Spin density and the real part of the heavy-ion potential

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The contribution of the spin density term in the Vautherin-Brink energy density functional to the real part of the heavy-ion potential is estimated. The explicit expression involving Hartree-Fock orbitals given by Vautherin and Brink is used to calculate the spin density where, instead of self-consistent orbitals, shell model orbitals have been used. Results are presented for target projectile combinations such that (a) one of the nuclei is spin unsaturated and (b) both are spin unsaturated. The contribution of the spin density term to the heavy-ion potential is found to be appreciable.

I. INTRODUCTION

The energy density formalism[1-3] has been used extensively in calculating the real part of the heavy ion potential.[4-8] The advantage of the method over other microscopic approaches lies in its computational simplicity. Among the various energy density functionals, the one given by Vautherin and Brink[3] (VB) derived from Skyrme interaction[9] enjoys special popularity because of its success in predicting properties of individual nuclei. The VB energy density is given in terms of nucleon mass density, the kinetic energy density, and the spin density (also referred to in the literature as "spin-orbit density").[10] The spin density arises out of the two-body spin-orbit interaction term in Skyrme interaction. The role of the spin density in determining the heavy ion potential is not adequately known. Either the systems studied had spin density equal to zero (spin saturated systems) or the term was neglected, assuming its contribution to be small.[5-6] If one wishes to extend the energy density formalism to deep inelastic collision processes, a proper evaluation of the importance of the term becomes necessary. Because of particle transfer, two spin saturated systems on collision will give rise to combinations which are not necessarily spin saturated. In fission also this term is expected to play a role, though the situation is more complicated by the presence of deformation. In this paper we present a systematic study of the contribution of the spin density term in the VB energy density functional to the heavy ion potential, confining our attention to spherical systems. In Sec. II the theory and the relevant mathematical details are given. In Sec. III the results of the computation are presented and discussed.

II. THE CONTRIBUTION OF SPIN DENSITY TO THE HEAVY ION POTENTIAL

The VB energy density functional for an even-even spherical nucleus is given by[3]

$$H(\mathbf{r},\rho,\tau,\mathbf{J})=\frac{\hbar^2}{2m}\tau+\tfrac{1}{2}t_0[(1+\tfrac{1}{2}x_0)\rho^2-(x_0+\tfrac{1}{2})(\rho_n^2+\rho_p^2)]+\tfrac{1}{4}(t_1+t_2)\rho\tau+\tfrac{1}{8}(t_2-t_1)(\rho_n\tau_n+\rho_p\tau_p)$$
$$+\tfrac{1}{16}(t_2-3t_1)\rho\nabla^2\rho+\tfrac{1}{32}(3t_1+t_2)(\rho_n\nabla^2\rho_n+\rho_p\nabla^2\rho_p)+\tfrac{1}{4}t_3\rho_n\rho_p\rho-\tfrac{1}{2}W_0(\rho\nabla\cdot\mathbf{J}+\rho_n\nabla\cdot\mathbf{J}_n+\rho_p\nabla\cdot\mathbf{J}_p)\ . \quad (1)$$

In (1), $\rho=\rho_n+\rho_p$ is the nucleon density (the subscripts n and p refer to neutron and proton, respectively), $\tau=\tau_n+\tau_p$ is the kinetic energy density, and $\mathbf{J}=\mathbf{J}_n+\mathbf{J}_p$ is the spin density. t_0, x_0, t_1, t_2, t_3, and W_0 are Skyrme interaction parameters. The above expression for energy density was obtained from a variational calculation using a wave function in the form of a Slater determinant.

The nucleon, kinetic energy, and spin density can be expressed in terms of self-consistent Hartree-Fock orbitals ϕ_i. Thus $\mathbf{J}$ in terms of ϕ_i is given as

$$\mathbf{J}_q(\mathbf{r})=(-i)\sum_{i,\sigma,\sigma'}\phi_i^*(\mathbf{r},\sigma,q)[\nabla\phi_i(\mathbf{r},\sigma',q)\times\langle\sigma\,|\,\boldsymbol{\sigma}\,|\,\sigma'\rangle]\ . \quad (2)$$

The summation over i runs over all occupied single particle orbitals. The subscript q refers to either neutrons ($q=$n) or protons ($q=$p).

The ion-ion potential in this formalism is calculated as the difference of total energies of the overlapping and isolated systems 1 and 2:

$$V(\mathbf{R})=\int H(\mathbf{r},\rho,\tau,\mathbf{J})d\mathbf{r}-\left[\int H_1(\mathbf{r}_1,\rho_1,\tau_1,\mathbf{J}_1)d\mathbf{r}_1+\int H_2(\mathbf{r}_2,\rho_2,\tau_2,\mathbf{J}_2)d\mathbf{r}_2\right]\ . \quad (3)$$

Equation (3) has been used by various authors to calculate the real part of the heavy ion potential. In such calculations many of the systems chosen for study were spin saturated with $\mathbf{J}_n=\mathbf{J}_p=0$. For systems in which these conditions were not satisfied the contribution of the term was neglected.

In principle, $\mathbf{J}_q(\mathbf{r})$ can be calculated for any even-even system using expression (2). Self-consistent calculations, however, involve large, time consuming computations[7] and become prohibitive for heavier systems. This is avoided in the present calculation by the use of shell model orbitals for ϕ_i. For closed j shells, expression (2) for $\mathbf{J}_q(\mathbf{r})$ simplifies considerably to

$$\mathbf{J}_q(\mathbf{r})=\frac{\mathbf{r}}{4\pi r^4}\sum_\alpha (2j_\alpha+1)[j_\alpha(j_\alpha+1)-l_\alpha(l_\alpha+1)-\tfrac{3}{4}]R^2_{\alpha,q}(r)\ , \tag{4}$$

where $R_{\alpha,q}(r)/r$ is the radial part of the single particle wave function $\phi_i(\mathbf{r},\sigma,q)$.

From Eqs. (1) and (3) the contribution of the spin density term in the energy density functional of VB to the heavy ion potential is found to be

$$V_S(\mathbf{R})=-\tfrac{3}{4}W_0\int[\rho_1\nabla\cdot(\mathbf{J}_{n_2}+\mathbf{J}_{p_2}) +\rho_2\nabla\cdot(\mathbf{J}_{n_1}+\mathbf{J}_{p_1})]d\mathbf{r}\ . \tag{5}$$

The subscripts 1 and 2 refer to the corresponding quantities for colliding nuclei 1 and 2, and R is the distance between their centers. In arriving at (5) it has been assumed that in a nucleus, $\rho_n\simeq\rho_p\simeq\frac{1}{2}\rho$. This last assumption is, however, not essential. The expression for $V_s(R)$ without this assumption will involve ρ_{n_1},ρ_{p_1} and ρ_{n_2},ρ_{p_2}. In evaluating the right-hand side of Eq. (5), the expression for $\mathbf{J}$ given in Eq. (4) has been used. In this equation, although the summation runs over the occupied levels, all pairs of orbitals corresponding to $j=l+\frac{1}{2}$ and $j=l-\frac{1}{2}$ contribute zero. The contribution to $\nabla\cdot\mathbf{J}$, therefore, comes from the outer unpaired orbitals.

III. RESULTS AND DISCUSSIONS

The contribution to the heavy ion potential from the spin density terms in the VB energy density functional has been calculated using Eqs. (4) and (5). The normalized radial part $R_{\alpha,q}(r)/r$ of the shell model orbitals is given by[11]

$$\frac{R_{nl}(r)}{r}=\left[\frac{2^{l-n+2}(2\nu)^{l+3/2}(2l+2n+1)!!}{\sqrt{\pi}[(2l+1)!!]^2 n!}\right]^{1/2} \times r^l e^{-\nu r^2}v_{nl}(2\nu r^2)\ , \tag{6}$$

where

$$v_{nl}(x)=\sum_{k=0}^{n}(-1)^k 2^k\begin{bmatrix}n\\k\end{bmatrix}\frac{(2l+1)!!}{(2l+2k+1)!!}x^k\ . \tag{7}$$

The scale factor

$$\nu=\frac{mw}{2\hbar}=\frac{0.4940}{A^{1/3}}\ \text{fm}^{-2} \tag{8}$$

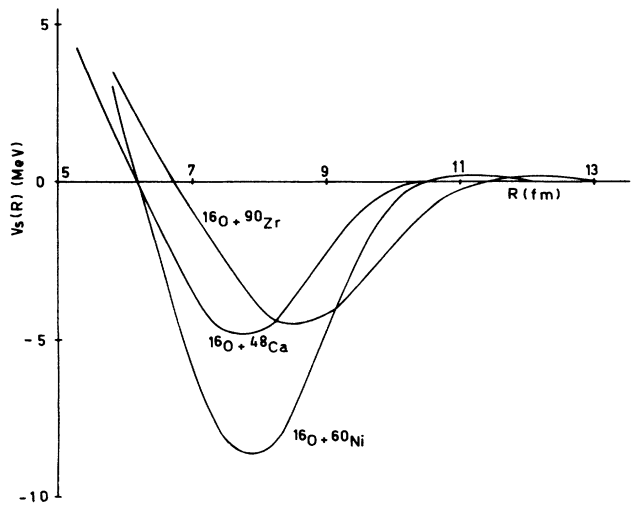

FIG. 1. The plot of $V_s(R)$ as a function of the separation distance R between the centers of the colliding nuclei. The nucleus ^{16}O is spin saturated with $\mathbf{J}_n=0$, $\mathbf{J}_p=0$.

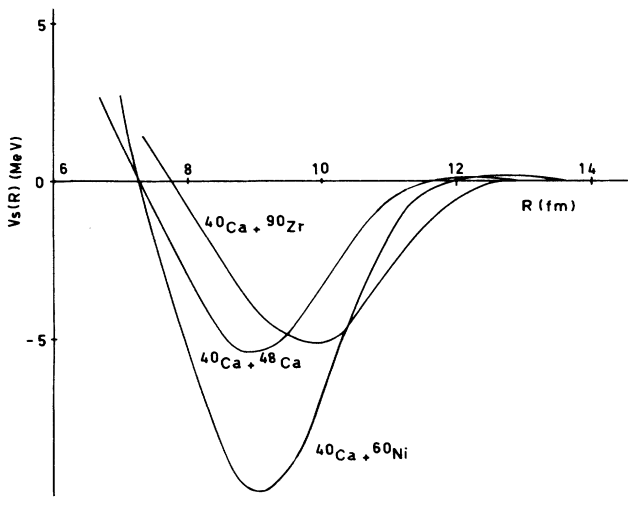

FIG. 2. The plot of $V_s(R)$ as a function of the separation distance R between the centers of the colliding nuclei. One of the nuclei (^{40}Ca) is spin saturated.

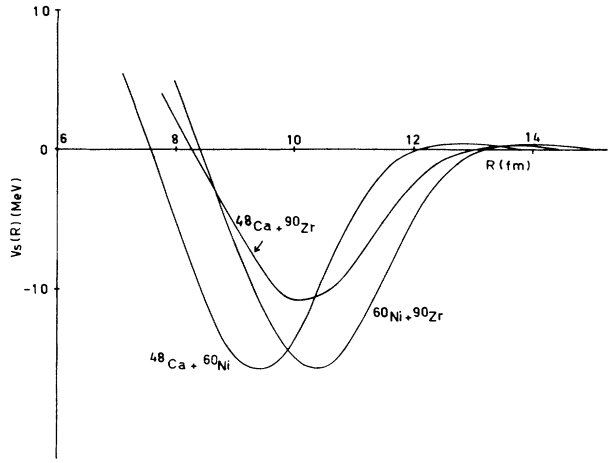

FIG. 3. The plot of $V_s(R)$ as a function of the distance of separation R between the colliding nuclei, where both nuclei are spin unsaturated.

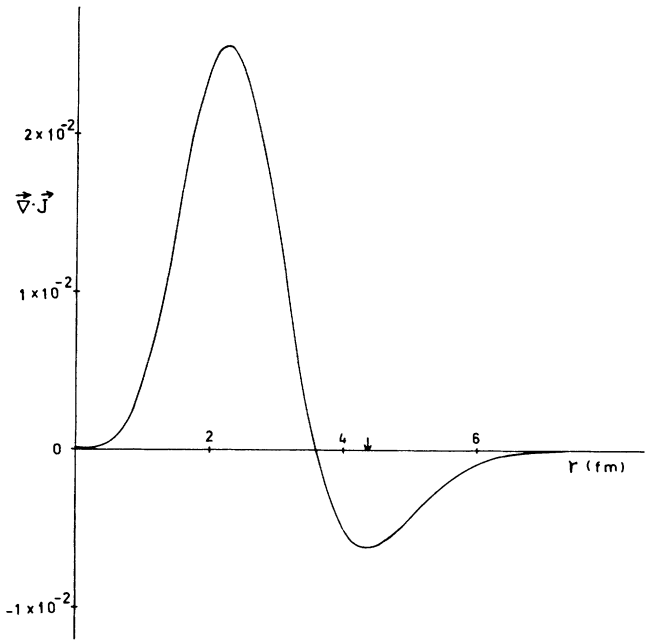

FIG. 4. The plot of $\nabla \cdot \mathbf{J}$ as a function of the radial distance r for ^{48}Ca. The arrow indicates the radius $R = r_0 A^{1/3}$ with $r_0 = 1.2$ fm.

is related to the oscillator parameter b by $\nu = 1/2b^2$. These oscillator wave functions could be used to calculate the density distributions of the colliding systems. Instead, parametrized Fermi-type distributions given by Stancu and Brink[6] have been used. The agreement between such parametrized densities and those calculated using wave functions has been shown to be very good in Ref. 6. The agreement is particularly impressive in the tail region, which makes the most significant contribution to the potential. One thus saves a lot of computational effort and time without sacrificing accuracy significantly, by using the parametrized density distributions. In obtaining the densities ρ and spin densities $\mathbf{J}$ of the overlapping systems, the sudden approximation has been used:

$$\rho = \rho_1 + \rho_2 \ , \qquad \mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2 \ . \tag{9}$$

This approximation is reliable only at high bombarding energies.

The plots of $V_s(R)$ as a function of the distance R between the centers of the colliding nuclei are given in Figs. 1–3. In all the target projectile combinations in Figs. 1 and 2, one of the nuclei is spin saturated ($\mathbf{J}=0$), while in the combinations of Fig. 3 both nuclei are spin unsaturated. One observes that the contribution of spin density to the potential is appreciable. In comparison, it should be noted that the depths of potentials obtained by Stancu and Brink[6] without the spin-density terms for the target projectile combinations ^{16}O+^{48}Ca and ^{40}Ca+^{56}Ni are -32 and -40 MeV, respectively. For combinations where both the colliding nuclei are spin unsaturated, $V_s(R)$ is much deeper compared to that for similar combinations where one nucleus is spin saturated. This is evident from a comparison of the curves corresponding to ^{48}Ca+^{60}Ni and ^{40}Ca+^{60}Ni, and also those for ^{40}Ca+^{90}Zr and ^{48}Ca+^{90}Zr. The tail parts of $V_s(R)$ indicate a slight repulsion. This arises because of a change of sign of $\nabla \cdot \mathbf{J}$ near the nuclear surface (Fig. 4). In the total potential this repulsion will be more than compensated for by the attractive contributions of the other terms.

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