Spin density contribution in heavy-ion interaction potentials using energy density formalism

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The result of adding the spin density term in heavy-ion interaction potentials is studied for the first time, especially for unclosed shell nuclei. For the energy density functional of Skyrme interaction, the spin density contribution is derived for nuclei with an even number of valence particles (or holes). The calculations are made for light nuclei, using both the shell-model and Fermi-type nucleon densities. The interaction potential is calculated in the proximity theorem, using corrected Thomas-Fermi approximation for the kinetic energy density. Only the repulsive spin density contribution is found to be significant, which cancels a part of attraction in the total interaction potential.

I. INTRODUCTION

Until recently, the contribution of the spin density term in heavy-ion potentials was neglected by either studying only the spin-saturated nuclei (i.e., nuclei with the major shell closed for both protons and neutrons) or taking its contribution to be small. Kaur and Chattopadhyay[1] have calculated the spin density part of the interaction potential in the energy density functional of Vautherin and Brink, derived for closed j-shell nuclei only.[2] However, the authors of Ref. 1 used the shell-model (harmonic-oscillator) orbitals, on one hand, and the parametrized Fermi-type density distribution, on the other hand. Thus, not only a proper evaluation of the spin density term is essential but also it is required to extend the formalism of Ref. 2 to nuclei having valence particles outside the closed shells.[3,4] During the particle transfer, for example, the spin-saturated (with both $j=l\pm\frac{1}{2}$ shells filled) or closed j-shell (either $j=l+\frac{1}{2}$ or $l-\frac{1}{2}$ shell filled) nuclei would become nuclei with valence particle configurations.

The aim of the present paper is, at least, threefold: (i) The spin density formalism is extended to nuclei with two and more (even) particles (or holes) outside the closed even-even core. (ii) The spin density part of the interaction potential is calculated more consistently by using the same shell-model wave functions also for determining the nucleon density distributions. A comparison of this calculation with that for the widely used two-parameter Fermi density distribution is then carried out. (iii) The contribution of the spin density term in the total interaction potential is studied for a number of $N\approx Z$, spherical or nearly spherical even-even nuclei. We have used here the energy density functional of Vautherin and Brink[2] for the Skyrme forces and, following Chattopadhyay and Gupta,[5] made our calculations of the interaction potential in the spirit of the proximity theorem. The calculations are carried out in the energy density formalism, using sudden approximation.

This paper is organized as follows. Section II gives a brief description of the formalism used to calculate the heavy-ion interaction potential. Neglecting the Coulomb potential effects, the spin density part of the potential and the nuclear proximity potential are discussed. The calculations are described in Sec. III and a summary of the results is presented in Sec. IV. The Appendix gives the derivation of spin density for closed j-shell nuclei[2] and its extension for nuclei with pairs of valence particles (or holes) outside the closed core.

II. THE FORMALISM

The energy density formalism has been used quite extensively for calculating the heavy-ion interaction potentials.[6-9] In this model, the interaction potential $V(R)$ is defined as the difference between the energy expectation value E of the colliding system at a finite separation distance R and at infinity,

$$V(R)=E(R)-E(\infty)\ . \tag{1}$$

The two nuclei are overlapping at R and completely separated at infinity. The energy expectation value E for the energy density functional $H(\mathbf{r})$ of Vautherin and Brink (VB),[2] obtained for the density-dependent Skyrme interaction and the single-particle orbitals, ϕ_i, defining a Slater determinant, is given by

$$E=\int H(\mathbf{r})d\mathbf{r}\ . \tag{2}$$

The $H(\mathbf{r})$ for an even-even spherical nucleus has the form (the subscripts n and p refer to neutron and proton, respectively)

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

The Coulomb interaction is not included here. In Eq. (3) m is the nucleon mass and t_0, x_0, t_1, t_2, t_3 and W_0 are Skyrme interaction parameters, obtained by different authors[2,10,11] in a self-consistent manner by fitting the binding energies, charge radii, and other single-particle properties of the spherical nuclei. The other terms are $\rho=\rho_n+\rho_p$, the nucleon density, $\tau=\tau_n+\tau_p$, the kinetic energy density, and $\mathbf{J}=\mathbf{J}_n+\mathbf{J}_p$, the spin density.

Different terms in (3) contribute to different effects in the interaction potential: whereas the last term is the spin density contribution, the other terms, involving ρ and τ and their powers, products, and derivatives, are shown[5] to constitute the nuclear proximity potential for the sudden approximation of $\rho=\rho_1+\rho_2$ and (corrected) Thomas-Fermi (TF) kinetic energy density. Thus, using (2) and (3) in (1), we can write

$$V(R)=\int\{H(\rho,\tau,\mathbf{J}) -[H_1(\rho_1,\tau_1,\mathbf{J}_1)+H_2(\rho_2,\tau_2,\mathbf{J}_2)]\}d\mathbf{r} =V_P(R)+V_J(R)\ , \tag{4}$$

with the nuclear proximity potential

$$V_P(R)=\int\{H(\rho,\tau)-[H_1(\rho_1,\tau_1)+H_2(\rho_2,\tau_2)]\}d\mathbf{r} \tag{5}$$

and the spin density part of the interaction potential

$$V_J(R)=\int\{H(\mathbf{J})-[H_1(\mathbf{J}_1)+H_2(\mathbf{J}_2)]\}d\mathbf{r}\ . \tag{6}$$

Here, $\mathbf{J}=\mathbf{J}_1+\mathbf{J}_2$, the spin density of the composite system.

For estimating $V_P(R)$, we notice from Blocki *et al.*[12] that according to the proximity theorem, the interaction potential between two spherical nuclei of radii C_1 and C_2, whose centers are separated by $R=R_{01}+R_{02}+s$ (see Fig. 1), is given by

$$V_P(R)=2\pi\bar{R}\int_s^\infty e(s)ds\ , \tag{7}$$

where

$$\bar{R}=C_1C_2/(C_1+C_2)$$

with $C_i=R_i-1/R_i$, the central radii, and

$$R_i=1.28A_i^{1/3}-0.76+0.8A_i^{-1/3}\ .$$

In Eq. (7) s_0 is the minimum value of separation distance s. Apparently, $s_0=0$ for the crevice formation (touching configuration), and is positive or negative for separated or overlapping nuclei, respectively. $e(s)$ is the interaction energy per unit area between two flat parallel surfaces separated by a disance s. Since $\int e(s)ds$ in (7) does not depend on the geometry of the two colliding nuclei, it is a universal function, $\Phi(s)$, characteristic of the matter. To calculate such a universal function, Chattopadhyay and Gupta[5] defined

$$\Phi(s)=\int e(s)ds =\int\{H(\rho,\tau)-[H_1(\rho_1,\tau_1)+H_2(\rho_2,\tau_2)]\}dz \tag{8}$$

for two slabs of semi-infinite nuclear matter with surfaces parallel to the X-Y plane, moving in the Z direction.

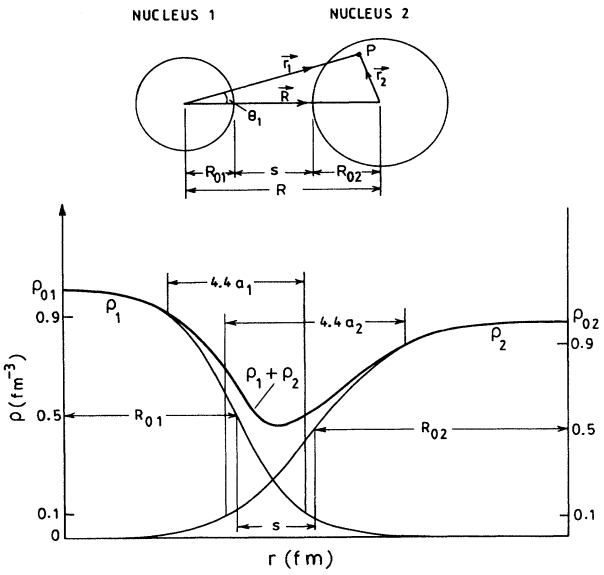

FIG. 1. Schematic two parameter Fermi density distributions and the relevant geometry of the two colliding nuclei.

These authors obtained an analytical expression for Φ, using TF densities in sudden approximation for both the nucleon and kinetic energy distributions. Here, in the following, we have solved the same problem for the two-parameter Fermi density distribution

$$\rho_i(r_i)=\rho_{0i}\left[1+\exp\left[\frac{r_i-R_{0i}}{a_i}\right]\right]^{-1},\quad i=1,2\ , \tag{9}$$

with

$$r_2=[r_1^2+R^2-2r_1R\cos\theta_1]^{1/2},\quad 0\le r\le\infty\ . \tag{10}$$

R_{0i} and a_i are the half-density radii and surface thickness parameters, respectively, taken (or intrapolated) from Refs. 13 and 14 (see Fig. 2). Such a density distribution is more realistic for heavy-ion collisions since, in contrast to TF distribution, it does not drop sharply to zero. For motion in a plane ($\theta_1=0$), in the Z direction,

$$z_2=R-z_1 \tag{11}$$

and the densities of the two nuclei become

$$\rho_1(z_1)=\rho_{01}\left[1+\exp\left[\frac{z_1-R_{01}}{a_1}\right]\right]^{-1},\quad -\infty\le z\le\infty\ , \tag{12a}$$

and

$$\rho_2(z_2)=\rho_{02}\left[1+\exp\left[\frac{z_2-R_{02}}{a_2}\right]\right]^{-1},\quad -\infty\le z\le\infty\ . \tag{12b}$$

Using (11) and $R=R_{01}+R_{02}+s$, we can write ρ_2 also in

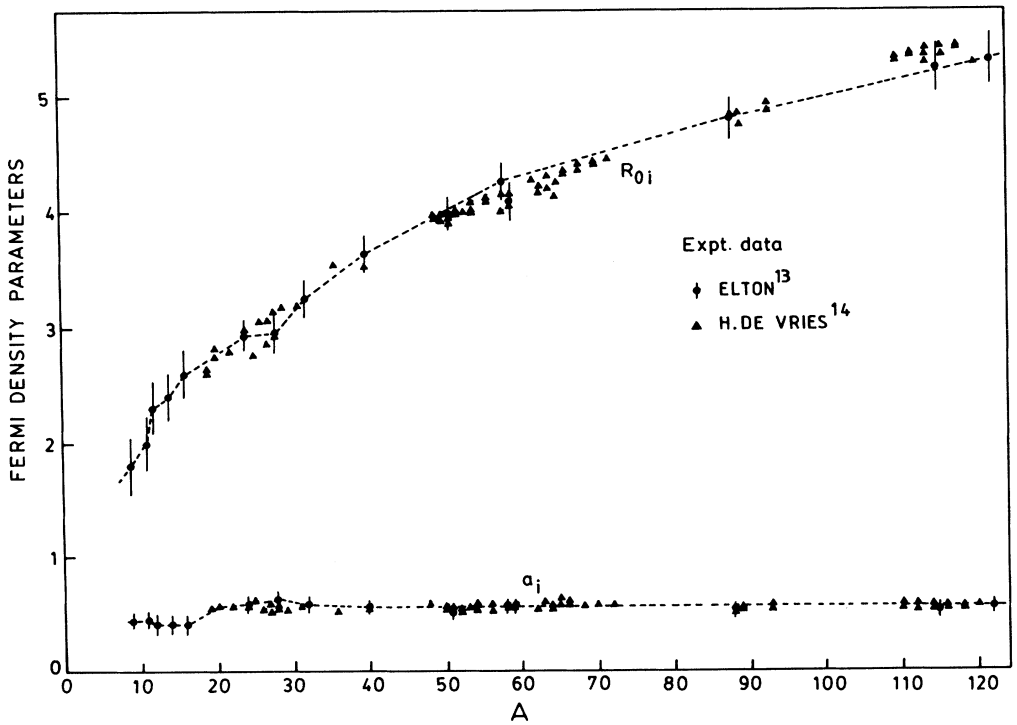

FIG. 2. The parameters R_{0i} (half-density radii) and a_i (surface thicknesses) of Fermi densities, as a function of mass number A of the nuclei. The circles and triangles represent, respectively, the data from Refs. 13 and 14, and the lines give the intrapolation used in the present work.

terms of the coordinate z_1,

$$\rho_2(z_1)=\rho_{02}\left[1+\exp\left[\frac{R_{01}+s-z_1}{a_2}\right]\right]^{-1} . \tag{12b'}$$

For the kinetic energy density, we use the TF approximation, corrected for additional surface effects due to von Weizsäcker,[15]

$$\tau=\tfrac{3}{5}(\tfrac{3}{2}\pi^2)^{2/3}\rho^{5/3}+\lambda(\nabla\rho)^2/\rho . \tag{13}$$

Here λ is a constant having the values[16] lying between $\frac{1}{36}$ and $\frac{9}{36}$. We choose $\lambda=\frac{1}{36}$ and the Skyrme force SII in view of the work of Chattopadhyay and Gupta.[5]

Combining (13) with (3), but without the spin density term, we get from (8) the following expression for universal function:[5]

$$\begin{aligned}\Phi(s)&=V_P(R)/2\pi\bar{R}\\&=\frac{3}{5}\frac{\hbar^2}{2m}(\tfrac{3}{2}\pi^2)^{2/3}I_{[5/3]}+\tfrac{3}{8}t_0I_{[2]}+\tfrac{1}{16}t_3I_{[3]}\\&\quad+\tfrac{1}{16}(3t_1+5t_2)\tfrac{3}{5}(\tfrac{3}{2}\pi^2)^{2/3}I_{[8/3]}+\Phi_{s\rho}+\Phi_{s\tau_\lambda} ,\end{aligned} \tag{14}$$

where the integrals, representing the volume effect in (3), are

$$I_{[n]}=\int[\rho^n-(\rho_1^n+\rho_2^n)]dz_1 \tag{15}$$

and $\Phi_{s\rho}$ and $\Phi_{s\tau_\lambda}$, giving the surface effects due to the ρ- and λ-dependent terms in τ, respectively, are

$$\begin{aligned}\Phi_{s\rho}&=\tfrac{1}{64}(9t_1-5t_2)\left\{\int\left[\left|\frac{\partial\rho}{\partial z_1}\right|^2-\left[\left|\frac{\partial\rho_1}{\partial z_1}\right|^2+\left|\frac{\partial\rho_2}{\partial z_1}\right|^2\right]\right]dz_1\right\}\\&=\tfrac{1}{64}(9t_1-5t_2)\Phi_0 ,\end{aligned} \tag{16}$$

$$\Phi_{s\tau_\lambda}=\tfrac{1}{16}(3t_1+5t_2)\lambda\Phi_0+\frac{\hbar^2}{2m}\lambda\left\{\int\left[\frac{1}{\rho}\left|\frac{\partial\rho}{\partial z_1}\right|^2-\left[\frac{1}{\rho_1}\left|\frac{\partial\rho_1}{\partial z_1}\right|^2+\frac{1}{\rho_2}\left|\frac{\partial\rho_2}{\partial z_1}\right|^2\right]\right]dz_1\right\} \tag{17}$$

Here $\rho=\rho_1+\rho_2$ and we have used $\rho_n=\rho_p$ for both the colliding nuclei. Equation (14), solved numerically for the Fermi densities (12), gives the nuclear proximity potential $V_P(R)$.

The estimation of the spin density part $V_J(R)$ of the interaction potential is straightforward. Using the approximation $\rho_n=\rho_p(=\frac{1}{2}\rho)$, we get from (3) and (6)

$$V_J(R)=-\tfrac{3}{4}W_0\int(\rho_1\nabla\cdot\mathbf{J}_2+\rho_2\nabla\cdot\mathbf{J}_1)d\mathbf{r} , \tag{18}$$

where $\mathbf{J}_1=\mathbf{J}_{n_1}+\mathbf{J}_{p_1}$ and $\mathbf{J}_2=\mathbf{J}_{n_2}+\mathbf{J}_{p_2}$ are the spin densities for the two colliding nuclei. In terms of the single-

particle orbitals ϕ_i that define a Slater determinant, the spin density for n or p in the energy density functional of VB (Ref. 2) is given as

$$\mathbf{J}_q(\mathbf{r})=(-i)\sum_{i,s,s'}\phi_i^*(\mathbf{r},s,q)[\nabla\phi_i(\mathbf{r},s',q)\times\langle s|\sigma|s'\rangle] \tag{19}$$

Here, the summation i runs over all the occupied single-particle orbitals and s and q ($=n$ or p) represent the spin and isospin indices, respectively. Since any self-consistent calculation is very time consuming, Eq. (19) is solved[2] by using the ansatz

$$\phi_i(\mathbf{r},s,q)=\frac{R_\alpha(r)}{r}y_{ljm}(\hat{r},s)\chi_q(t) \tag{20}$$

where

$$y_{ljm}(\hat{r},s)=\sum_{m_l m_s}\langle l\tfrac{1}{2}m_l m_s|jm\rangle Y_l^{m_l}(\hat{r})\chi_{m_s}(s) \tag{21}$$

and $\chi_q(t)$ is the isospin part of the wave function. The index $\alpha(\equiv q,n,l)$ specifies the radial part of the wave function, $R_\alpha(r)$.

Dropping the quantum number q, i.e., considering the spin density to arise from either the occupied neutron or proton orbitals, for a completely filled j shell, Eq. (19) simplifies to

$$\mathbf{J}(\mathbf{r})=\frac{\mathbf{r}}{4\pi r^4}\sum_\alpha(2j_\alpha+1)[j_\alpha(j_\alpha+1)-l_\alpha(l_\alpha+1)-\tfrac{3}{4}]R_\alpha^2(r). \tag{22}$$

Notice that in this equation, though the summation is over all the (fully) occupied levels, the contribution for pairs of orbitals with $j=l+\frac{1}{2}$ and $l-\frac{1}{2}$ is zero. In other words, $\mathbf{J}_n=\mathbf{J}_p=0$ for nuclei with major shells completely filled, called the spin-saturated nuclei.

For even-even nuclei with valence particles (or holes) outside the closed shells, we divide the contribution to $\mathbf{J}(\mathbf{r})$ in two parts: one due to the core consisting of closed shells and another due to the valence n_v particles (or holes),

$$\mathbf{J}(\mathbf{r})=\mathbf{J}_c(\mathbf{r})\pm\mathbf{J}_{n_v}(\mathbf{r}) . \tag{23}$$

The + sign is for particles and − sign for holes (see the Appendix). The first term, $\mathbf{J}_c(\mathbf{r})$ in (23) is apparently the same as Eq. (22). Since the ground state of all the even-even nuclei is observed to have zero angular momentum, considering that the valence nucleons couple to zero angular momentum, we get for

$$\mathbf{J}_{n_v}(\mathbf{r})=\frac{n_v\mathbf{r}}{4\pi r^4}[j(j+1)-l(l+1)-\tfrac{3}{4}]R_l^2(r) . \tag{24}$$

Here all the quantities on the right-hand side of (24) refer to the last occupied (unfilled) shell only. The details of derivation of Eqs. (22)–(24) are given in the Appendix.

The normalized radial wave functions $R_{nl}(r)$ in Eqs. (20), (22), and (24) are taken from the shell model,[17]

$$R_{nl}(r)=\left[\frac{2^{l-n+2}(2\nu)^{l+3/2}(2l+2n+1)!!}{\sqrt{\pi}[(2l+1)!!]^2 n!}\right]^{1/2} r^{l+1}\times e^{-\nu r^2}v_{nl}(2\nu r^2) \tag{25}$$

where

$$v_{nl}(x)=\sum_{k=0}^{n}(-1)^k 2^k\binom{n}{k}\frac{(2l+1)!!}{(2l+2k+1)!!}x^k \tag{26}$$

and the scale factor ν, related to oscillator parameter b, is

$$\nu=\frac{1}{2b^2}=\frac{m\omega}{2\hbar}\ (\text{in fm}^{-2})$$

with

$$\hbar\omega=41A^{-1/3} . \tag{27}$$

For a consistent evaluation of the spin density part of the interaction potential, Eq. (18), we use the oscillator wave functions (25) also to calculate the nucleon density distributions $\rho(\mathbf{r})$. This is defined as

$$\rho(\mathbf{r})=\sum_{i,s}|\phi_i(\mathbf{r},s,q)|^2 , \tag{28a}$$

where the summation index i ($=nl$) runs over all occupied single-particle states. This means that Eq. (28a) defines the nucleon density distribution for closed major shell (both $j=l\pm\frac{1}{2}$ filled) nuclei. In order to use this relation for closed j-shell nuclei or for a nucleus with n_v valence particles (or holes), we make the following ansatz, respectively, as

$$\rho(\mathbf{r})=\begin{cases}\rho_{cc}(\mathbf{r})+\dfrac{(2j+1)}{2(2l+1)}\left|\phi_{nlj}(\mathbf{r},s,q)\right|^2 \\ \quad\text{(for closed } j \text{ shell)} \qquad (28b)\\ \rho_c(\mathbf{r})\pm\dfrac{n_v}{2(2l+1)}\left|\phi_{nlj}(\mathbf{r},s,q)\right|^2 \\ \quad\text{(for } n_v \text{ valence nucleons)} \qquad (28c)\end{cases}$$

Here $\rho_{cc}(\mathbf{r})$ in (28b) is the nucleon density distribution due to the closed major shell core, given by Eq. (28a), and $\rho_c(\mathbf{r})$ in (28c) is the nucleon density distribution, respectively, due to the closed major shell core or closed j-shell core, depending on whether the valence nucleons are outside the closed major shell core or closed j-shell core, and are given by (28a) or (28b), respectively. In (28c), the + sign is for valence particles and the − sign for valence holes. The single-particle orbitals ϕ_{nlj} in (28b) and (28c) refer to the last filled or unfilled j shell, respectively.

Using in (18), Eqs. (22) and (28b) or (23) and (28c), we can calculate the spin density contribution $V_J(R)$ of the interaction potential. Here, some integrals are solvable analytically, whereas others involving radial wave functions have to be solved numerically. Alternatively, instead of (28), we can use the Fermi distribution (9) for the nucleon densities. We shall see in the following that in

the tail region not only shell-model densities match very well with the Fermi densities but also the calculated $V_J(R)$ are very much identical for the two density distributions. This is important, since in heavy-ion collisions only the tail part of densities overlap.

III. CALCULATIONS AND DISCUSSION OF RESULTS

In this section we present our calculations first for the spin density part of the interaction potential, using both the shell-model and Fermi density distributions. We find that the two density distributions give very much identical results. Then, using only the Fermi density distribution, the total interaction potential is calculated. The spin density is found to contribute to the reduction of attraction of the interaction potential, which could be significant for many fusion reactions.

Figure 3 shows a plot of the nucleon density distributions for a few representative nuclei from 0*p* and 0*s*-1*d* shells. The solid and dashed lines represent, respectively, the Fermi distribution (9) and the shell-model distribution (28). Interesting enough, the two distributions are nearly the same, at least in the surface region. This is true even for the deformed *s*-*d* shell nuclei, like ^{24}Mg and ^{28}Si. In heavy-ion collisions only the surface regions of densities are important. This is demonstrated in Fig. 4 where the spin density part of the interaction potential $V_J(R)$ is plotted. For the relevant region of R (beyond the repulsive maximum, as discussed below) the two calculations do not differ much, particularly if one of the reaction partners (like ^{16}O, ^{40}Ca) is a spin-saturated nucleus ($J=0$). In these later cases, we notice from Eq. (18) that only one term contributes and the nucleon density of the spin-unsaturated partner does not contribute to $V_J(R)$. Also, Fig. 3 shows that the differences in the two model density distributions are somewhat larger in the surface regions for the spin-unsaturated nuclei. Therefore, in the following, we have used only the Fermi density distribution for the calculation of $V_J(R)$ and the total interaction $V(R)$.

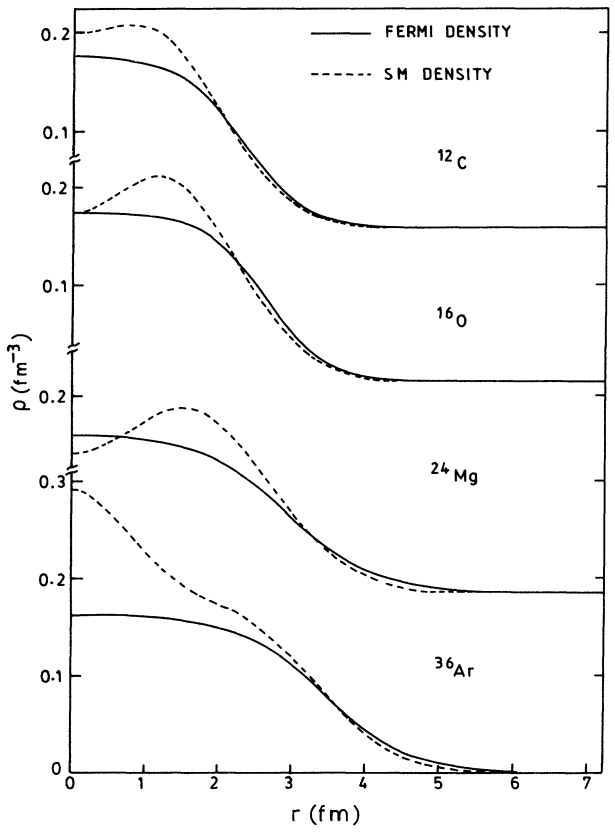

FIG. 3. The shell-model (dashed lines) and Fermi (solid lines) nucleon density distributions for ^{12}C, ^{16}O, ^{24}Mg, and ^{36}Ar nuclei.

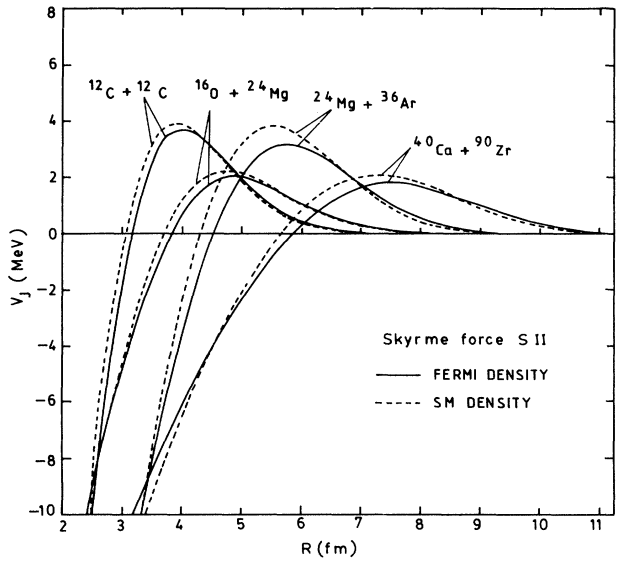

FIG. 4. The spin density part of the interaction potential $V_J(R)$ for various reactions, using the shell-model (dashed lines) and Fermi (solid lines) density distributions. The Skyrme force SII is used.

Figure 5 shows the spin density part of the interaction $V_J(R)$ for an assortment of target-projectile combinations, having one nucleus spin-saturated (^{40}Ca+^{60}Ni) or both spin unsaturated with the j shell completely filled (^{48}Ca+^{60}Ni, ^{60}Ni+^{90}Zr) or with valence particles or holes outside the closed core (^{14}C+^{46}Ti, ^{20}Ne+^{52}Fe). Only light target projectiles are considered where the approximation of equal proton and neutron densities is justified. We have also included here in Fig. 5 some of the cases of Ref. 1, since a numerical error was detected in the calculations reported in that work. We notice in Fig. 5 that the spin density contribution in the interaction potential can be very large, of the order of 5–7 MeV repulsive. This is studied in the following.

Figure 6 gives the total interaction potential $V(R)$ and its contributing terms $V_J(R)$ and $V_P(R)$, for an illustrative example of ^{56}Ni+^{56}Ni, for the case of $\lambda=0$. We notice that the signs of the two contributing terms are different. Also, the important region of the R value in $V_J(R)$ is on the right-hand side of the repulsive maximum $V_J^{\max}$, which adds to $V_P(R)$ and reduces the attraction of the resultant $V(R)$ considerably. The same result is presented in another example of ^{36}Ar+^{36}Ar in Fig. 7,

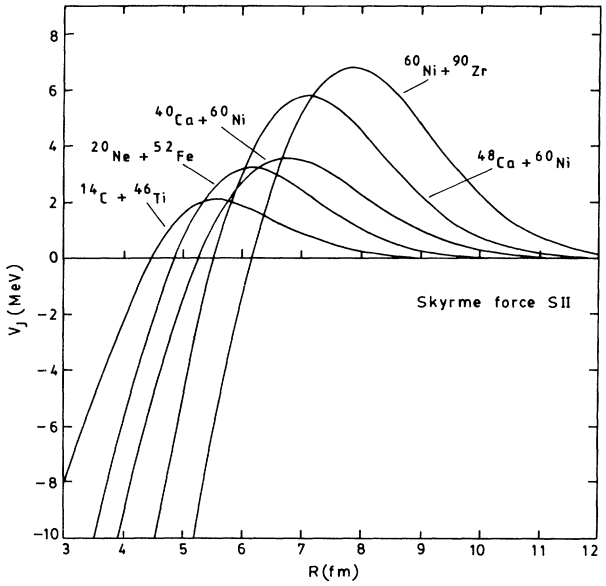

FIG. 5. The spin density part of the interaction potential $V_J(R)$ for reactions with one nucleus spin-saturated ($^{40}Ca+^{60}Ni$), both spin unsaturated but with the j shell completely filled ($^{48}Ca+^{60}Ni$, $^{60}Ni+^{90}Zr$) or with valence particles (or holes) outside the closed core ($^{14}C+^{46}Ti$, $^{20}Ne+^{52}Fe$), using Fermi density distribution and Skyrme force SII.

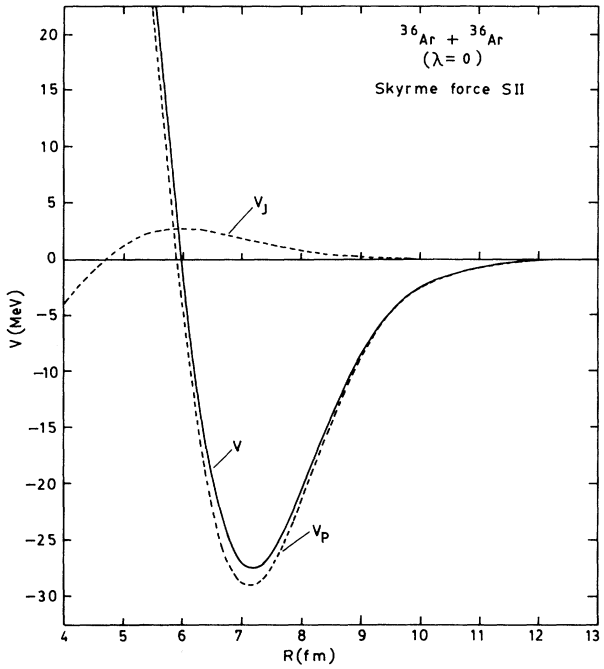

FIG. 7. Same as in Fig. 6 but for the $^{36}Ar+^{36}Ar$ system.

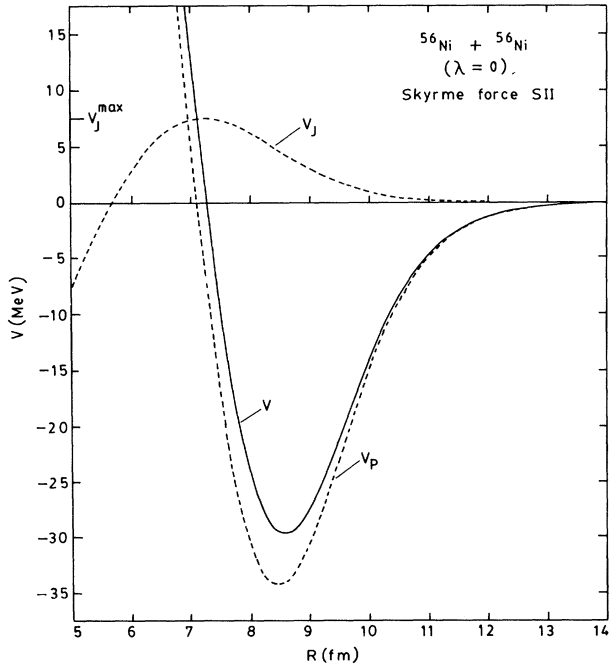

FIG. 6. The total interaction potential $V(R)$ for the surface term $\lambda=0$ and its contributing terms $V_P(R)$, the proximity potential, and $V_J(R)$, the spin density part for the $^{56}Ni+^{56}Ni$ system. The force parameters are of Skyrme SII and the nucleon density is of Fermi type.

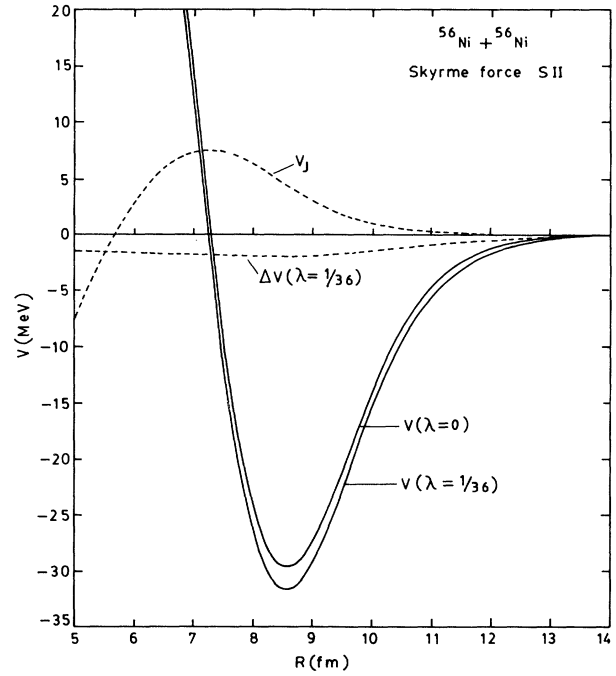

FIG. 8. Same as in Fig. 6 but for both $\lambda=0$ and $\frac{1}{36}$. The proximity potential $V_P(R)$ is not shown here but the contribution of the $\lambda=\frac{1}{36}$ term is shown explicitly.

but to a lesser extent.

Finally, Fig. 8 shows the result of adding the λ term to the total interaction potential of ^{56}Ni+^{56}Ni. We notice that the λ term compensates for a part of the repulsion due to $V_J(R)$. This is not surprising since both terms represent the surface effects (with opposite signs)—one of nucleon density and the other of spin density.

IV. SUMMARY

The purpose of this paper has been to estimate the contribution of spin density in heavy-ion interaction potentials. With this aim in mind, the spin density formalism of Vautherin and Brink[2] for the energy density functional of Skyrme interactions is first generalized to unclosed shell nuclei, i.e., to nuclei with $2n$ (even integers) valence particles or holes outside the closed even-even core. The spin density part of the interaction potential is then calculated consistently for the shell-model densities and compared with that for the Fermi density distributions. The similarity between the two calculations, especially when one of the colliding nuclei is spin saturated, justifies the use of Fermi density distribution for this purpose.

The total interaction potential is obtained by adding the spin density contribution to the potential calculated in the method of proximity theorem.[5] The relevant portion of the potential due to the spin density term is found to be repulsive, which reduces the attraction of the total potential by as much as 5–7 MeV for light spherical nuclei.

ACKNOWLEDGMENTS

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APPENDIX:

Spin density for nuclei with a closed j shell and pairs of particles (or holes) outside the closed even-even core

Spin density for nuclei with a closed j shell is calculated by Vautherin and Brink.[2] In the following, we first reproduce their steps for completeness and then extend this formalism to obtain spin density for nuclei with an even number of particles (or holes) outside the closed core. Spin density for nuclei with a closed j shell is then shown to be given as a special case of the spin density for nuclei with valence particles (or holes).

Using the ansatz (20) in the definition (19), the spin density due to proton or neutron occupied orbitals is given by

$$\mathbf{J}(\mathbf{r})=(-i)\sum_{\alpha}\frac{R_\alpha^2(r)}{r^2}\sum_{m_l m_l'}\sum_{m_s m_s'}\sum_{m}\langle l\tfrac{1}{2}m_l m_s|jm\rangle\langle l\tfrac{1}{2}m_l' m_s'|jm\rangle Y^*_{lm_l}(\Omega)(\nabla Y_{lm_l'}(\Omega)\times\langle m_s|\boldsymbol{\sigma}|m_s'\rangle)\ . \tag{A1}$$

In this relation, the product in parentheses gets simplified by noting[2] the following. (i) In an orthonormal basis $\{\mathbf{e}_\mu\}$, defined as

$$\mathbf{e}_0=\mathbf{e}_z,\quad \mathbf{e}_{\pm1}=\mp\frac{1}{\sqrt{2}}(\mathbf{e}_x\pm i\mathbf{e}_y)\ , \tag{A2}$$

the components of the outer product of the two vectors are

$$(\mathbf{A}\times\mathbf{B})_\mu=-i\sqrt{2}\sum_{\mu_1\mu_2}\langle 11\mu_1\mu_2|1\mu\rangle A_{\mu_1}B_{\mu_2} \tag{A3}$$

and (ii)

$$\nabla Y_{lm_l}(\Omega)f(r)=\frac{\mathbf{r}}{r}\frac{\partial f}{\partial r}Y_{lm_l}(\Omega)+f(r)\nabla Y_{lm_l}(\Omega)\ , \tag{A4}$$

where for the parentheses in (A1), the first term in (A4) vanishes since it involves radial derivative of the component of the Pauli spin matrix. (iii) By use of the Wigner-Eckart theorem,

$$\begin{aligned}\langle m_s|\boldsymbol{\sigma}|m_s'\rangle_{\mu_2}=\langle\tfrac{1}{2}m_s|\boldsymbol{\sigma}|\tfrac{1}{2}m_s'\rangle_{\mu_2}&=(-1)^{1/2-m_s}\begin{pmatrix}\frac{1}{2}&1&\frac{1}{2}\\-m_s&\mu_2&m_s'\end{pmatrix}\langle\tfrac{1}{2}\|\boldsymbol{\sigma}\|\tfrac{1}{2}\rangle\\&=\sqrt{6}(-1)^{1/2-m_s}\begin{pmatrix}\frac{1}{2}&1&\frac{1}{2}\\m_s'&\mu_2&-m_s\end{pmatrix}\ .\end{aligned} \tag{A5}$$

Then, the parentheses in (A1) become

$$\begin{aligned}[\nabla Y_{lm_l'}(\Omega)\times\langle m_s|\boldsymbol{\sigma}|m_s'\rangle]&=-i\sqrt{2}\sum_{\mu_1\mu_2}\langle 11\mu_1\mu_2|1\mu\rangle\nabla_{\mu_1}Y_{lm_l'}(\Omega)\langle m_s|\boldsymbol{\sigma}|m_s'\rangle_{\mu_2}\\&=-i2\sqrt{3}(-1)^{1/2-m_s}\sum_{\mu_1\mu_2}\langle 11\mu_1\mu_2|1\mu\rangle\begin{pmatrix}\frac{1}{2}&1&\frac{1}{2}\\m_s'&\mu_2&-m_s\end{pmatrix}\nabla_{\mu_1}Y_{lm_l'}(\Omega)\ .\end{aligned} \tag{A6}$$

Substituting (A6) in (A1) and changing all the Clebsch-Gordan coefficients into $3j$ symbols, we get

$$J_\mu(\mathbf{r})=-6\sum_\alpha \frac{R_\alpha^2(r)}{r^2}(2j_\alpha+1)$$
$$\times \sum_{m_l m_l'}\sum_{m_s m_s'}\sum_{m}\sum_{\mu_1\mu_2}(-1)^{1/2-m_s-\mu+2j-2m}\begin{pmatrix} l & \frac{1}{2} & j \\ m_l & m_s & -m\end{pmatrix}\begin{pmatrix} \frac{1}{2} & l & j \\ -m_s' & -m_l' & m\end{pmatrix}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 1 \\ m_s' & -m_s & \mu_2\end{pmatrix}\begin{pmatrix} 1 & 1 & 1 \\ \mu_1 & \mu_2 & -\mu\end{pmatrix}$$
$$\times Y^*_{lm_l}\nabla_{\mu_1}Y_{lm_l'}(\Omega)\ . \tag{A7}$$

Here we have used some simple symmetry relations of $3j$ symbols.

The gradient formula for the spherical harmonics, to be inserted into (A7), is given by

$$\nabla_{\mu_1}Y_{lm_l'}(\Omega)=\sum_{LM}\frac{f(l,L)}{r}(-1)^{1-l-M}(2L+1)^{1/2}\begin{pmatrix} l & 1 & L \\ m_l' & \mu_1 & -M\end{pmatrix}Y_{LM}(\Omega) \tag{A8}$$

with

$$f(l,L)=\begin{cases} -l\left[\dfrac{l+1}{2l+3}\right]^{1/2} & \text{if } L=l+1 \\ -(l+1)\left[\dfrac{l}{2l-1}\right]^{1/2} & \text{if } L=l-1 \\ 0, \quad \text{otherwise}\ . \end{cases} \tag{A9}$$

Inserting (A8) into (A7) and summing over indices m, m_s, m_s' and m_l', μ_1, μ_2, respectively, by using the standard $3j$ symbol formulas and then recoupling the product of the two spherical harmonics by carrying out the summation over m_l and M, we obtained

$$\mathbf{J}_\mu(\mathbf{r})=2\sqrt{3}\sum_\alpha\frac{R_\alpha^2(r)}{r^3}(2j_\alpha+1)\sum_L(-1)^{j+1/2}(2L+1)f(l,L)\left[\frac{2l+1}{4\pi}\right]^{1/2}$$
$$\times\begin{Bmatrix} l & l & 1 \\ \frac{1}{2} & \frac{1}{2} & j\end{Bmatrix}\begin{Bmatrix} L & l & 1 \\ 1 & 1 & l\end{Bmatrix}\begin{Bmatrix} l & L & 1 \\ 0 & 0 & 0\end{Bmatrix}Y_{1\mu}(\Omega)\ . \tag{A10}$$

Then, using the explicit expressions for $3j$ and $6j$ symbols, the following sum over L can be obtained:

$$\sum_L(2L+1)f(l,L)\begin{Bmatrix} L & l & 1 \\ 1 & 1 & l\end{Bmatrix}\begin{Bmatrix} l & L & 1 \\ 0 & 0 & 0\end{Bmatrix}$$
$$=\frac{1}{\sqrt{6}}(-1)^l[l(l+1)]^{1/2}\ . \tag{A11}$$

Also, for the basis $\{\mathbf{e}_\mu\}$

$$\frac{\mathbf{r}}{r}=\sqrt{4\pi/3}\,Y_{1\mu}$$

with

$$r_\mu=\begin{cases} -\dfrac{1}{\sqrt{2}}(x+iy) & \text{for } \mu=1 \\ Z \quad \text{for } \mu=0 \\ \dfrac{1}{\sqrt{2}}(x-iy) & \text{for } \mu=-1 \end{cases}\ . \tag{A12}$$

Substituting (A11), (A12), and the explicit expression for the remaining $6j$ symbol into (A10), we get the final result

$$\mathbf{J}(\mathbf{r})=\frac{\mathbf{r}}{4\pi r^4}\sum_\alpha(2j_\alpha+1)$$
$$\times[j_\alpha(j_\alpha+1)-l_\alpha(l_\alpha+1)-\tfrac{3}{4}]R_\alpha^2(r)\ . \tag{A13}$$

Notice that here the summation over α refers to over all the fully occupied orbitals. Then, two different cases arise for the last occupied orbital: it is either completely filled (closed j shell) or partially filled (valence nucleons outside the closed core). For a completely filled major shell (i.e., $j=l\pm\frac{1}{2}$ both), $\mathbf{J}(\mathbf{r})=0$. The coupling of angular momentum quantum numbers (j,m) of the individual nucleons in each case now has to be carried out. In the following, we begin with the case of a nucleus with a partially filled last orbital, since the other case of a completely filled orbital then follows simply as a corollary of the first one.

We limit ourselves to even-even nuclei, with n_v particles (or holes) in the last unfilled shell. Thus, for the valence nucleons to be the particles, the closed core consists of the already filled orbitals, whereas for the holes the last, originally unfilled, orbit is considered to be filled and belonging to the core. We can thus write

$$\mathbf{J}(\mathbf{r})=\mathbf{J}_c(\mathbf{r})\pm\mathbf{J}_{n_v}(\mathbf{r}) , \tag{A14}$$

where $\mathbf{J}_c(\mathbf{r})$ and $\mathbf{J}_{n_v}(\mathbf{r})$ are, respectively, the contributions of closed core and valence particles (or holes). The + sign is for particles and the − sign is for holes. In the following, we first obtain $\mathbf{J}_{n_v}(\mathbf{r})$, say, for $n_v=4$ particles and then generalize it to any even number of valence particles (or holes).

Since even-even nuclei have the experimental ground-state angular momentum $J^\pi=0^+$, the valence particles must couple to zero angular momentum. This means that each pair of particles must couple to zero angular momentum and their magnetic quantum numbers m must have the values, say, $(r_1,-r_1)$, $(r_2,-r_2)$,—etc., so that the total magnetic quantum number $M=0$ also. This means that for, say, four particles in the last unfilled shell ($n_v=4$), the magnetic quantum m has only four values $(r_1,-r_1,r_2,-r_2)$, instead of all the allowed $(2j+1)$ values. Introducing this restricted summation (denoted by primes) over m (and so also over m_l,m_s, etc. since $m=m_l+m_s=m_l'+m_s'$) in (A1) or directly in (A7), since there are no changes in steps from (A1) to (A7), we get for n_v particles

$$\begin{aligned}\mathbf{J}_{n_v}(\mathbf{r})=&-6\frac{R_\alpha^2(r)}{r^2}(2j+1)\\&\times\sum_{m_lm_l'}{}'\sum_{m_sm_s'}{}'\sum_{m}^{n_v\text{ values}}{}'\sum_{\mu_1\mu_2}(-1)^{2j-2m+1/2-m_s-\mu}\\&\times\begin{bmatrix} l & \frac{1}{2} & j\\ m_l & m_s & -m\end{bmatrix}\begin{bmatrix}\frac{1}{2} & l & j\\ -m_s' & -m_l' & m\end{bmatrix}\begin{bmatrix}\frac{1}{2} & \frac{1}{2} & 1\\ m_s' & -m_s & \mu_2\end{bmatrix}\\&\times\begin{bmatrix}1 & 1 & 1\\ \mu_1 & \mu_2 & -\mu\end{bmatrix}Y^*_{lm_l}\nabla_{\mu_i}Y_{lm_l'}(\Omega) .\end{aligned} \tag{A15}$$

Notice that here we have dropped the summation over α, since we are now estimating the spin density due to valence particles alone. Equation (A15) is true for any even number of valence particles in the last orbital, $(j,m)^{n_v}$. If this orbital was completely filled, then $n_v=2j+1$ and Eq. (A15) reduces back to (A7).

Now, to evaluate (A15) further, for a one-body operator $\hat{O}$ like the spin density, we notice the following result:[18]

$$\begin{aligned}\left\langle\phi_{jr_1}\phi_{jr_2}\phi_{jr_3}\cdots\phi_{jn_v}\left|\sum_{i=1}^{n_v}\hat{O}\right|\phi_{jr_1}\phi_{jr_2}\phi_{jr_3}\cdots\phi_{jn_v}\right\rangle\\=\langle\phi_{jr_1}|\hat{O}|\phi_{jr_1}\rangle+\langle\phi_{jr_2}|\hat{O}|\phi_{jr_2}\rangle+\langle\phi_{jr_3}|\hat{O}|\phi_{jr_3}\rangle+\cdots+\langle\phi_{jn_v}|\hat{O}|\phi_{jn_v}\rangle .\end{aligned} \tag{A16}$$

Using (A16) in (A15) and noting that the variable r in (A16) is equivalently the dummy summation index m in (A15), we get

$$\begin{aligned}\mathbf{J}_{n_v}(\mathbf{r})=&-6n_v\frac{R_\alpha^2(r)}{r^2}(2j+1)\\&\times\sum_{m_lm_l'}{}'\sum_{m_sm_s'}{}'\sum_{\mu_1\mu_2}(-1)^{2j-2m+1/2-m_s-\mu}\\&\times\begin{bmatrix} l & \frac{1}{2} & j\\ m_l & m_s & -m\end{bmatrix}\begin{bmatrix}\frac{1}{2} & l & j\\ -m_s' & -m_l' & m\end{bmatrix}\begin{bmatrix}\frac{1}{2} & \frac{1}{2} & 1\\ m_s' & -m_s & \mu_2\end{bmatrix}\begin{bmatrix}1 & 1 & 1\\ \mu_1 & \mu_2 & -\mu\end{bmatrix}\\&\times Y^*_{lm_l}\nabla_{\mu_1}Y_{lm_l'}(\Omega) .\end{aligned} \tag{A17}$$

Note that here $m=r$ (for a single nucleon) and there is no summation over m. In order to restore the summation over m to all the allowed $(2j+1)$ values, we multiply and divide through (A17) by the $(2j+1)$ factor [see Eqs. (13.59)–(13.61) in Ref. 17],

$$\mathbf{J}_{n_v}(\mathbf{r})=-\frac{6n_v}{(2j+1)}\frac{R_\alpha^2(r)}{r^2}(2j+1)$$
$$\times\sum_{m_l m_l' m_s m_s'}\sum_{m}\sum_{\mu_1\mu_2}(-1)^{2j-2m+1/2-m_s-\mu}\begin{pmatrix} l & \frac{1}{2} & j \\ m_l & m_s & -m\end{pmatrix}\begin{pmatrix} \frac{1}{2} & l & j \\ -m_s' & -m_l' & m\end{pmatrix}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 1 \\ m_s' & -m_s & \mu_2\end{pmatrix}$$
$$\times\begin{pmatrix} 1 & 1 & 1 \\ \mu_1 & \mu_2 & -\mu\end{pmatrix}Y_{lm_l}^{*}\nabla_{\mu_1}Y_{lm_l'}(\Omega)\ . \tag{A18}$$

The summations over m_l, m_s, and m_l', m_s' are also no longer restricted since m is now allowed all the $2j+1$ values. This relation differs from (A7) only by a multiplicative factor $n_v/(2j+1)$. Therefore, substituting in (A18) the solution (A13) of (A7) (without the summation over α), we get

$$\mathbf{J}_{n_v}(\mathbf{r})=\frac{n_v}{(2j+1)}\frac{\mathbf{r}}{4\pi r^4}(2j+1)$$
$$\times[j(j+1)-l(l+1)-\tfrac{3}{4}]R_l^2(r) \tag{A19}$$
$$=\frac{n_v\mathbf{r}}{4\pi r^4}[j(j+1)-l(l+1)-\tfrac{3}{4}]R_l^2(r)\ . \tag{A20}$$

For a completely filled shell, $n_v=2j+1$, which means for a closed core nucleus (including the closed j-shell nucleus), (A19) gives (A13) after the summation over all the filled shells (α values) is allowed,

$$\mathbf{J}_c(\mathbf{r})=\frac{\mathbf{r}}{4\pi r^4}\sum_\alpha(2j_\alpha+1)[j_\alpha(j_\alpha+1)-l_\alpha(l_\alpha+1)$$
$$-\tfrac{3}{4}]R_\alpha^2(r)\ . \tag{A21}$$

Vautherin and Brink[2] have also used the same argument of all the allowed $(2j+1)$ values of m, to call Eq. (A13) as the spin density for a closed j-shell nucleus.

Equation (A20) is derived for n_v particles in the last unfilled j shell. In shell-model theory,[18] a hole state (j,m) is the equivalent of a particle state $(j,-m)$. Therefore, Eq. (A20) is valid also for n_v holes in the last j shell, since here the magnetic quantum number m is already summed over. However, for the hole configuration the last j shell is considered filled and belonging to the closed core. This means that the contribution of the hole state is absent and is thus taken with a $-$ sign in Eq. (A14)

Finally, for two particles (or two holes), Eq. (A20) is also obtained by simply arguing[19] that the $J^\pi=0^+$ ground state is formed by the coupling of the two particles in $m=+r$ and $m=-r$ states, such that Eq. (A15) gets multiplied by the Clebsch-Gordan coefficient $\langle jjr-r|00\rangle$ with a summation over r. Then, the spin density being a one-body operator [Eq. (A16)], the expectation value of the spin density $\mathbf{J}_2(\mathbf{r})$ (for $n_v=2$) between the determinental wave functions will be the sum of contributions corresponding to $m=+r$ and $m=-r$ with a summation over r and the additional factor $|\langle jjr-r|00\rangle|^2=1/(2j+1)$. The restriction over the summation m in (A15) is thus removed[19] and the summation is carried out as in (A7) to (A13). Since the contributions of $m=+r$ and $m=-r$ are the same because of the summation over r, an overall factor of $2/(2j+1)$ is obtained, as in (A19) for $n_v=2$. The same argument can be extended[20] to any number of even particles (or holes). For each pair of particles (or holes), (A15) gets multiplied by an additional Clebsch-Gordan coefficient, giving rise to an additional factor of $n_v/(2j+1)$ for n_v particles (or holes), as in Eq. (A19)

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