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Energy dependence of the real part of ion-ion interaction potential

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A simple derivation for the energy dependence of the real part of ion-ion interaction potential is given in the framework of Brueckner's energy density formalism. This is based on the decreasing effect of antisymmetrization on the kinetic energy densities of the two ions which is studied in a Fermi gas model and tends to make the ion-ion potential more and more attractive with increasing relative energy $E_{\mathrm{c.m.}}$. On the other hand, the linear dependences of the kinetic energy densities and the momentum densities on $E_{\mathrm{c.m.}}$, through the effective mass term in the energy density, introduce a repulsion which increases directly as the relative energy. At low values of $E_{\mathrm{c.m.}}$ the first effect dominates over the second one, thereby making the ion-ion potential more and more attractive. However, at relatively high energies, the repulsion caused by the second effect dominates completely and makes the potential less and less attractive.

[NUCLEAR REACTIONS Antisymmetrization effects, Fermi gas model, momentum density, effective mass term, energy dependence of ion-ion interaction potential.]

I. INTRODUCTION

In a previous publication[1] we had reported the results of our calculation for the real part of the ion-ion interaction potentials for several pairs of spherical nuclei in the framework of Brueckner's energy density formalism.[2] It was shown there that the positions and heights of the calculated Coulomb barriers for all the pairs of nuclei considered agree well with those referred to in the literature. However, in the above mentioned calculation the effects arising out of the relative motion of the two colliding ions on the interaction potential were not taken into account. Brink and Stancu[3] have shown in detail the dependence of the real part of the potential for the system ^{16}O-^{16}O on this relative motion by taking proper account of the antisymmetrization effects on the particle densities and kinetic energy densities of the two colliding ions by evaluating them in a two-center harmonic oscillator potential. However, the numerical difficulties pose a serious problem in extending these calculations to pairs of medium and heavy nuclei.

Recently, Moszkowski[4] has shown how the dependence of the ion-ion interaction potential on the relative energy of the ions can be included in a very simple but approximate way. Using the simple energy density introduced by Skyrme,[5] the effects of relative energy of the two ions were taken into account by adding correction terms to the energy independent potential. These correction terms arise from (i) the antisymmetrization effects on the kinetic energy and (ii) the effective mass term. In Ref. 4, while the first correction was calculated by using a Fermi gas model, the correction arising out of the effective mass term was estimated by considering the energy dependence of the nucleon-nucleus optical potential in an empirical way. Besides, the necessary modification[3] of the effective mass term in the energy density when the nuclei are in relative motion is not taken into account in the work of Moszkowski.[4] As shown in Ref. 3, this modification introduces an extra repulsion in the ion-ion interaction potential at any energy.

In the present work, where we have extended our earlier calculation[1] of the real part of ion-ion potential to include the effects arising out of relative motion, the antisymmetrization on the kinetic energy densities of the colliding ions is taken into account by evaluating the kinetic energy density of the composite system of two ions in a Fermi gas model. However, since we use the sudden approximation of Brueckner[2] in our calculation, the antisymmetrization effects arising out of the modifications on the particle densities of the two ions are completely ignored. This is justified to a good extent because most of the antisymmetrization corrections come from the modifications of the kinetic energy densities.[3] Besides, this approach of calculating the ion-ion interaction potential has the advantage that it can be extended to any pair of nuclei without facing the problem of complicated numerical calculations. Moreover, since the energy density used in our calculation is derived from a simple two-body effective interaction,[6] the necessary modification[3] of the effective mass term when the nuclei are in relative motion can be easily taken into account and the energy dependence of the ion-ion potential arising out of this term, as will be shown in what follows, is included automatically and one need not consider it separately in an empirical way as in Ref. 4.

II. BASIC FORMALISM

The nuclear part of the ion-ion interaction potential as a function of the separation distance R between the centers of the two colliding ions can be given by,

$$V(R) = \int [H(\rho,\zeta) - H(\rho_1,\zeta_1) - H(\rho_2,\zeta_2)]d^3r \,, \tag{1}$$

where $H(\rho,\zeta)$ is the energy density of the composite system, $H(\rho_1,\zeta_1)$ and $H(\rho_2,\zeta_2)$ are the same for the two separate nuclei, and ρ and ζ are, respectively, the particle density and the kinetic energy density. In the framework of the density matrix expansion proposed by Negele and Vautherin,[7] the energy density of a nucleus derived from a two-body effective interaction can be given by

$$H(\rho,\zeta) = \frac{\hbar^2}{2m}\zeta + A(\rho) + B(\rho)\zeta + C(\rho)(\nabla\rho)^2 \,. \tag{2}$$

While the first term in Eq. (2) is the pure kinetic energy term, the third term comes from the exchange part of the two-body effective interaction and determines the density dependence of the nucleon effective mass. This term gets modified[3] when the nuclei are in relative motion with respect to each other. This modification is done in replacing $\rho\zeta$ by $\rho\zeta - j^2$ where $\vec{j}$ is the momentum density. With this change, the energy density becomes

$$H(\rho,\zeta) = \frac{\hbar^2}{2m}\zeta + A(\rho) + \frac{B(\rho)}{\rho}(\rho\zeta - j^2) + C(\rho)(\nabla\rho)^2 \,. \tag{3}$$

If in the center of mass system the two nuclei are moving towards each other with momenta $\vec{K}$ and $-\vec{K}$ respectively, it can be shown that[3] this motion can be approximated by a plane wave. Under this approximation the densities $\rho_{1,2}$ of the two separate nuclei are independent of the relative energy whereas the kinetic energy densities $\zeta_{1,2}$ are linear in $k_{1,2}{}^2$:

$$\zeta_{1,2} = \zeta^s_{1,2} + k_{1,2}{}^2\rho_{1,2} \,, \tag{4}$$

where $k_{1,2} = K/A_{1,2}$ and $\zeta^s_{1,2}$ are the static kinetic energy densities. In the same approximation, the momentum densities of the two nuclei can be given by

$$\vec{j}_1 = \vec{k}_1\rho_1 \,, \qquad \vec{j}_2 = -\vec{k}_2\rho_2 \,. \tag{5}$$

The calculation of the interaction potential $V(R)$ in Eq. (1) requires the knowledge of the density ρ, the momentum density $\vec{j}$, and the kinetic energy density ζ of the composite system of the two nuclei. For the sake of simplicity, we use the sudden approximation in our calculation so that $\rho = \rho_1 + \rho_2$. For the momentum density $\vec{j}$, we use the approximation of Brink and Stancu,[3] namely $\vec{j} = \vec{j}_1 + \vec{j}_2$. In Ref. 1 we had approximated the static kinetic energy densities in Eq. (4) by

$$\zeta^s_{1,2} = \tfrac{3}{5}k_{F_{1,2}}{}^2\rho_{1,2} + \tfrac{1}{2}\nabla^2\rho_{1,2} \,. \tag{6}$$

However, in the present work we have used for the Thomas-Fermi term in Eq. (6), the approximation due to Kirzhnit[8] so that

$$\zeta^s_{1,2} = \tfrac{3}{5}k_{F_{1,2}}{}^2\rho_{1,2} + \tfrac{1}{36}\frac{(\nabla\rho_{1,2})^2}{\rho_{1,2}} + \tfrac{1}{3}\nabla^2\rho_{1,2} \,. \tag{7}$$

This approximation for $\zeta^s_{1,2}$ has been examined by Brink and Stancu[9] and also by one of the present authors,[10] and it has been observed that this leads to a better description of the ion-ion potential in the tail region than the relation in Eq. (6). The Thomas-Fermi term in the kinetic energy densities takes account of the antisymmetrization corrections in the ion-ion potential. When the ions have relative motion, the necessary modification of this term for the composite system of the two ions is done by using a Fermi gas model.[4] In this model, while the Fermi spheres of the two colliding ions overlap perfectly at zero relative energy, they overlap partially at finite energy and do not overlap at all beyond a critical energy. Defining a reduced energy $\mathcal{E}$ by

$$\mathcal{E} = E_{\text{c.m.}}/a \,, \tag{8}$$

where $\mathcal{E}_{\text{c.m.}}$ is the total relative energy in the center of mass system and a is the reduced mass number $A_1A_2/(A_1+A_2)$, it can be shown[4] that the Fermi seas of the two ions do not overlap at all if

$$\mathcal{E} \geq 4T_F \,, \tag{9}$$

where T_F is the Fermi kinetic energy at the Fermi surface. For $\mathcal{E} < 4T_F$, the Fermi seas of the two ions overlap partially, and in that case the Thomas-Fermi term in the kinetic energy density of the composite system will be proportional to

$$F(\rho_1{}^{5/3} + \rho_2{}^{5/3}) + (1-F)(\rho_1+\rho_2)^{5/3} \,, \tag{10}$$

where F is the fractional volume of each Fermi sphere which does not overlap with the other. We take the following relation of F given by Moszkowski[4]:

$$F = \tfrac{3}{2}\left(\frac{\mathcal{E}}{4T_F}\right)^{1/2} - \tfrac{1}{2}\left(\frac{\mathcal{E}}{4T_F}\right)^{3/2} \,, \tag{11}$$

and use for the Fermi kinetic energy T_F at the Fermi surface, the value corresponding to nuclear matter at normal density. With these modifications in the Thomas-Fermi term, we approximate the kinetic energy density for the composite system as

$$\zeta = \tfrac{3}{5}\left(\frac{3\pi^2}{2}\right)^{2/3}\left[F(\rho_1{}^{5/3}+\rho_2{}^{5/3}) + (1-F)(\rho_1+\rho_2)^{5/3}\right] + \tfrac{1}{36}\frac{(\nabla\rho)^2}{\rho} + \tfrac{1}{3}\nabla^2\rho + k_1{}^2\rho_1 + k_2{}^2\rho_2\,, \tag{12}$$

where $\rho = \rho_1 + \rho_2$. From Eqs. (10) and (11) it is seen that for $\mathcal{E} = 0$ there is perfect overlap of the Fermi levels whereas this overlap decreases to zero as $\mathcal{E}$ approaches $4T_F$.

III. RESULTS AND DISCUSSIONS

Using the formalism of Sec. II and the parametrized versions of the density functionals $A(\rho)$, $B(\rho)$, and $C(\rho)$ obtained in Ref. 1, we have calculated the real part of the ion-ion interaction potential for the system ^{16}O-^{16}O at different relative energy $E_{c.m.}$. This result is shown in Fig. 1, where the interaction potential is plotted as a function of the separation distance R. It is seen that the potential becomes more and more attractive when $E_{c.m.}$ varies from 0 to 250 MeV. Beyond this range of $E_{c.m.}$ the potential curve starts to move in the opposite direction and for large values of energy, for example $E_{c.m.} = 1000$ MeV, rises above the curve for zero energy. This behavior of the ion-ion potential $V(R)$ with energy agrees with the findings of Brink and Stancu,[3] at least qualitatively.

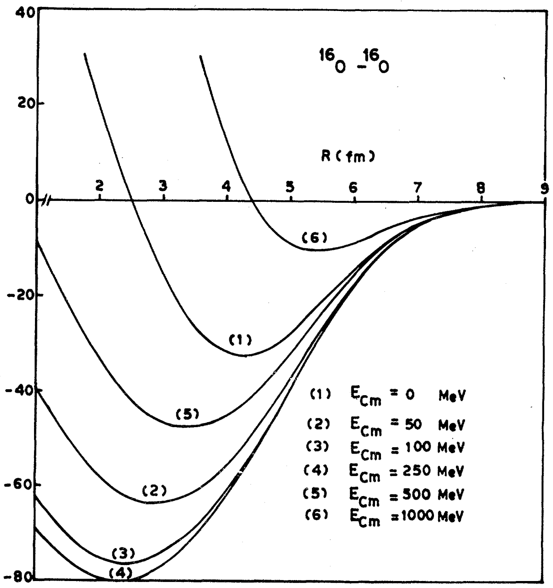

FIG. 1. The real part of ion-ion interaction potential $V(R)$ as a function of the separation distance R, at different energy $E_{c.m.}$.

From Eq. (12) it is readily seen that the antisymmetrization effects on the kinetic energy density decreases as $E_{c.m.}$ increases. This effect, which causes the potential to become more and more attractive for low values of $E_{c.m.}$ is shown in Fig. 2, where we have plotted $V_A(R)$ as a function of R for different energies. The quantity $V_A(R)$ represents the antisymmetrization correction due to the modifications made on the Thomas-Fermi term in the kinetic energy density of the composite system of both the ions through Eq. (10) and can be given by

$$V_A(R) = \int\left[\left(\frac{\hbar^2}{2m} + B(\rho)\right)\zeta_{TF}(C) - \left(\frac{\hbar^2}{2m} + B(\rho_1)\right)\zeta_{TF}(1) - \left(\frac{\hbar^2}{2m} + B(\rho_2)\right)\zeta_{TF}(2)\right] d^3r\,. \tag{13}$$

Here $\zeta_{TF}(C)$ is the Thomas-Fermi term of the kinetic energy density of the composite system

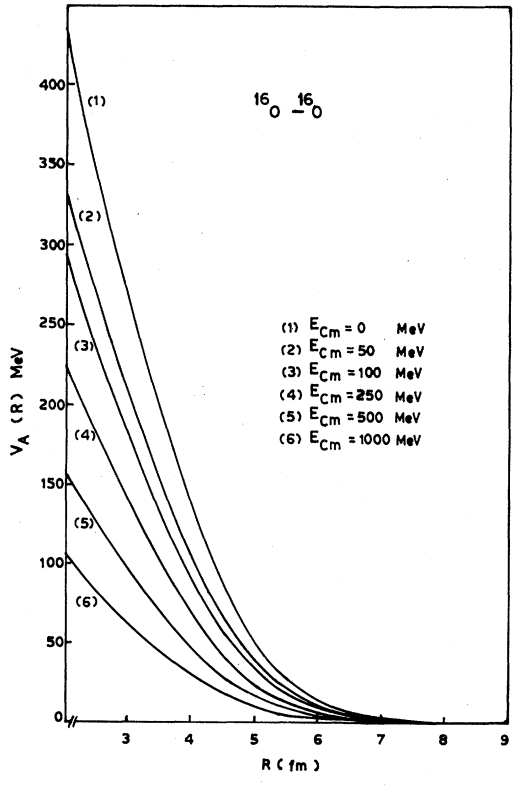

FIG. 2. $V_A(R)$ [Eq. (12)] as a function of the separation distance R, at different energy $E_{c.m.}$.

and $\zeta_{TF}(1)$ and $\zeta_{TF}(2)$ are the same for the two separate ions. The major contribution to $V_A(R)$ comes from the pure kinetic energy term and this contribution vanishes for energies $\mathcal{E} \geq 4T_F$. However, the contribution from the other term associated with the density functional (the so called effective mass term) does not vanish at this critical energy because $B(\rho)$ is always greater than $B(\rho_1)$, as well as $B(\rho_2)$.

Besides the decreasing effect of antisymmetrization, there is an additional energy dependence of $V(R)$ at any energy which comes from the linear dependence of ζ and j^2 on k^2. From the relation of $\zeta_{1,2}$ and $j_{1,2}{}^2$ in Eqs. (4) and (5) we see that

$$(\rho_{1,2}\zeta_{1,2} - j_{1,2}{}^2) = \rho_{1,2}\zeta^s_{1,2}$$

and the contribution $V_E(R)$ from this additional energy dependence to the potential $V(R)$ can be obtained as

$$V_E(R) = (k_1 + k_2)^2 \int \frac{B(\rho)}{\rho} \rho_1 \rho_2 \, d^3r \, . \tag{15}$$

This is linear in $E_{\text{c.m.}}$ and is determined completely by the density functional B. In Fig. 3 we have shown this energy dependence of the potential where $V_E(R)$ is plotted as a function of R at different energy.

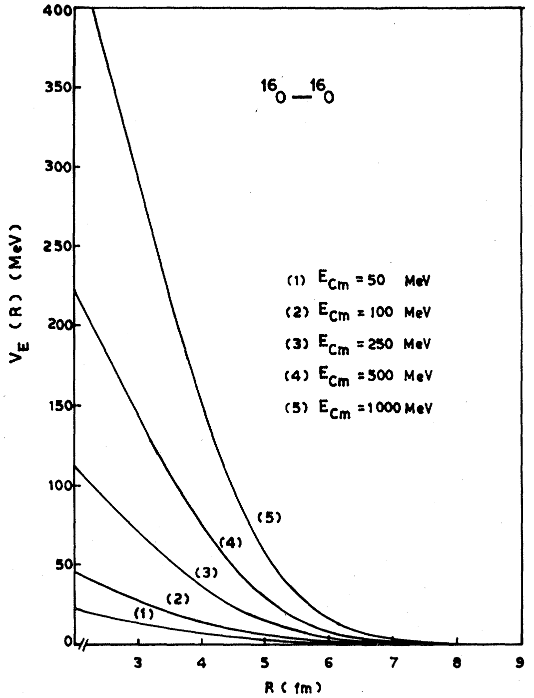

FIG. 3. $V_E(R)$ [Eq. (15)] as a function of the separation distance R, at different energy $E_{\text{c.m.}}$.

Thus we see that the complete energy dependence of the potential $V(R)$ comes from two distinct effects, namely (i) the decreasing effect of antisymmetrization on the kinetic energy densities which causes the potential to be more and more attractive with increasing energy and (ii) the linear dependence of ζ and j^2 on k^2 which tends to decrease the strength of the potential as energy increases. While both the kinetic term and the effective mass term contribute to the first effect, the contribution to the second effect comes only from the effective mass term. The increasing attraction brought into the potential due to the first effect through $V_A(R)$ dominates the repulsive effect $V_E(R)$ coming from the effective mass term and this causes the total potential $V(R)$ to be more and more attractive at low energies. However, at relatively high energies, $V_E(R)$ completely dominates over $V_A(R)$, thereby making the ion-ion potential $V(R)$ less and less attractive. These findings are in conformity with those of Moszkowski.[4] However, as mentioned earlier, the contribution from the effective mass term which has two opposite effects, comes automatically in our calculation through the density functional B whereas these effects are treated phenomenologically in Ref. 4. Moreover, the extra repulsion brought by the j^2 term in the energy density is not taken into account in the work of Ref. 4.

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