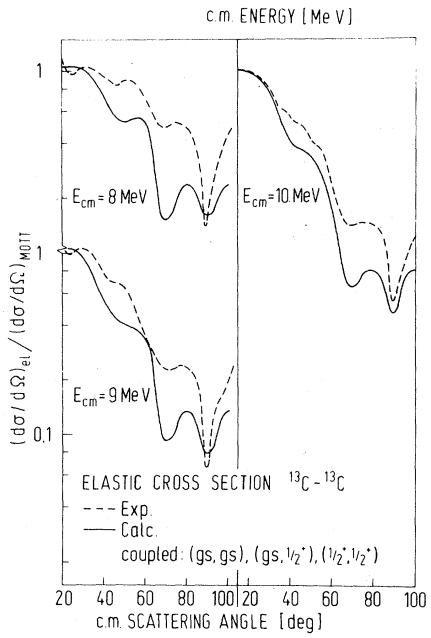


FIG. 13. Angular distributions of the elastic ^{13}C-^{13}C scattering. The experimental data are measured by Helb *et al.* (Ref. 14). The same channels as in Fig. 12 have been coupled.

^{13}C-^{13}C excitation functions reveal intermediate structures which arise by the excitation of quasibound resonances via the double resonance mechanism.[19] Up to now no experimental data have been published for a comparison with the theoretical curves.

To investigate the influence of the radial and rotational coupling potentials we have calculated the inelastic excitation function separately with the radial coupling and with the rotational one. As shown in Fig. 14 the rotational coupling is of minor influence on the inelastic cross section. The strength of the radial coupling grows with increasing relative velocity since the radial matrix elements in Eq. (30a) are multiplied by the relative momentum p_r.

The influence of the channel coupling on the intermediate structure in the elastic 90°-excitation function is illustrated in Fig. 15. When only the ground-state channels are coupled [dashed line in Fig. 15(a)] the elastic excitation function is completely smooth. On the other hand when all considered channels are coupled [solid line in Fig. 15(b)], the excitation function shows strong intermediate structures.

IV. CONCLUSIONS

The intention of this paper was to develop a practicable method for the use of molecular single-

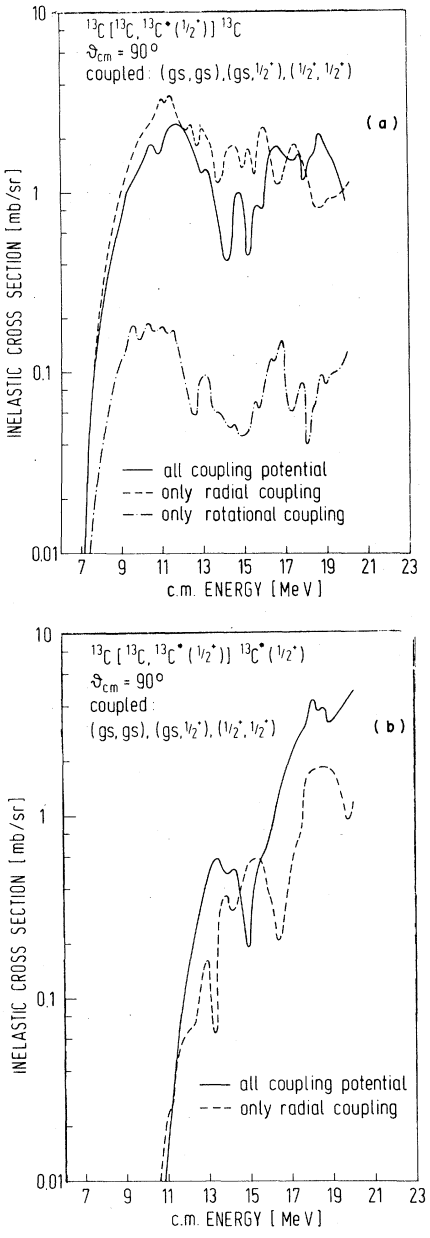


FIG. 14. The 90°-differential cross section for the single (a) and mutual (b) excitation of the first $\frac{1}{2}^+$ state in ^{13}C (solid line). The cross sections shown by the dashed and dotted-dashed lines demonstrate the effects of the radial and rotational coupling separately. One notes the importance of the radial coupling.

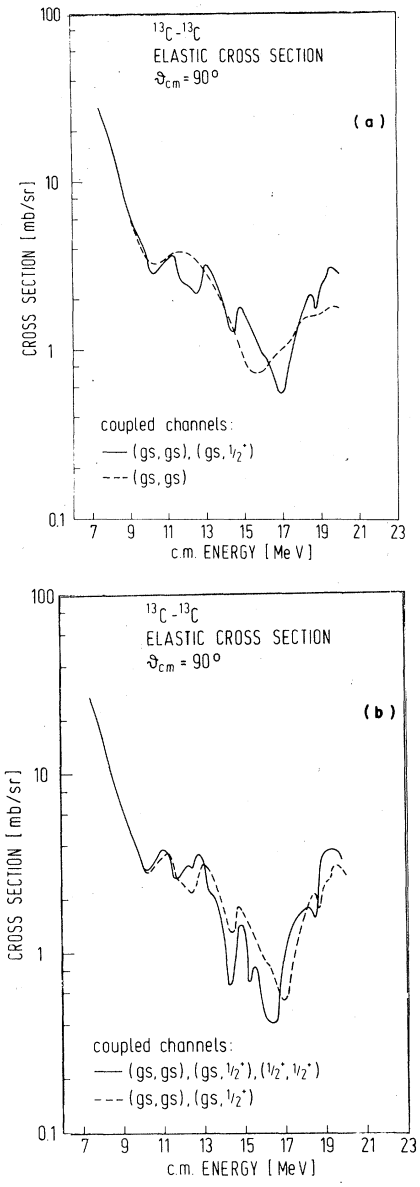


FIG. 15. The dependence of the intermediate structure on the number of coupled channels in the 90°-differential cross section for elastic ^{13}C-^{13}C scattering. The coupled channels are (a) (gs,gs) (dashed line), (gs,gs) and (gs,$\frac{1}{2}^+$) (solid line); (b) (gs,gs) and (gs,$\frac{1}{2}^+$) (dashed line), (gs,gs), (gs,$\frac{1}{2}^+$), and ($\frac{1}{2}^+$,$\frac{1}{2}^+$) (solid line).

particle wave functions in nucleus-nucleus collisions. The molecular method has the advantage that the mean interaction between all nucleons, represented by the potential of the two-center shell model, is treated correctly. A further advantage is that molecular single-particle states are orthogonal. On the contrary, single particle states, concentrated around different nuclear centers and widely used in reaction theories, do not possess this orthogonality. However, the molecular wave functions are referred to a body-fixed, rotating coordinate system and, therefore, rotational coupling enters the Hamiltonian. Our calculations (see Fig. 14) show that the diagonal part of the rotational coupling is the important one. A much stronger coupling arises through the

dependence of the molecular wave functions on the two-center distance. The radial coupling leads to the excitation of nucleons when their states, at first centered at the individual nuclei, pass into the molecular states of the compound system.

The model can be extended in two main directions: the inclusion of the transfer channels and the excitation of collective states of the cores. The treatment of the transfer channels needs a careful investigation of TCSM potentials. Various kinds of realistic TCSM potentials as given in Refs. 4, 5, 26, and 27 should be tested. Also the change of the relative coordinates in the entrance and final channels has to be taken into account.[20] The core excitation and its coupling to the single-particle motion leads to a dynamical treatment of polarization effects.

The molecular single-particle states can be experimentally verified by measuring inelastic excitation functions. As shown in Ref. 21 the intermediate structures in the inelastic cross sections depend quite sensitively on the position of the resonance states in the nucleus-nucleus potentials. Analyzing the S matrix we can explain the origin of each individual structure in the calculated inelastic cross section shown in Fig. 14. As a result we find that the positions of the structures depend on the molecular core-core potential, the excitation energy of the nucleons in the molecular orbits, and the centrifugal potentials.

Further work has to be done to reveal specific signatures in the inelastic cross sections which arise from the molecular single-particle states. Especially the study of crossings of molecular levels can become an important tool for detecting molecular single-particle effects in heavy ion collisions. At points of level crossing the excitation of nucleons becomes enhanced. This effect was studied by Fano and Lichten[22] for the analogous excitation of electrons in atomic collisions.

We thank Professor Jae Park for fruitful discussions.

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 extra particles which are measured from an arbitrary coordinate origin. If we denote the momenta canonically conjugate to the 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 as[8]

$$T=\frac{\vec{P}_{C_1}^{\,2}}{2C_1M}+\frac{\vec{P}_{C_2}^{\,2}}{2C_2M}+\sum_{i=1}^{N}\frac{\vec{p}_i^{\,2}}{2M}. \tag{A1}$$

The cores have $C_i=A_i-N_i$ nucleons ($i=1,2$) where A_i is the atomic number and N_i the number of extra particles of each nucleus. The relative motion of the two nuclei is described by the relative coordinate $\vec{r}$ between the nuclei. Since the relative coordinate is not symmetric in the particle coordinates, 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 particles. For the partition of the extra particles $i\leq N_1$ to nucleus A_1 and $N_1+1\leq i\leq N$ to nucleus A_2 the relative coordinate is given by

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

In the following we consider two canonical transformations of the kinetic energy. We transform the coordinates $\vec{R}_{C_1}$, $\vec{R}_{C_2}$, and $\vec{r}_i$ to the center-of-mass coordinate

$$\vec{R}_{\text{c.m.}}=\frac{1}{A}\left(C_1+\vec{R}_{C_1}+C_2\vec{R}_{C_2}+\sum_{i=1}^{N}\vec{r}_i\right), \tag{A3}$$

with $A=A_1+A_2$, to the relative coordinate $\vec{r}$ and N independent particle coordinates. Depending whether we use atomic or molecular coordinates for the extra particles we distinguish the following two cases.

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

$$\begin{aligned}\vec{r}_{iA_1}&=\vec{r}_i-\vec{R}_{A_1}\\&=\vec{r}_i-\frac{1}{A_1}\left(\sum_{i=1}^{N_1}\vec{r}_i+C_1\vec{R}_{C_1}\right)\quad\text{for } i\leq N_1,\\ \vec{r}_{iA_2}&=\vec{r}_i-\vec{R}_{A_2}\\&=\vec{r}_i-\frac{1}{A_2}\left(\sum_{i=N_1+1}^{N}\vec{r}_i+C_2\vec{R}_{C_2}\right)\quad\text{for } i>N_1.\end{aligned} \tag{A4}$$

The atomic coordinates (A4) are useful if one describes the motion of the extra particles by one-center shell model states concentrated around each center at $\vec{R}_{A_1}$ and $\vec{R}_{A_2}$. Introducing the momenta $\vec{P}_{\text{c.m.}}$, $\vec{p}_r$, $\vec{p}_{iA_1}$, and $\vec{p}_{iA_2}$ canonically conjugate to the coordinates $\vec{R}_{\text{c.m.}}$, $\vec{r}$, $\vec{r}_{iA_1}$, and $\vec{r}_{iA_2}$, respectively, the kinetic energy (A1) becomes

$$T=\frac{1}{2AM}\vec{P}_{\text{c.m.}}^{\,2}+\frac{1}{2\mu}\vec{p}_r^{\,2}+\frac{1}{2M}\sum_{i=1}^{N_1}\vec{p}_{iA_1}^{\,2}+\frac{1}{2M}\sum_{i=N_1+1}^{N}\vec{p}_{iA_2}^{\,2}-\frac{1}{2A_1M}\left(\sum_{i=1}^{N_1}\vec{p}_{iA_1}\right)^2-\frac{1}{2A_2M}\left(\sum_{i=N_1+1}^{N}\vec{p}_{iA_2}\right)^2, \tag{A5}$$

where μ is the reduced mass of the relative motion.

(b) In the second case, the coordinates of the extra particles are measured from the center of mass at $\vec{R}_{\text{c.m.}}$ (see Fig. 2):

$$\vec{r}_{i\text{c.m.}}=\vec{r}_i-\vec{R}_{\text{c.m.}}. \tag{A6}$$

The molecular coordinates (A6) are applicable if the motion of the extra particles is described by two-center wave functions, as we have done in our calculations. 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[8]:

$$T=\frac{1}{2AM}\vec{P}_{\text{c.m.}}^{\,2}+\frac{1}{2\mu}\vec{p}_r^{\,2}+\frac{1}{2M}\sum_{i=1}^{N}\vec{p}_{i\text{c.m.}}^{\,2}+\left(\frac{1}{A_1M}\sum_{i=1}^{N_1}\vec{p}_{i\text{c.m.}}-\frac{1}{A_2M}\sum_{i=N_1+1}^{N}\vec{p}_{i\text{c.m.}}\right)\cdot\vec{p}_r-\frac{1}{2AM}\left(\sum_{i=1}^{N}\vec{p}_{i\text{c.m.}}\right)^2. \tag{A7}$$

In Eq. (A7) the last term can be neglected when the number of the extra particles is small compared to the number of nucleons in the cores, i.e.,

$$N_i/(A_i-N_i)\ll 1,\quad i=1,2. \tag{A8}$$

The fourth term in (A7) contains the coupling between the extra particles and the relative motion and has to be taken into account for large relative velocities. Although the masses of nuclei A_1M and A_2M stand in the denominators of this expression, the term is not negligible for small ratios $N_i/A_i\ll 1$ as can be seen by the following argument: Replacing $\vec{p}_r=\mu\vec{v}_r$ one recognizes that the fourth term in Eq. (A7) is proportional to the relative velocity and the difference of the momenta of the extra particles.

As discussed in Sec. II C, it is convenient to introduce a rotating coordinate system with the z' axis coinciding with the direction of $\vec{r}$. The particle coordinates in the rotating frame are denoted by $\vec{r}'_{iA_1}$, $\vec{r}'_{iA_2}$, and $\vec{r}'_{i\text{c.m.}}$. Here 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 $\vec{p}'_{i\text{c.m.}}$ of the rotating frame. The momentum of the relative motion transforms as follows:

$$\vec{p}_r=\frac{\hbar}{i}\vec{e}_r\frac{\partial}{\partial r}-\frac{\vec{e}_r}{r}\times(\vec{I}-\vec{J}') \tag{A9}$$

with $\vec{e}_r=\vec{e}_{r'}$, the total angular momentum $\vec{I}$ and the angular momentum $\vec{J}'$ of the extra nucleons. When the coordinates $\vec{r}'_{iA_1}$ and $\vec{r}'_{iA_2}$ are used, $\vec{J}'$ is the sum of the angular momenta of the extra particles including their spin with respect to the two nuclear centers:

$$\vec{J}'=\sum_{i=1}^{N_1}\vec{r}'_{iA_1}\times\vec{p}'_{iA_1}+\sum_{i=N_1+1}^{N}\vec{r}'_{iA_2}\times\vec{p}'_{iA_2}+\sum_{i=1}^{N}\vec{s}'_i. \tag{A10}$$

In molecular coordinates the angular momentum $\vec{J}'$ of the extra particles is measured from the center of mass in the rotating frame,

$$\vec{J}'=\sum_{i=1}^{N}\vec{r}'_{i\text{c.m.}}\times\vec{p}'_{i\text{c.m.}}+\sum_{i=1}^{N}\vec{s}'_i. \tag{A11}$$

With the angular momentum $\vec{J}_A$ of the extra particles measured from the center of mass of the individual nuclei, the angular momentum $\vec{J}'$ given in Eq. (A11) can be written in the form

$$\vec{J}'=\vec{J}_a+\vec{J}_0 \tag{A12}$$

with

$$\vec{J}_a=\sum_{i=1}^{N_1}\vec{r}'_{iA_1}\times\vec{p}'_{i\text{c.m.}}+\sum_{i=N_1+1}^{N}\vec{r}'_{iA_2}\times\vec{p}'_{i\text{c.m.}}+\sum_{i=1}^{N}\vec{s}'_i,$$
$$\vec{J}_0=\frac{1}{A}\vec{r}\times\left(A_2\sum_{i=1}^{N_1}\vec{p}'_{i\text{c.m.}}-A_1\sum_{i=N_1+1}^{N}\vec{p}'_{i\text{c.m.}}\right). \tag{A13}$$

Here we have used the relations

$$\vec{r}'_{i\text{c.m.}}=\vec{r}'_{iA_1}+\frac{A_2}{A}\vec{r}\quad\text{for } i\leq N_1$$

and (A14)

$$\vec{r}'_{i\text{c.m.}}=\vec{r}'_{iA_2}-\frac{A_1}{A}\vec{r}\quad\text{for } i>N_1.$$

Inserting (A12) into (A7) and using the relation (A9) we finally obtain the following expression for the kinetic energy (A7):

$$T=\frac{1}{2AM}\vec{P}_{\text{c.m.}}^{\,2}-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\left(\frac{\partial}{\partial r}+D\right)r^2\left(\frac{\partial}{\partial r}+D\right)\right]+\frac{(\vec{I}-\vec{J}_a)^2}{2\mu r^2}+\frac{1}{2M}\sum_{i=1}^{N}\vec{p}'^{\,2}_{i\text{c.m.}}-\frac{1}{2A_1M}\left(\sum_{i=1}^{N_1}\vec{p}'_{i\text{c.m.}}\right)^2-\frac{1}{2A_2M}\left(\sum_{i=N_1+1}^{N}\vec{p}'_{i\text{c.m.}}\right)^2 \tag{A15}$$

with

$$D=\frac{1}{A}\left(A_2\sum_{i=1}^{N_1}\frac{\partial}{\partial z'_{i\text{c.m.}}}-A_1\sum_{i=N_1+1}^{N}\frac{\partial}{\partial z'_{i\text{c.m.}}}\right). \tag{A16}$$

If we replace $\vec{p}'_{c.m.}$ by $\vec{p}'_{tA_1}$ and $\vec{p}'_{tA_2}$ and $(\hbar/i)(\partial/\partial r + D)$ by $(\hbar/i)(\partial/\partial r)$ in (A15) we obtain the analogous expression of the kinetic energy T written in atomic coordinates. The kinetic energies in the atomic and molecular coordinates differ in the radial part of the operator $\vec{p}_r^{\,2}$, since the molecular single-particle wave functions depend on the relative distance r in contrary to the one-center single-particle wave functions.

APPENDIX B: THE TWO-CENTER SHELL MODEL

The wave functions of the symmetric two-center shell model solve the Schrödinger equation:

$$\left(-\frac{\hbar^2}{2M}\Delta + V(\rho, z; z_0) + V_{ls} + V_{l^2} - \epsilon^{g,u}_{\lambda(j)lm}\right) \times \chi^{g,u}_{\lambda(j)m}(\rho, \varphi, z; z_0) = 0 . \quad \text{(B1)}$$

According to Maruhn *et al.*[23] the potential $V(\rho, z; z_0)$ in (B1) is given for identical and spherical nuclei by

$$|z| < z_0: \quad V(\rho, z; z_0) = \tfrac{1}{2}M\omega^2(z_0)[\rho^2 + z'^2 f_0(1 + cz' + dz'^2)] , \quad \text{(B2)}$$

$$|z| > z_0: \quad V(\rho, z; z_0) = \tfrac{1}{2}M\omega^2(z_0)(\rho^2 + z'^2) \quad \text{(B3)}$$

with

$$z' = |z| - z_0 ,$$

where M is the nucleon mass. The potential and the corresponding nuclear surface are depicted in Fig. 4. The constants c and d are fixed by the condition that the potential and its derivative are continuous at $z = 0$. The parameter f_0 may be obtained by minimizing the liquid drop energy of the nuclear system.[7] For simplicity we have calculated the wave functions of the extra particles with the two-center oscillator potential, i.e., $c = d = 0$ and $f_0 = 1$.

In the adiabatic approximation the oscillator frequency $\omega(z_0)$ is determined with the condition of volume conservation. In that case the equipotential surface describing the nuclear surface has the value

$$V_0 = \tfrac{1}{2}M\omega_\infty^2 R_0^2 . \quad \text{(B4)}$$

Here R_0 denotes the radius: $R_0 = r_0(A/2)^{1/3}$ of the separated nuclei and ω_∞ the asymptotic frequency: $\omega_\infty = \omega(z_0 \to \infty)$. In the sudden approximation the frequency ω is independent of $r = 2z_0$ and is set equal to its asymptotic value ω_∞ also in the interaction region.

In addition the realistic two-center shell potential in (B1) includes the spin-orbit potential V_{ls} of Thomas-type

$$V_{ls}(\vec{r}, \vec{p}, \vec{s}) = -\frac{2\kappa\hbar}{M\omega_0}(\vec{\nabla}V \times \vec{p}) \cdot \vec{s} \quad \text{(B5)}$$

and a l^2 type term

$$V_{l^2}(\vec{r}, \vec{p}) = -\hbar\omega_0\kappa\mu\left[\left(\frac{1}{2\hbar}\vec{\nabla}(\rho^2 + z'^2) \times \vec{p}\right)^2 - \frac{N(N+3)}{2}\delta_{lf}\right] . \quad \text{(B6)}$$

The second term of (B6) is diagonal in the basis states of the two-center oscillator defined in (B7) because of the Kronecker symbol δ_{lf}. $N = N_\rho + n_z$ denotes the principal quantum numbers of the two-center oscillator. The parameters ω_0, κ, and μ are interpolated between the values of the united and separated systems as proposed in Ref. 23.

The eigenfunctions and eigenvalues of the two-center shell model are obtained by diagonalizing the Schrödinger equation (B1) with the eigenfunctions of the symmetric two-center oscillator given by

$$\left(-\frac{\hbar^2}{2M}\Delta + \tfrac{1}{2}M\omega^2(z_0)(\rho^2 + z'^2) - \epsilon_{n_z N_\rho |m|}\right) \times \psi_{n_z N_\rho m m_s}(\rho, \varphi, z; z_0) = 0 . \quad \text{(B7)}$$

The functions ψ factorize in the coordinates ρ, φ, and z and the spin part. They can be written in terms of Laguerre polynomials and confluent hypergeometric functions as shown in Ref. 5.

Asymptotically the wave functions $\chi^{g,u}_{\lambda(j)m}$ approach a superposition of solutions $\varphi_{\lambda ljm}$ of the one-center oscillator shell model:

$$\chi^{g,u}_{\lambda(j)m}(\vec{r}, z_0 \to \infty) = \frac{1}{\sqrt{2}}[\varphi_{\lambda ljm}(\vec{r} - z_0\vec{e}_z) \pm (-1)^l \varphi_{\lambda ljm}(\vec{r} + z_0\vec{e}_z)] . \quad \text{(B8)}$$

The phase factor $(-1)^l$ is the parity of the functions $\varphi_{\lambda ljm}(\vec{r})$ with respect to the center of the oscillator.

APPENDIX C: THE S MATRIX AND THE CROSS SECTION

The total wave function (8) can be written asymptotically in the form[16]

$$\Psi = \sum_{k,k',I,M} A^{IM}_k(\delta_{k'k}J_{k'} - S^I_{k'k}O_{k'}) \times [i^{l'}Y_{l'} \otimes \Phi^A_{\alpha_1\alpha_2 J}(1, 2, \vec{r})]^{[I]}_M . \quad \text{(C1)}$$

The abbreviations are $k = \{\alpha_1, \alpha_2, l, J\}$ and J_k and O_k for the ingoing and outgoing Coulomb functions. $S^I_{k'k}$ is the S matrix, Y_{lm} the orbital wave functions, and the intrinsic wave functions are taken as

$$\Phi^{A}_{\alpha_1\alpha_2 JM}(1,2,\vec{r}) = \frac{1}{2(1+\delta_{\alpha_1\alpha_2})^{1/2}} A(1,2)[\varphi_{\alpha_1}(\vec{r}_{1c.m.},\vec{r}/2)\otimes\varphi_{\alpha_2}(\vec{r}_{2c.m.},-\vec{r}/2) - (-1)^{l}\varphi_{\alpha_1}(\vec{r}_{2c.m.},-\vec{r}/2)\otimes\varphi_{\alpha_2}(\vec{r}_{1c.m.},\vec{r}/2)]^{[J]}_{M}, \quad \alpha_i=\{\lambda_i, I_i=j_i\}. \tag{C2}$$

In the one-center wave function φ_α we denote the position of the cores by $\pm\vec{r}/2$ to which the extra particles 1 and 2 belong. The coefficients A^{IM}_k are determined by the asymptotic form of the wave function Ψ. The wave function (C1) has incoming and outgoing waves in the channels k, whereas in all other channels only outgoing waves are present. To specify the initial conditions we assume that the nuclei are in the initial states, defined by the quantum numbers $\mu_1=\{\lambda_1, I_1=j_1, M_1\}$ and $\mu_2=\{\lambda_2, I_2=j_2, M_2\}$. These conditions are fulfilled by the coefficients

$$A^{IM}_k = \frac{i}{k_k}[\pi(2l+1)(1+\delta_{\alpha_1\alpha_2})]^{1/2}\delta_{\alpha_1,(\lambda_1 I_1)}\delta_{\alpha_2,(\lambda_2 I_2)} \times (lOJM|IM)(I_1M_1I_2M_2|JM). \tag{C3}$$

Inserting (C3) into (C1) and using the definitions of the Coulomb functions J_k, O_k and the wave function $u_C(\vartheta)$ for the Coulomb scattering of two point charges we get the following expression for the asymptotic wave function (C1):

$$\Psi = \tfrac{1}{2}\{u_c(\vartheta)A(1,2)\varphi_{\mu_1}(\vec{r}_{1c.m.},\vec{r}/2)\varphi_{\mu_2}(\vec{r}_{2c.m.},-\vec{r}/2) - u_c(\pi-\vartheta)A(1,2)\varphi_{\mu_1}(\vec{r}_{2c.m.},-\vec{r}/2)\varphi_{\mu_2}(\vec{r}_{1c.m.},\vec{r}/2)\}$$
$$+\frac{1}{2}\sum_{\mu_1',\mu_2',\mu}\frac{i^{l'+1}}{k_k}[\pi(2l+1)]^{1/2}\left(\frac{1+\delta_{\alpha_1\alpha_2}}{1+\delta_{\alpha_1'\alpha_2'}}\right)^{1/2}(I_1M_1I_2M_2|JM)(I_1'M_1'I_2'M_2'|J'M')$$
$$\times(lOJM|IM)(l'm'J'M'|IM)(e^{2i\sigma_{l'}}\delta_{k'k}-S^{I}_{k'k})Y_{l'm'}(\Omega)O_{k'}$$
$$\times A(1,2)\{\varphi_{\mu_1'}(\vec{r}_{1c.m.},\vec{r}/2)\varphi_{\mu_2'}(\vec{r}_{2c.m.},-\vec{r}/2) - (-1)^{l'}\varphi_{\mu_1'}(\vec{r}_{2c.m.},-\vec{r}/2)\varphi_{\mu_2'}(\vec{r}_{1c.m.},\vec{r}/2)\},$$
$$\mu=\{l,J,l',m',J',M',I,M\}. \tag{C4}$$

The Coulomb phase is denoted by σ_l. The sum represents the waves scattered by the nuclear interaction. The nuclear part of the scattering amplitude for the scattering from the initial states μ_1, μ_2 into the final states μ_1', μ_2' is derived from wave function (C4) according to the method given in Refs. 12 and 16:

$$f^{\mu_1'\mu_2'}_{\mu_1\mu_2}(\vartheta,\varphi) = \sum_{\mu}\frac{i}{k_k}[\pi(2l+1)]^{1/2}[(1+\delta_{\alpha_1\alpha_2})(1+\delta_{\alpha_1'\alpha_2'})]^{1/2}(I_1M_1I_2M_2|JM) \times (I_1'M_1'I_2'M_2'|J'M')(lOJM|IM)(l'm'J'M'|IM)(e^{2i\sigma_{l'}}\delta_{k'k}-S^{I}_{k'k})Y_{l'm'}(\vartheta,\varphi). \tag{C5}$$

With the Coulomb scattering amplitude $f_c(\vartheta)$ we finally obtain for the differential cross section for the scattering from the initial states μ_1 and μ_2 into the final states μ_1' and μ_2' observed in the direction ϑ, φ and $\pi-\vartheta$, $\varphi+\pi$, respectively:

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mu_1\mu_2\to\mu_1'\mu_2'} = |f_c(\vartheta)\delta_{\mu_1'\mu_1}\delta_{\mu_2'\mu_2} - f_c(\pi-\vartheta)\delta_{\mu_1'\mu_2}\delta_{\mu_2'\mu_1} + f^{\mu_1'\mu_2'}_{\mu_1\mu_2}(\vartheta,\varphi)|^2. \tag{C6}$$

Since usually the magnetic quantum numbers are not measured, we have to average over the initial states and to sum over the final states:

$$\left(\frac{d\sigma}{d\Omega}\right)_{\alpha_1\alpha_2\to\alpha_1'\alpha_2'} = \frac{1}{(2I_1+1)(2I_2+1)} \times \sum_{M_1',M_2',M_1,M_2}\left(\frac{d\sigma}{d\Omega}\right)_{\mu_1\mu_2\to\mu_1'\mu_2'}. \tag{C7}$$

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