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Hartree-Fock Calculations with Skyrme's Interaction. I. Spherical Nuclei*

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Hartree-Fock calculations for spherical nuclei using Skyrme's density-dependent effective nucleon-nucleon interaction are discussed systematically. Skyrme's interaction is described and the general formula for the mean energy of a spherical nucleus derived. Hartree-Fock equations are obtained by varying the mean energy with respect to the single-particle wave functions of occupied states. Relations between the parameters of the Skyrme force and various general properties of nuclear matter and finite nuclei are analyzed. Calculations have been made for closed-shell nuclei using two rather different sets of parameters, both of which give good binding energies and radii for ^{16}O and ^{208}Pb. Both interactions give good binding energies and charge radii for all closed-shell nuclei. Calculated electron scattering angular distributions agree qualitatively with experiment, and for one interaction there is good quantitative agreement. The single-particle energies calculated with the two interactions are somewhat different owing to a different nonlocality of the Hartree-Fock potentials, but both interactions give the correct order and density of single-particle levels near the Fermi level. They differ most strongly in their predictions for the energies of 1s single-particle states.

I. INTRODUCTION

It now seems clear that the average field in nuclei should emerge from an approximation more or less closely connected to the Hartree-Fock method. However, the exact nature of the relation between the observed single-particle properties of nuclei and the nucleon-nucleon force has not yet been resolved. Several attempts to clarify this relation have been made in the past few years by means of two rather different approaches. The first one is to use soft potentials and the framework of the usual Goldstone expansion. This point of view has been adopted in particular by Kerman and his group, who have solved, for Tabakin's potential, the Hartree-Fock problem with second- and third-order corrections.[1-3] With such calculations, however, difficulties are encountered in explaining nuclear radii and densities. Even though the rate of convergence of the expansion does not appear to be satisfactory[3] the discrepancy has to be attributed to the improper saturation properties of the Tabakin potential. The second approach is appropriate for interactions with a strong short-range repulsion and the framework of the Brueckner-Goldstone expansion is used. Even though it has been reputed to be difficult, a certain number of complete Brueckner-Hartree-Fock calculations of finite nuclei, including double self-consistency, are now available.[4,5] Among these the most recent one is the work of Davies and McCarthy, who have used Reid's soft-core potential and included also renormalized occupation probabilities. Here again, however, the fit to nuclear radii and binding energies turns out to be rather poor, and the origin of the discrepancy is not clear. It could be due either to the importance of higher-order diagrams or to the fact that Reid's soft-core potential is an inadequate description of the nucleon-nucleon force. An evaluation of higher-order terms in the expansion – in particular a calculation of the three-body cluster diagram – would be necessary in order to settle this question.

The present status of realistic calculations, and also their complexity, therefore explains the coexistence of calculations of another type, namely Hartree-Fock calculations with effective interactions, which leave out completely the problem of higher-order corrections and, rather, try to reproduce in lowest order as many nuclear properties as possible. Although less fundamental, this approach is extremely useful: It allows one to calculate in regions where realistic calculations become impracticable. It also allows one to make systematic studies with the least amount of numerical work.

Calculations with effective forces can be divided into two distinct groups. In the first group the effective interaction is first derived in lowest order from a realistic two-body force, and higher-order corrections to it are then parametrized. In contrast, for the second group one leaves out any idea of a relation with a realistic force and one rather parametrizes the effective interaction directly as a whole.

All calculations belonging to the first group[6-9] use the framework of Brueckner's theory in the local-density approximation; it is stated that in lowest order the interaction between two nucleons in a finite nucleus is given by the nuclear-matter G matrix calculated at the density of the center of mass of the nucleon pair. Since Brueckner theory of nuclear matter leads to a defect of the order of 4 MeV for the binding energy per particle, it is necessary to include higher-order terms which, it is hoped, will account for this difference. Rather than calculating these terms, a phenomenological correction is added in order to compensate for this missing binding energy. In Ref. 6 this correction is carried out by reducing by 10% the strength of the short-range "core term," whereas, in Ref. 7 it is taken to be proportional to the interaction itself. In Refs. 8 and 9 multiplicative factors are introduced to allow variations of the strength and relative intensities of the short- and long-range terms, and also of the like and unlike interactions in order to be able to adjust the binding energy, symmetry energy, and incompressibility of nuclear matter at a given density. A common feature of these calculations is that they all lead to a significant density dependence of the effective force. In addition to this density dependence two of them[8,9] also give a starting energy dependence. Most of them give a rather satisfactory description of the radii, binding energies, and single-particle energies of doubly-closed-shell nuclei.

The approach consisting of a direct parametrization of the effective force is obviously less fundamental than the previous one but nevertheless has a certain number of advantages. First of all, from the simplicity of the calculations involved one can get a somewhat better physical insight because simple relations connecting different nuclear properties can often be derived. Also it is a useful tool to extrapolate in a rather simple and reliable way to nuclei far from the stability line and to superheavy nuclei. Among the interactions belonging to this group one finds: (i) density-independent forces,[10-13] which usually involve some difficulties in explaining either the nuclear radii or the total binding energies, and always the single-particle level densities of heavy nuclei; (ii) density-dependent forces which generally allow, in contrast, a fair description of these properties. Among these forces are Moszkowski's modified δ interaction[14] and also Skyrme's interaction,[15] which is the object of the present study.

The results of several calculations using Skyrme's interaction have already appeared in previous publications.[16-19] The purpose of the present paper is to give a systematic presentation of the theory and results for closed-shell nuclei. A description of this force, together with the motivation for such a parametrization of the effective interaction is given in the next section. The simple structure of the Skyrme force allows one to express the Hamiltonian density for a system described by a Slater determinant as an algebraic function of the nuclear and kinetic energy densities. This relation is derived in Sec. III where it is also shown that, applied to infinite nuclear matter, this relation yields simple expressions for the parameters of the force in terms of the nuclear-matter constants. In the same section we apply the variational principle to derive the Hartree-Fock equations. These equations exhibit a particularly simple structure, since it is found that the average nuclear field can be also expressed as an algebraic function of the densities. This structure is used to work out the physical meaning of the parameters. For doubly-closed-shell nuclei the reduction of angular variables can be carried out to yield a set of radial equations which is derived in Sec. IV. Section V deals with the problem of adjusting the parameters of the force. These are essentially fitted to the binding energies and equilibrium densities of oxygen-16 and lead-208. Two sets of parameters, yielding similar results but corresponding to different density-dependent terms, are constructed in this way. The numerical method of solving the Hartree-Fock equations is indicated in Sec. VI, and the results obtained for the radii, binding energies, and single-particle energies of doubly-closed-shell nuclei are presented and discussed in Sec. VII. In particular, a comparison of the results obtained with the two previous sets of parameters is made and contrasted with the predictions of Sec. III concerning the effect of changing the parameters. Finally, a summary of the main conclusions and perspectives is given in Sec. VIII.

II. DESCRIPTION OF SKYRME'S INTERACTION

In its original form Skyrme's interaction can be written as a potential,

$$V=\sum_{i<j} v_{ij}^{(2)} + \sum_{i<j<k} v_{ijk}^{(3)}, \tag{1}$$

with a two-body part v_{ij} and three-body part v_{ijk}.

To simplify calculations Skyrme used a short-range expansion for the two-body interaction. The matrix elements in momentum space are

$$\langle\vec{k}\,|\,v_{12}\,|\,\vec{k}'\rangle = t_0(1+x_0P_\sigma)+\tfrac{1}{2}t_1(k^2+k'^2)+t_2\vec{k}\cdot\vec{k}'$$
$$+\,iW_0(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{k}\times\vec{k}', \tag{2}$$

where $\vec{k}$ and $\vec{k}'$ are relative wave vectors of two nucleons. In Eq. (2) P_σ is a spin-exchange operator, and the $\vec{\sigma}$ are Pauli spin matrices. The reason why this expression corresponds to a short-range expansion can be seen in the following way. Consider, for instance, a Gaussian central force with exchange terms,

$$V=e^{-(r_{12}/\mu)^2}(W+BP_\sigma-HP_\tau-MP_\sigma P_\tau). \tag{3}$$

Only low-momentum matrix elements $(k, k' \leq 2k_F)$ are important for Hartree-Fock calculations. Now if the range μ in Eq. (3) is small compared to k_F^{-1}, then one can retain only the first few terms in the Taylor series for the matrix elements of V in momentum space, and one is left finally with an expression of the form

$$\langle\vec{k}\,|\,V\,|\,\vec{k}'\rangle=(\mu\sqrt{\pi}\,)^3[W+M+(B+H)P_\sigma][1-\tfrac{1}{4}(k^2+k'^2)\mu^2]$$
$$+\,\tfrac{1}{2}(\mu\sqrt{\pi}\,)^3[W-M+(B-H)P_\sigma]\mu^2\vec{k}\cdot\vec{k}', \tag{4}$$

which is identical to Eq. (2) except for the last term. In a similar way one can show[20] that this last term can be generated by a two-body spin-orbit force $V_{LS}(r_{12})\vec{L}\cdot\vec{S}$, where in the short-range limit

$$W_0=-\tfrac{2}{3}\pi\int_0^{+\infty}V_{LS}(r)r^4dr. \tag{5}$$

To see how one deals with such an interaction in practical calculations it is convenient to write it in configuration space. It can be expressed as

$$v_{12}=t_0(1+x_0P_\sigma)\delta(\vec{r}_1-\vec{r}_2)$$
$$+\,\tfrac{1}{2}t_1[\delta(\vec{r}_1-\vec{r}_2)k^2+k'^2\delta(\vec{r}_1-\vec{r}_2)]$$
$$+\,t_2\vec{k}'\cdot\delta(\vec{r}_1-\vec{r}_2)\vec{k}+iW_0(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{k}'\times\delta(\vec{r}_1-\vec{r}_2)\vec{k}, \tag{6}$$

where $\vec{k}$ now denotes the operator $(\vec{\nabla}_1-\vec{\nabla}_2)/2i$ acting on the right; whereas, $\vec{k}'$ is the operator $-(\vec{\nabla}_1-\vec{\nabla}_2)/2i$ acting on the left. By considering the matrix elements of expression (6) in a state of relative motion $\Psi(\vec{r})=R(r)Y_{lm}(\Omega)$ one can see that the first two terms correspond to S-wave interactions [since the matrix elements are proportional to $|\Psi(0)|^2$ and $\Psi(0)\nabla^2\Psi(0)$, respectively]; whereas, the last two terms correspond to P-wave interactions, since the matrix elements are proportional to $|\vec{\nabla}\Psi(0)|^2$.

For the three-body force Skyrme also assumed a zero-range force

$$v_{123}^{(3)}=t_3\delta(\vec{r}_1-\vec{r}_2)\delta(\vec{r}_2-\vec{r}_3). \tag{7}$$

In the following we will show that for Hartree-Fock calculations of even-even nuclei, this force is equivalent to a two-body density-dependent interaction:

$$v_{12}=\tfrac{1}{6}t_3(1+P_\sigma)\delta(\vec{r}_1-\vec{r}_2)\rho\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right). \tag{8}$$

Such a term provides a simple phenomenological representation of many-body effects, and describes the way in which the interaction between two nucleons is influenced by the presence of others. Skyrme's interaction can be considered as a kind of phenomenological G matrix which already includes the effect of short-range correlations, notably through the density-dependent term. This is one reason why it would be meaningless to calculate second-order corrections with Skyrme's force, and a perturbation calculation would actually diverge because of the zero range. As mentioned earlier, Skyrme's interaction is an approximate representation of the effective nucleon force which is only valid for low relative momenta.

A similar type of interaction has been investigated recently by Moszkowski.[14] His force differs from the present one by the absence of P-wave interactions and also by a density dependence proportional to $\rho^{2/3}$ rather than to ρ. The $\rho^{2/3}$ density dependence was suggested by Bethe.[21] For most G matrices[6-9] the convergence of the short-range expansion (4) is not rapid enough to allow a restriction to the first two lowest-order terms. A much more satisfactory derivation of Skyrme's interaction, based on an expansion for the mixed density will be presented in a forthcoming publication.[22]

III. HARTREE-FOCK EQUATIONS

For the Skyrme interaction there exists a very simple way of deriving the Hartree-Fock equations, which we will now describe. Consider a nucleus whose ground state is represented by a Slater determinant ϕ of single-particle states ϕ_i:

$$\phi(x_1,x_2,\ldots,x_A)=\frac{1}{\sqrt{A!}}\det|\,\phi_i(x_j)|, \tag{9}$$

where x denotes the set $\vec{r},\sigma,q$ of space, spin, and isospin coordinates ($q=+\tfrac{1}{2}$ for a proton, $-\tfrac{1}{2}$ for a neutron). The expectation value of the total energy is

$$
\begin{aligned}
E &= \langle \phi, (T+V)\phi \rangle \\
&= \sum_i \left\langle i \left| \frac{p^2}{2m} \right| i \right\rangle + \frac{1}{2} \sum_{ij} \langle ij | \bar{v}_{12} | ij \rangle \\
&\quad + \frac{1}{6} \sum_{ijk} \langle ijk | \bar{v}_{123} | ijk \rangle \\
&= \int H(\vec{r})\, d^3r \,, \qquad (10)
\end{aligned}
$$

where the notation $\bar{v}$ denotes an antisymmetrized matrix element. For the Skyrme interaction the energy density $H(\vec{r})$ is an algebraic function of the nucleon densities $\rho_n(\rho_p)$, the kinetic energy τ_n (τ_p), and spin densities $\vec{J}_n$ $(\vec{J}_p)$. These quantities depend in turn on the single-particle states ϕ_i defining the Slater-determinant wave function ϕ,

$$
\begin{aligned}
\rho_q(\vec{r}) &= \sum_{i,\sigma} | \phi_i(\vec{r}, \sigma, q)|^2 \,, \\
\tau_q(\vec{r}) &= \sum_{i,\sigma} | \vec{\nabla}\phi_i(\vec{r}, \sigma, q)|^2 \,, \qquad (11) \\
\vec{J}_q(\vec{r}) &= (-i) \sum_{i,\sigma,\sigma'} \phi_i^*(\vec{r}, \sigma, q)[\vec{\nabla}\phi_i(\vec{r}, \sigma', q) \times \langle \sigma | \vec{\sigma} | \sigma' \rangle] \,.
\end{aligned}
$$

The sums in Eq. (11) are taken over all occupied single-particle states. The expression for $H(\vec{r})$ is derived explicitly in Appendix A for the central term and in Appendix B for the spin-orbit term. Assuming that the subspace of occupied single-particle states is invariant under time reversal (which implies an even-even nucleus) one gets the following result:

$$
\begin{aligned}
H(\vec{r}) = {} & \frac{\hbar^2}{2m} \tau(\vec{r}) + \tfrac{1}{2} t_0 [(1+\tfrac{1}{2}x_0)\rho^2 - (x_0 + \tfrac{1}{2})(\rho_n^2 + \rho_p^2)] + \tfrac{1}{4}(t_1+t_2)\rho\tau + \tfrac{1}{8}(t_2 - t_1)(\rho_n \tau_n + \rho_p \tau_p) + \tfrac{1}{16}(t_2 - 3t_1)\rho\nabla^2\rho \\
& + \tfrac{1}{32}(3t_1 + t_2)(\rho_n \nabla^2 \rho_n + \rho_p \nabla^2 \rho_p) + \tfrac{1}{16}(t_1 - t_2)(\vec{J}_n^2 + \vec{J}_p^2) + \tfrac{1}{4} t_3 \rho_n \rho_p \rho + H_C(\vec{r}) - \tfrac{1}{2} W_0 (\rho \vec{\nabla} \cdot \vec{J} + \rho_n \vec{\nabla} \cdot \vec{J}_n + \rho_p \vec{\nabla} \cdot \vec{J}_p) \,, \qquad (12)
\end{aligned}
$$

where $\rho = \rho_n + \rho_p$, $\tau = \tau_n + \tau_p$, and $\vec{J} = \vec{J}_n + \vec{J}_p$. The direct part of the Coulomb interaction in $H_C(\vec{r})$ is $\frac{1}{2} V_C(\vec{r})\rho_p(\vec{r})$, where

$$
V_C(\vec{r}) = \int \rho_p(\vec{r}) \frac{e^2}{|\vec{r} - \vec{r}'|} d^3r' \,. \qquad (13)
$$

By comparing the terms proportional to t_0 and t_3 in Eq. (12) one can see that the three-body contact interaction (7) is equivalent to the density-dependent two-body force defined by Eq. (8). This equivalence, however, is valid only for the case we have investigated, namely that of an even-even nucleus.

In a nucleus with $N = Z$ and no Coulomb field we have

$$
\rho_n = \rho_p = \tfrac{1}{2} \rho, \quad \tau_n = \tau_p = \tfrac{1}{2} \tau, \quad \vec{J}_n = \vec{J}_p = \tfrac{1}{2} \vec{J} \,, \qquad (14)
$$

and the expression for $H(\vec{r})$ simplifies to

$$
\begin{aligned}
H(\vec{r}) = {} & \frac{\hbar^2}{2m} \tau + \tfrac{3}{8} t_0 \rho^2 + \tfrac{1}{16} t_3 \rho^3 + \tfrac{1}{16}(3t_1 + 5t_2)\rho\tau \\
& + \tfrac{1}{64}(9t_1 - 5t_2)(\vec{\nabla}\rho)^2 - \tfrac{3}{4} W_0 \rho \vec{\nabla} \cdot \vec{J} \,. \qquad (15)
\end{aligned}
$$

From this expression one can get immediately the binding energy per particle in nuclear matter. In nuclear matter $\vec{\nabla}\rho = \vec{\nabla} \cdot \vec{J} = 0$, $\rho = (\frac{2}{3}\pi^2)k_F^3$, $\tau = \frac{3}{5} k_F^2$, so that

$$
\frac{E}{A} = \frac{H}{\rho} = \tfrac{3}{5} T_F + \tfrac{3}{8} t_0 \rho + \tfrac{1}{16} t_3 \rho^2 + \tfrac{3}{80}(3t_1 + 5t_2)\rho k_F^2 \,, \qquad (16)
$$

where $T_F = \hbar^2 k_F^2 / 2m$ is the kinetic energy of a particle at the Fermi surface. Differentiating the previous expression twice with respect to the Fermi momentum k_F yields the following value of the nuclear-matter incompressibility K:

$$
K = k_F^2 \frac{\partial^2 (E/A)}{\partial k_F^2} = \tfrac{6}{5} T_F + \tfrac{9}{4} t_0 \rho + \tfrac{15}{8} t_3 \rho^2 + \tfrac{3}{4}(3t_1 + 5t_2)\rho k_F^2 \,. \qquad (17)
$$

If one now adds to these two equations the saturation condition $\partial(E/A)/\partial k_F = 0$, one gets a system of three linear equations for the quantities t_0, t_3, and $3t_1 + 5t_2$. Next, solving this system allows one to express the parameters of the interaction in terms of the nuclear-matter constants E/A, k_F, K:

$$
\begin{aligned}
t_0 \rho &= \tfrac{40}{9} E/A + \tfrac{4}{9} K - \tfrac{16}{5} T_F \,, \\
\tfrac{3}{16} t_3 \rho^2 &= 15E/A + K - \tfrac{9}{5} T_F \,, \qquad (18) \\
\tfrac{1}{16}(3t_1 + 5t_2)\rho k_F^2 &= 2T_F - 15E/A - \tfrac{5}{6} K \,.
\end{aligned}
$$

The second of these equations shows that for given values of E/A and k_F in nuclear matter, the coefficient t_3 of the density-dependent term increases linearly with the nuclear-matter incompressibility.

The Hartree-Fock equations for Skyrme's interaction are obtained by writing that the total energy E is stationary with respect to individual variations of the single-particle states ϕ_i, with the subsidiary condition that ϕ_i are normalized

$$
\frac{\delta}{\delta\phi_i} \left(E - \sum_i e_i \int |\phi_i(\vec{r})|^2 d^3r \right) = 0 \,. \qquad (19)
$$

Using the explicit expression (12) for $H(\vec{r})$, one concludes that the single-particle wave functions ϕ_i have to satisfy the following set of equations (see Appendix C):

$$\left[-\vec{\nabla}\cdot\frac{\hbar^2}{2m_q^*(\vec{r})}\vec{\nabla}+U_q(\vec{r})+\vec{W}_q(\vec{r})\cdot(-i)(\vec{\nabla}\times\vec{\sigma})\right]\phi_i=e_i\phi_i\,, \tag{20}$$

where q stands for the charge of the single-particle state i. Equation (20) has the form of a local Schrödinger equation with an effective mass $m^*(\vec{r})$ which depends on the density only,

$$\frac{\hbar^2}{2m_q^*(\vec{r})}=\frac{\hbar^2}{2m}+\tfrac{1}{4}(t_1+t_2)\,\rho+\tfrac{1}{8}(t_2-t_1)\,\rho_q\,; \tag{21}$$

whereas, the potential $U(\vec{r})$ also depends on the kinetic energy density,

$$\begin{aligned}U_q(\vec{r})={}&t_0[(1+\tfrac{1}{2}x_0)\rho-(x_0+\tfrac{1}{2})\rho_q]+\tfrac{1}{4}t_3(\rho^2-\rho_q^2)\\&-\tfrac{1}{8}(3t_1-t_2)\nabla^2\rho+\tfrac{1}{16}(3t_1+t_2)\nabla^2\rho_q+\tfrac{1}{4}(t_1+t_2)\tau\\&+\tfrac{1}{8}(t_2-t_1)\tau_q-\tfrac{1}{2}W_0(\vec{\nabla}\cdot\vec{J}+\vec{\nabla}\cdot\vec{J}_q)+\delta_{q,+\frac{1}{2}}V_C(\vec{r})\,.\end{aligned} \tag{22a}$$

The form factor $\vec{W}$ of the one-body spin-orbit potential is

$$\vec{W}_q(\vec{r})=\tfrac{1}{2}W_0(\vec{\nabla}\rho+\vec{\nabla}\rho_q)+\tfrac{1}{8}(t_1-t_2)\vec{J}_q(\vec{r})\,. \tag{22b}$$

In expression (22a) V_C is the direct part of the Coulomb potential defined by equation (13). The Coulomb exchange term has been neglected. One can notice in Eq. (22b) that the central force contributes to the one-body spin-orbit potential in those cases where the spin density $\vec{J}_q(\vec{r})$ is not zero. However, we will see in Sec. VII D that the contribution of this term to $\vec{W}$ is quite small. Since it is difficult to include such a term in the case of deformed nuclei, it has been neglected in our calculations. The variational principle has been preserved by neglecting also the term $\frac{1}{16}(t_1-t_2)(\vec{J}_n^{\,2}+\vec{J}_p^{\,2})$ in Eq. (12).

For a nucleus with $N=Z$ and no Coulomb interaction the effective mass, the potential $U_q(\vec{r})$, and the form factor $\vec{W}_q$ of the one-body spin-orbit potential are independent of q and are given by

$$\frac{\hbar^2}{2m^*(\vec{r})}=\frac{\hbar^2}{2m}+\tfrac{1}{16}(3t_1+5t_2)\,\rho(\vec{r})\,, \tag{23}$$

$$\begin{aligned}U(\vec{r})={}&\tfrac{3}{4}t_0\rho+\tfrac{3}{16}t_3\rho^2+\tfrac{1}{16}(3t_1+5t_2)\tau\\&+\tfrac{1}{32}(5t_2-9t_1)\nabla^2\rho-\tfrac{3}{2}W_0\vec{\nabla}\cdot\vec{J}\,,\end{aligned} \tag{24a}$$

$$\vec{W}(\vec{r})=\tfrac{3}{4}W_0\vec{\nabla}\rho+\tfrac{1}{16}(t_1-t_2)\vec{J}\,. \tag{24b}$$

From the previous expressions one can guess more or less the physical meaning of the parameters. From the expression (15) for $H(\vec{r})$ one can see that the parameter $9t_1-5t_2$ is important for surface effects, since it determines the importance of the term $(\vec{\nabla}\rho)^2$ in the energy density. In fact, in Thomas-Fermi theory[15] one can show that densities can be written explicitly in the form

$$\rho=\rho_0 th^2\,\frac{r-R}{b}$$

with

$$b=0.16\left[\frac{1}{T_F}(9t_1-5t_2)\rho\right]^{1/2}\,, \tag{25}$$

so that in this case surface thicknesses and surface energies are completely determined by the value of $9t_1-5t_2$. For Hartree-Fock calculations such a simple expression does not hold any more, but as will be seen in Sec. VII, larger values of $9t_1-5t_2$ give larger surface thicknesses. From the expression (23) of $\hbar^2/2m^*$ one can also see that the parameter $3t_1+5t_2$ is important for single-particle energy levels, since it determines the density dependence of the effective mass. In the present paper we will discuss only the case of spherical nuclei, but it can be noticed, however, that from the expression (15) for $H(\vec{r})$, deformation energies depend only on the kinetic energy, on $3t_1+5t_2$, $9t_1-5t_2$, and the spin-orbit strength W_0, since, for terms containing ρ only, a deformation is just a scale transformation, $\tilde{\rho}(r,z)=\rho(r/b,b^2z)$.

IV. CASE OF DOUBLY-CLOSED-SHELL NUCLEI

For doubly-closed-shell nuclei the reduction of angular variables in the Hartree-Fock equations can be carried out by making the ansatz

$$\phi_i(\vec{r},\sigma,\tau)=\frac{R_\alpha(r)}{r}\mathcal{Y}_{ljm}(\hat{r},\sigma)\chi_q(\tau)\,, \tag{26}$$

where

$$\mathcal{Y}_{ljm}(\hat{r},\sigma)=\sum_{m_l m_s}\langle l\tfrac{1}{2}m_l\,m_s|jm\rangle\,Y_{lm_l}(\hat{r})\chi_{m_s}(\sigma)\,,$$

and where the index i now stands for the following set of quantum numbers: the charge q, the principal quantum number n, the orbital angular momentum l, the total angular momentum j, and the magnetic quantum number m. We have also introduced the notation $\alpha\equiv q,n,l,j$ for simplicity.

From the definitions (11) for the density $\rho(\vec{r})$ and the kinetic energy density $\tau(\vec{r})$ one concludes that these functions depend on the radial coordinate r only. Explicitly,

$$\begin{aligned}\rho(r)&=\frac{1}{4\pi r^2}\sum_\alpha(2j_\alpha+1)R_\alpha^{\,2}(r)\,,\\\tau(r)&=\frac{1}{4\pi}\sum_\alpha(2j_\alpha+1)\left[\left(\frac{d\varphi_\alpha}{dr}\right)^2+\frac{l_\alpha(l_\alpha+1)}{r^2}\varphi_\alpha^{\,2}\right],\end{aligned} \tag{27}$$

where $\varphi_\alpha(r) = R_\alpha(r)/r$. The sums in Eq. (27) are restricted to neutron (proton) orbitals to obtain the neutron (proton) densities. We have used the relation

$$\nabla^2\rho(r) = 2\sum_i \phi_i^* \nabla^2 \phi_i + 2\tau(r) \tag{28}$$

to obtain the expression for $\tau(r)$. Similarly, one can show that the modulus of the spin density $\vec{J}(\vec{r})$ defined by Eq. (11) depends on the radial coordinate r only. A detailed derivation is given in Appendix D. However, one can guess the result from the following simple argument. For symmetry reasons $\vec{J}(\vec{r})$ is proportional to $\vec{r}$ for a doubly-closed-shell nucleus, so that

$$\vec{J}(\vec{r}) = \left(\frac{\vec{r}}{r}\cdot\vec{J}\right)\frac{\vec{r}}{r} = \frac{\vec{r}}{r^2}\sum_i \phi_i^* \vec{l}\cdot\vec{\sigma}\,\phi_i\,, \tag{29}$$

where $\vec{l}$ denotes the orbital angular momentum operator. Using the explicit expression (26) for the single-particle wave functions ϕ_i, one gets the following expression:

$$\vec{J}(\vec{r}) = \frac{\vec{r}}{r} J(r),$$
$$J(r) = \frac{1}{4\pi r^3}\sum_\alpha (2j_\alpha+1)[j_\alpha(j_\alpha+1) - l_\alpha(l_\alpha+1) - \tfrac{3}{4}]R_\alpha^{\,2}(r)\,, \tag{30}$$

which is identical to the result obtained in Appendix D. Inserting the values (27) and (30) of the densities into the definition (21), (22) of the Hartree-Fock potential, one finds that the average field U and the effective mass m^* are spherically symmetric. Also, due to Eq. (30) and to the fact that the density is spherically symmetric, the one-body spin-orbit term in Eq. (20) reduced to the usual form

$$\frac{1}{r}W_q(r)\vec{l}\cdot\vec{\sigma}\,, \tag{31}$$

where

$$W_q(r) = \tfrac{1}{2}W_0\frac{d}{dr}(\rho+\rho_q) + \tfrac{1}{8}(t_1 - t_2)J_q(r)\,. \tag{32}$$

Rewriting Eq. (20) as

$$-\frac{\hbar^2}{2m_q^*}\nabla^2\phi_i - \left(\vec{\nabla}\frac{\hbar^2}{2m_q^*}\right)\cdot\vec{\nabla}\phi_i + \left(U_q + \frac{1}{r}W_q\vec{l}\cdot\vec{\sigma}\right)\phi_i = e_i\phi_i\,, \tag{33}$$

and using the following expressions for the gradient and Laplacian operators in spherical coordinates:

$$\nabla^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2}r - \frac{\vec{l}^{\,2}}{r^2}\,,$$
$$\vec{\nabla}\frac{\hbar^2}{2m_q^*} = \frac{\vec{r}}{r}\frac{d}{dr}\frac{\hbar^2}{2m_q^*}\,, \tag{34}$$

one concludes that the radial wave functions $R_\alpha(r)$ have to satisfy the following set of equations:

$$\frac{\hbar^2}{2m_q^*}\left[-R_\alpha''(r) + \frac{l_\alpha(l_\alpha+1)}{r^2}R_\alpha(r)\right] - \frac{d}{dr}\left(\frac{\hbar^2}{2m_q^*}\right)R_\alpha'(r) + \left\{U_q(r) + \frac{1}{r}\frac{d}{dr}\left(\frac{\hbar^2}{2m_q^*}\right) + [j_\alpha(j_\alpha+1) - l_\alpha(l_\alpha+1) - \tfrac{3}{4}] \times\frac{1}{r}W_q(r)\right\}R_\alpha(r) = e_\alpha R_\alpha(r)\,. \tag{35}$$

V. CHOICE OF PARAMETERS

In his original work Skyrme fixed the numerical values of the parameters by fitting the binding energy and density of nuclear matter ($E/A = -17.04$ MeV, $k_F = 1.37\ \mathrm{fm}^{-1}$) and also binding energies and mass differences of some light nuclei calculated with oscillator wave functions. However, we found that Skyrme's parameters gave too small radii for heavy nuclei and for this reason we have determined better sets of parameters in the following way. In the first step the parameters were adjusted to fit the binding energy and density of nuclear matter and also the binding energy and radius of O^{16} with harmonic-oscillator wave functions. For nuclear matter the relevant formula is given by Eq. (16). For light nuclei the binding energy calculated from Eq. (15) with harmonic-oscillator wave functions is given by Skyrme's formula[15]

$$E = A\frac{\hbar^2}{2mb^2} + \frac{6}{(2\pi b^2)^{3/2}}\left(B_0t_0 + B_1t_1\frac{3}{2b^2} + B_2t_2\frac{5}{2b^2}\right) + \frac{4B_3t_3}{(\pi b^2\sqrt{3})^3}\,, \tag{36}$$

where b denotes the oscillator parameter $(\hbar/m\omega)^{1/2}$. The values of the coefficients A and B are given in Table I for helium-4, oxygen-16, and calcium-40. The previous procedure determines the four parameters t_0, t_1, t_2, t_3. The parameter x_0 which determines symmetry effects was adjusted to give a value of the order of 30 MeV for the symmetry-energy coefficient in nuclear matter

$$a_\tau = \tfrac{1}{3}T_F - \tfrac{1}{4}t_0(x_0+\tfrac{1}{2})\rho - \tfrac{1}{16}t_3\rho^2 + \tfrac{1}{6}t_2\rho k_F^{\,2}\,. \tag{37}$$

Finally the strength W_0 of the one-body spin-orbit

TABLE I. Numerical values of the coefficients A and B to be used in Eq. (36) for helium-4, oxygen-16, and calcium-40.

Nucleus	A	B_0	B_1	B_2	B_3
^{4}He	$\frac{9}{2}$	1	1	0	1
^{16}O	$\frac{69}{2}$	$\frac{31}{4}$	$\frac{35}{4}$	4	$\frac{116}{9}$
^{40}Ca	$\frac{237}{2}$	$\frac{1945}{64}$	$\frac{2625}{4}$	$\frac{1760}{64}$	$\frac{2060}{27}$

force was adjusted to fit the experimental value of 6.15 MeV for the splitting of the $1p$ levels in oxygen-16. In the second step Hartree-Fock calculations were carried out for doubly-closed-shell nuclei, and the nuclear matter and oxygen-16 input values were corrected to obtain a better fit to oxygen-16 and lead-208, so that the parameters were adjusted in fact on oxygen and lead. Using this procedure we have been able to find several sets of parameters giving a good description of closed-shell nuclei in Hartree-Fock calculations. Particularly good fits were obtained with the two sets of parameters defined in Table II. Both of these interactions exhibit a strong density dependence. For interaction (I) the contribution of the density-dependent term in nuclear matter is of the order of 22 MeV per particle. Comparing this number with the average kinetic energy per particle in this case, $\frac{3}{5} T_F = 21$ MeV, shows that the three-body term cannot be considered as a small correction. We have also indicated in Table II the corresponding input values of E/A, k_F, $E(^{16}\mathrm{O})$, and $b(^{16}\mathrm{O})$ together with the calculated values of the nuclear-matter incompressibility K and the symmetry-energy coefficient a_τ. As we might have expected from Eq. (18) the large values of t_3 for both of these interactions are associated with rather large values of K.

TABLE II. Numerical values of the parameters t_0 (MeV fm^3), t_1 (MeV fm^5), t_2 (MeV fm^5), t_3 (MeV fm^6), W_0 (MeV fm^5), and x_0 corresponding to interactions I and II. The equilibrium oscillator parameter b (in fm) and the associated total binding energy E (in MeV) of oxygen-16 have also been indicated, together with the Fermi momentum k_F (fm^{-1}), the binding energy per particle E/A (in MeV), the symmetry-energy coefficient a_τ (in MeV), and the incompressibility K (in MeV) of nuclear matter.

Force	t_0	t_1	t_2	t_3	x_0	W_0
I	−1057.3	235.9	−100.	14 463.5	0.56	120.
II	−1169.9	585.6	−27.1	9331.1	0.34	105.
	$E(^{16}\mathrm{O})$	$b(^{16}\mathrm{O})$	E/A	k_F	K	a_τ
I	−140.	1.71	−16	1.32	370	29.3
II	−135.	1.76	−16	1.30	342	34.1

VI. NUMERICAL SOLUTION FOR SPHERICAL NUCLEI

Eliminating the potential U, the form factor $\vec{W}$ of the one-body spin-orbit potential, and the effec-

TABLE III. Root mean square radii (in fm) and total binding energies per particle (in MeV) calculated with interactions I and II.

		^{16}O	^{40}Ca	^{48}Ca	^{90}Zr	^{208}Pb	^{298}114
	r_c (exp)	2.73 [a]	3.49 [b]	3.48 [b]	4.27 [c]	5.50 [d]	
	(E/A) (exp)	−7.98 [e]	−8.55 [e]	−8.67 [e]	−8.71 [e]	−7.87 [e]	
Force I	r_m	2.55	3.29	3.43	4.17	5.45	6.15
	r_n	2.53	3.27	3.48	4.19	5.49	6.18
	r_p	2.56	3.31	3.36	4.14	5.38	6.09
	r_c	2.68	3.41	3.46	4.22	5.44	6.14
	E/A	−8.22	−8.64	−8.93	−8.81	−7.89	−7.08
Force II	r_m	2.62	3.38	3.55	4.29	5.61	6.34
	r_n	2.61	3.35	3.63	4.32	5.69	6.41
	r_p	2.63	3.40	3.45	4.24	5.49	6.22
	r_c	2.75	3.49	3.54	4.31	5.55	6.27
	E/A	−7.89	−8.41	−8.39	−8.43	−7.54	−6.74
Ref. 8	r_p	2.71	3.41	3.45	4.18	5.37	
	E/A	−6.75	−7.49	−7.48	−7.85	−7.53	
Ref. 7	r_c	2.76	3.45	3.52	4.23	5.44	
	E/A	−7.73	−8.32	−7.87	−8.07	−7.31	

[a] I. Sick and J. S. McCarthy, Nucl. Phys. A150, 631 (1970).

[b] R. F. Frosh *et al.*, Phys. Rev. 174, 1380 (1968).

[c] L. A. Fajardo, J. R. Ficenec, W. P. Trower, and I. Sick, Phys. Letters 37B, 363 (1971).

[d] J. Heisenberg *et al.*, Phys. Rev. Letters 23, 1402 (1969).

[e] J. H. E. Mattauch, W. Thiele, and A. H. Wapstra, Nucl. Phys. 67, 1 (1965).

tive mass $\hbar^2/2m^*$ between Eqs. (35) and (21), (22) yields a nonlinear system of *differential* equations. In contrast, Hartree-Fock calculations made with finite-range interactions yield in general systems of integrodifferential equations. This important difference makes the solution of the Hartree-Fock equations particularly simple for Skyrme's interaction. It is related to the fact that (i) the average field (21), (22) is an algebraic function of the densities; (ii) the Schrödinger equation (35) is a differential equation even though it is nonlocal, owing to the presence of a radius-dependent effective mass.

In the present case the Hartree-Fock equations were solved by the following usual iteration procedure. Let $R_\alpha^{(0)}$ denote a first approximation to the unknown radial wave functions, e.g., harmonic-oscillator wave-functions or Woods-Saxon wave functions. Inserting these functions into Eqs. (27) and (30) yields first approximations $\rho^{(0)}$, $\tau^{(0)}$, and $\vec{J}^{(0)}$ to the densities, and therefore from Eqs. (21), (22) first approximations $U^{(0)}$, $\vec{W}^{(0)}$, $\hbar^2/2m^{*(0)}$ to the potential, to the form factor of the one-body spin-orbit potential, and to the effective mass. Substituting these values into the Schrödinger equation (35) yields a new approximation $R_\alpha^{(1)}$ to the radial wave functions, and so on. Eventually this procedure converges to the exact solution R_α. In practice we have found that, starting from Woods-Saxon wave functions, 10 to 15 iterations for light nuclei, and 15 to 20 iterations for heavy and superheavy nuclei are sufficient to obtain a good convergence, namely, a relative variation smaller than 10^{-4} for the single-particle energies between the last two iterations.

The calculation of the average field from the radial wave functions via Eqs. (21), (22), (27), and (30) involves only a few elementary operations and has been found to be a negligible fraction of the total computing time. To solve the Schrödinger equation (35) with an effective mass, we have used a slight modification of the standard methods available to solve local Schrödinger equations. This technique is described in Appendix E.

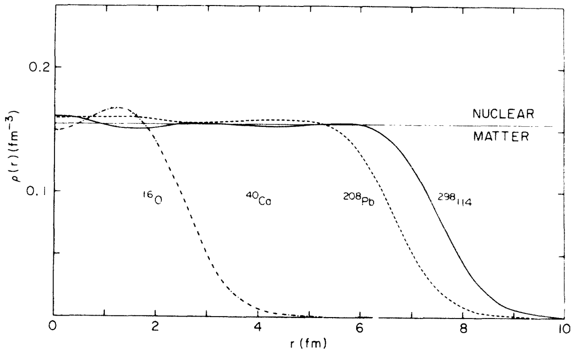

FIG. 1. Mass distributions $\rho(r)$ calculated with interaction I for the nuclei ^{16}O, ^{40}Ca, ^{208}Pb, and ^{298}114.

Because of the simple structure of the Hartree-Fock equations for Skyrme's interaction, the calculations are extremely fast. The complete iteration procedure in lead-208 takes only 3 min for 20 iterations on a UNIVAC 1108; whereas, the solution of the integrodifferential system for a finite-range interaction as simple as the Brink and Boeker force requires 120 min.

VII. RESULTS

The present section is concerned with the results obtained for doubly-closed-shell nuclei by solving the Hartree-Fock equations (35), (21), (22) for the two sets of parameters defined in Table II.

Center-of-mass corrections to the total energy can be made by subtracting the center-of-mass kinetic energy $P^2/2mA$ from the many-particle Hamiltonian. This prescription improves the total energy, but it is not clear that it improves the wave functions. As the total momentum $\vec{P}=\sum_{i=1}^{A}\vec{p}_i$ is a sum of single-particle momenta, the center-of-mass kinetic energy splits up into a sum of two terms:

$$\frac{1}{2mA}\vec{P}^2=\frac{1}{2mA}\sum_{i=1}^{A}\vec{p}_i^{\,2}+\frac{1}{2mA}\sum_{i\neq j}\vec{p}_i\cdot\vec{p}_j\,.$$

The effects of the first term can be included by multiplying the factor $\hbar^2/2m$ in the kinetic energy term of Eq. (21) by a factor $(A-1)/A$. The second term gives rise only to exchange corrections. It

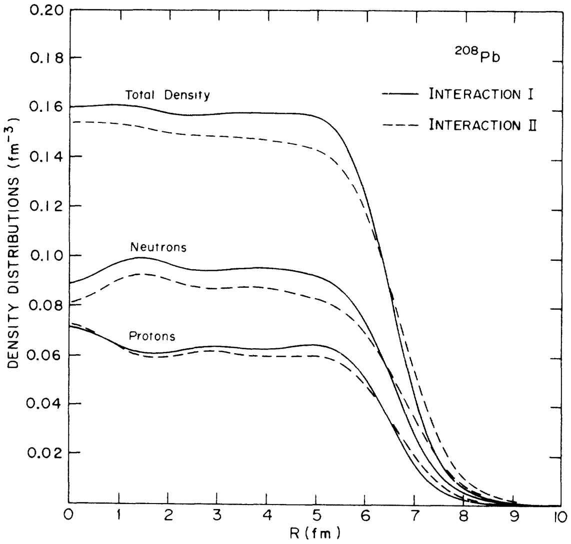

FIG. 2. Neutron, proton, and mass densities of ^{208}Pb obtained from interactions I and II.

is difficult to calculate and has been neglected in the present work. We recall that the exchange term from the Coulomb force and the spin-orbit term coming from the central force have also been neglected.

A. Density Distributions and Electron Scattering

Table III shows the calculated values of r.m.s. radii of the neutrons (r_n), protons (r_p), and the charge distribution (r_c) and of the binding energies of several closed-shell nuclei. Corrections to the nuclear-charge distribution to allow for the finite extent of the proton-charge distribution have been made with a proton form factor:

$$f_p(r)=\frac{1}{(r_0\sqrt{\pi})^3}e^{-r^2/r_0^2}\,,\quad r_0=0.65\text{ fm}.$$

This form factor is folded with the proton density distribution $\rho_p(r)$ to get the charge distribution $\rho_c(r)$:

$$\rho_c(\vec{r})=\int f_p(\vec{r}-\vec{s})\rho_p(\vec{s})d^3\vec{s}\,.$$

The calculated charge radii in Table III agree remarkably well with experiment for both sets of parameters, though the agreement is somewhat better for interaction II than for interaction I.

The mass distributions $\rho(r)$ calculated for the closed-shell nuclei ^{16}O, ^{40}Ca, ^{208}Pb and the superheavy nucleus ^{298}114 with interaction I are graphed in Fig. 1. These densities are similar to those obtained from other Hartree-Fock calculations made with density-dependent forces,[7,8] in particular as far as saturation properties are concerned. Indeed, for the heavier elements the calculated density is found to be nearly constant inside the nucleus and is close to the equilibrium density in nuclear matter calculated with the same force (0.155 fm^{-3}). In contrast, calculations made with density-independent forces always suffer from a serious lack of saturation, which is reflected in excessively high central densities.[23,24] This difference is probably a consequence of a higher value of the nuclear-matter incompressibility K. For instance, $K=370$ MeV for interaction I, 310 MeV in Ref. 7, while it is only 190 MeV in Ref. 23. As in all Hartree-Fock calculations[6-8,13,23,24] there are small oscillations in the density with a wave length of the order of π/k_F.[25] These oscillations are less pronounced, however, than in Hartree-Fock calculations made with density-independent forces.[23,24] Here again we attribute this difference to a higher value of the compression modulus. Figure 2 compares the neutron and proton densities calculated in ^{208}Pb with interactions I and II. A notable difference between the two calculations is that the surface thickness is slightly larger in the case of interaction II. We expect the surface thickness to depend both on K[14,15] and also, as argued in Sec. III, on the parameter combination $9t_1-5t_2$, larger values of this quantity corresponding to a larger surface thickness. Since interactions I and II correspond to very similar values of K, and the parameter combination $9t_1-5t_2$ is larger for interaction II, the difference in surface thickness is in qualitative agreement with the predictions of Sec. III.

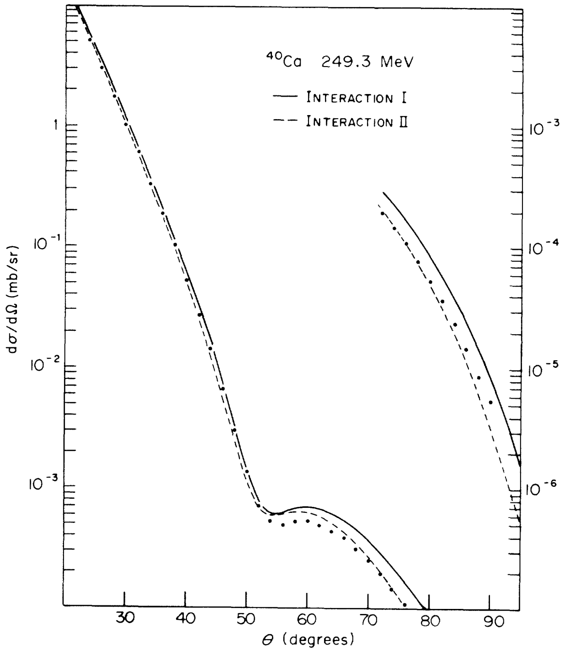

FIG. 3. Elastic electron scattering from ^{40}Ca at 249.3 MeV. Experimental data points are taken from Ref. 26.

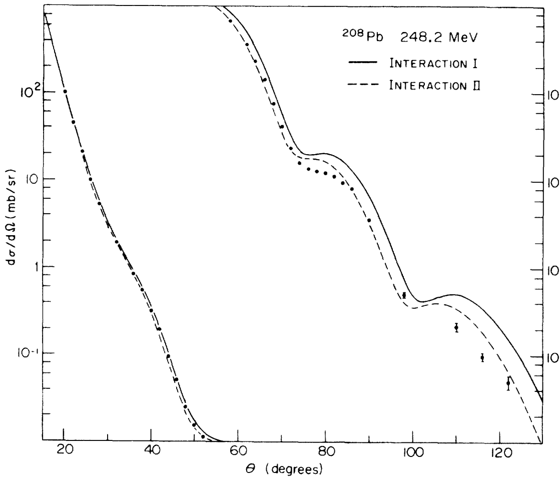

FIG. 4. Elastic electron scattering from ^{208}Pb at 248.2 MeV. Experimental data points are taken from Ref. 26.

Figures 3–5 compare experimental differential cross sections for electron scattering from ^{40}Ca at 250 MeV and ^{208}Pb at 250 MeV and 500 MeV with cross sections calculated from Hartree-Fock charge distributions. The charge distributions and electron scattering were calculated for both interactions I and II. The cross sections were calculated by solving the Dirac equation by the phase-shift method. Vacuum-polarization corrections are not included. The calculated cross sections for electron scattering agree quite well with experimental values for both the interactions I and II. As for charge radii the agreement is quantitatively much better for interaction II. In this case the calculated values fit the experimental points very well except for angles near diffraction minima. We should point out that the fit to electron scattering data with the Hartree-Fock charge distribution given by interaction II is still not as good as fits made with phenomenological charge distributions.[26] For example the χ^2 value for electron scattering from ^{40}Ca at 250 MeV is 540 for the charge distribution found from interaction II, while the χ^2 value for a phenomenological charge distribution is 20.[26] Also, the fit for ^{40}Ca with interaction II is quantitatively not as good as that obtained by Negele.[8]

Figure 6 shows the Hartree-Fock charge distributions for ^{208}Pb calculated with interactions I and II and compares them with a phenomenological charge distribution determined from electron scattering by Heisenberg *et al.*[26] The phenomenological charge distribution tends to decrease towards the center of the nucleus. The Hartree-Fock charge distribution from interaction I also shows this tendency, but has too small a surface thickness compared with the phenomenological distribution. The charge distribution for interaction II is not so good inside the nucleus, but compares well with the phenomenological charge distribution in the surface region. This is the reason why the charge distribution from interaction II fits the electron scattering data better than the charge distribution from interaction I. Both Hartree-Fock charge distributions have oscillations in the nuclear interior. These have a smaller amplitude than for other Hartree-Fock calculations, but are still larger than the amplitude of the oscillations in the phenomenological charge distribution. The Hartree-Fock charge distributions always have a small bump at $r=0$ for ^{208}Pb. This is because the $3s_{1/2}$ proton shell-model orbit has a density peaked at $r=0$.

B. Binding Energies

The calculated binding energies listed in Table III also agree well with experimental values. This agreement is closely connected with the density dependence of the Skyrme force. For density-independent forces the total binding energy in the Hartree-Fock approximation is given by

$$E=\tfrac{1}{2}\sum_i (t_i+e_i)\,,$$

where t_i and e_i denote single-particle kinetic energies and single-particle energies, respectively. Owing to this relation it is well-known[27] that it is not possible to fit the radius, single-particle energies, and total binding energy of ^{16}O and ^{40}Ca in a Hartree-Fock calculation using a single density-

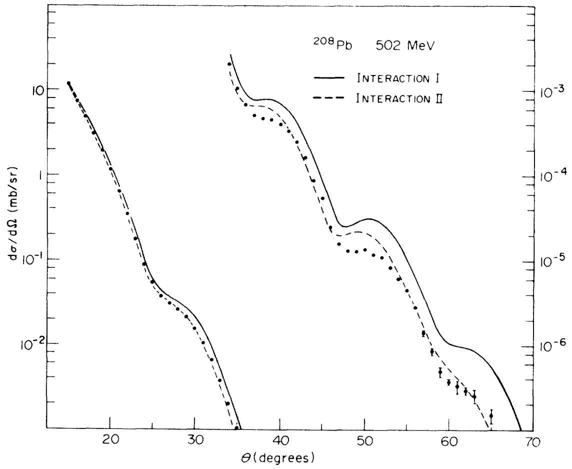

FIG. 5. Elastic electron scattering from ^{208}Pb at 502 MeV. Experimental data points are taken from Ref. 26.

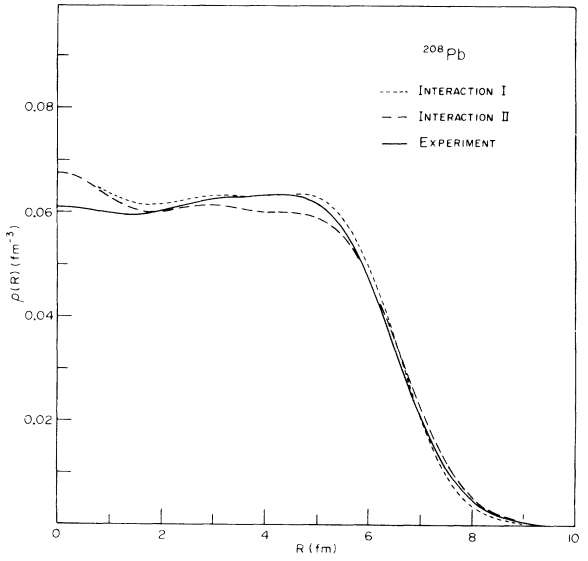

FIG. 6. Charge distribution of ^{208}Pb calculated with interactions I and II. The experimental charge distribution is that of Ref. 26.

TABLE IV. Single-particle energies (in MeV) calculated with interactions I and II. Occupied and unoccupied levels are separated by a horizontal line.

	Neutrons			Protons		
	(I)	(II)	(Exp)	(I)	(II)	(Exp)
$^{16}\mathrm{O}$						
$1s_{1/2}$	32.96	42.22		28.76	38.01	40 ± 8[a]
$1p_{3/2}$	20.81	22.22	21.8[b]	16.77	18.28	18.4[b]
$1p_{1/2}$	13.84	16.80	15.7[b]	9.94	12.97	12.1[b]
$1d_{5/2}$	8.16	5.31	4.14[b]	4.33	1.78	0.60[b]
$2s_{1/2}$	3.27	2.14	3.27[b]			0.10[b]
$^{40}\mathrm{Ca}$						
$1s_{1/2}$	41.04	55.33		32.84	47.11	50 ± 11[a]
$1p_{3/2}$	32.17	39.22		24.18	31.30	34 ± 6[a]
$1p_{1/2}$	28.44	36.08		20.51	28.23	
$1d_{5/2}$	22.16	23.26		14.37	15.67	
$2s_{1/2}$	15.67	17.08	18.1[b]	7.88	9.57	10.9[b]
$1d_{3/2}$	14.95	17.53	15.6[b]	7.31	10.10	8.3[b]
$1f_{7/2}$	11.25	8.34	8.36[b]	3.69	1.22	1.4
$2p_{3/2}$	4.46	3.02	6.2[b]			
$2p_{1/2}$	2.37	1.56				
$1f_{5/2}$	1.23	1.21				
$^{48}\mathrm{Ca}$						
$1s_{1/2}$	40.40	55.74		39.36	53.21	55 ± 9[a]
$1p_{3/2}$	30.39	39.80		31.28	38.73	35 ± 7[a]
$1p_{1/2}$	28.36	37.60		28.26	36.24	
$1d_{5/2}$	20.86	23.86		21.84	23.47	
$2s_{1/2}$	15.44	18.10	12.55[b]	14.73	16.48	15.3[b]
$1d_{3/2}$	14.64	18.95	12.52[b]	15.46	18.48	15.7[b]
$1f_{7/2}$	10.48	9.10	9.94[b]	11.36	8.61	9.6[b]
$2p_{3/2}$	4.91	4.13	5.14[b]	3.22	1.72	1.9[b]
$2p_{1/2}$	2.98	2.60	3.11[b]	1.32	0.23	0.0[b]
$1f_{5/2}$	0.71	2.02		1.74	1.69	
$^{90}\mathrm{Zr}$						
$1s_{1/2}$	44.69	62.12		36.29	52.68	54 ± 8[a]
$1p_{3/2}$	37.97	50.35		30.78	42.19	43 ± 8[a]
$1p_{1/2}$	36.63	49.17		29.07	40.80	
$1d_{5/2}$	30.27	37.47		23.87	30.22	27 ± 8[a]
$1d_{3/2}$	26.89	34.68		20.11	27.20	
$2s_{1/2}$	25.49	31.99		17.65	23.70	
$1f_{7/2}$	21.90	24.33		15.87	17.57	
$1f_{5/2}$	15.78	19.42	13.50[c]	9.60	12.62	
$2p_{3/2}$	15.76	17.63	13.10[c]	7.83	9.48	
$2p_{1/2}$	13.73	15.90	12.60[c]	6.05	7.91	
$1g_{9/2}$	12.96	11.53	12.00[c]	6.99	4.92	
$2d_{5/2}$	6.22	5.07	7.20[c]	...	...	
$3s_{1/2}$	4.07	3.12	5.63[c]	...	...	
$2d_{3/2}$	3.40	2.88	4.88[c]	...	...	
$1g_{7/2}$	3.93	4.64	4.46[c]	...	...	
$^{208}\mathrm{Pb}$						
$1s_{1/2}$	44.63	62.92		36.60	53.36	
$1p_{3/2}$	40.91	56.17		33.07	46.89	
$1p_{1/2}$	40.31	55.70		32.48	46.43	
$1d_{5/2}$	36.17	48.07		28.41	38.94	
$1d_{3/2}$	34.75	46.97		27.00	37.83	
$2s_{1/2}$	32.45	43.88		24.03	34.01	
$1f_{7/2}$	30.64	38.96		22.91	29.93	
$1f_{5/2}$	27.98	36.90		20.27	27.86	
$2p_{3/2}$	25.43	32.83		17.08	23.12	
$^{208}\mathrm{Pb}$ *(Continued)*						
$2p_{1/2}$	24.22	31.87		15.98	22.20	
$1g_{9/2}$	24.47	29.18		16.73	20.24	15.43[b]
$1g_{7/2}$	20.16	25.83		12.51	16.91	11.43[b]
$2d_{5/2}$	18.12	21.84		9.68	12.16	9.70[b]
$1h_{11/2}$	17.75	19.07		9.95	10.18	9.37[b]
$2d_{3/2}$	15.93	20.05		7.74	10.54	8.38[b]
$3s_{1/2}$	15.60	19.00		6.80	8.95	8.03[b]
$1h_{9/2}$	11.48	14.15	10.85[b]	3.88	5.38	3.77[b]
$2f_{7/2}$	10.55	11.23	9.72[b]	1.84	1.36	2.87[b]
$1i_{13/2}$	10.55	8.92	9.01[b]	2.63		2.16[b]
$3p_{3/2}$	7.49	7.92	8.27[b]			0.95[b]
$2f_{5/2}$	7.48	8.73	7.95[b]			0.47[b]
$3p_{1/2}$	6.35	7.00	7.38[b]			
$2g_{9/2}$	2.84	1.47	3.94[b]			
$1i_{11/2}$	2.14	2.42	3.15[b]			
$1j_{15/2}$	2.89		2.53[b]			
$3d_{5/2}$	0.19		2.36[b]			
$4s_{1/2}$			1.91[b]			
$2g_{7/2}$			1.45[b]			
$3d_{3/2}$			1.42[b]			
$^{298}114$						
$1s_{1/2}$	44.58	62.01		34.56	50.74	
$1p_{3/2}$	41.84	57.31		31.19	45.40	
$1p_{1/2}$	41.41	57.03		30.93	45.23	
$1d_{5/2}$	38.16	51.17		27.21	38.91	
$1d_{3/2}$	37.18	50.48		26.41	38.33	
$2s_{1/2}$	34.86	46.84		25.07	35.48	
$1f_{7/2}$	33.74	43.94		22.63	31.50	
$1f_{5/2}$	31.94	42.62		20.99	30.27	
$2p_{3/2}$	29.10	38.02		18.76	26.14	
$2p_{1/2}$	28.31	37.47		18.13	25.69	
$1g_{9/2}$	28.70	35.89		17.50	23.37	
$1g_{7/2}$	25.80	33.69		14.73	21.24	
$2d_{5/2}$	22.91	28.64		12.07	16.40	
$1h_{11/2}$	23.13	27.24		11.87	14.75	
$2d_{3/2}$	21.29	27.50		10.68	15.35	
$3s_{1/2}$	20.53	25.75		10.10	13.75	
$1h_{9/2}$	18.83	23.92		7.70	11.47	
$1i_{13/2}$	17.08	18.24		5.78	5.82	
$2f_{7/2}$	16.37	19.18		5.16	6.62	
$2f_{5/2}$	13.84	17.23		2.99	4.92	
$3p_{3/2}$	13.27	15.43		2.62	3.16	
$3p_{1/2}$	12.39	14.73		1.91	2.59	
$1i_{11/2}$	11.13	13.56			1.22	
$1j_{15/2}$	10.60	9.08				
$2g_{9/2}$	9.52	9.79				
$2g_{7/2}$	6.22	7.24				
$3d_{5/2}$	6.04	5.95				
$3d_{3/2}$	4.69	4.92				
$4s_{1/2}$	4.56	4.47				
$1k_{17/2}$	3.71	...				
$1j_{13/2}$	2.83	2.99				
$2h_{11/2}$	2.47	0.94				

[a] Reference 28.

[b] A. Bohr and B. Mottelson, *Nuclear Structure* (Benjamin, New York, 1969), Vol. I.

[c] G. Bassani *et al.*, J. Phys. Soc. Japan, Suppl. 24, 649 (1968); E. Cosman *et al.*, to be published; E. Cosman, private communication.

independent force. For Skyrme's interaction, however, the situation is different, since the above relation no longer holds and is replaced by

$$E=\tfrac{1}{2}\sum_i (t_i+e_i)+E_{\mathrm{R}}\,, \tag{38}$$

where

$$\begin{aligned} E_{\mathrm{R}} &= -\tfrac{1}{12}\sum_{ijk}\langle ijk|\bar{v}_{123}|ijk\rangle \\ &= -\tfrac{1}{8}t_3\int \rho_n(\vec{r})\rho_p(\vec{r})\rho(\vec{r})d^3r\,. \end{aligned} \tag{39}$$

The term E_{R} comes from the density dependence of the interaction and is sometimes called the rearrangement term. For interaction I the single-particle levels of oxygen-16 are a little too weakly bound so that the first term in Eq. (38) is of the order of only 2 MeV. However, the rearrangement term E_{R} is found to be of the order of 6 MeV, therefore allowing a good fit to the binding energy of oxygen-16. From expression (30) for the spin density, one can see that the contribution E_{so} of the two-body spin-orbit force to the total binding energy has to be very small for spin-satured nuclei, i.e., nuclei such that both doublets $j=l+\frac{1}{2}$, $j=l-\frac{1}{2}$ are occupied. In fact, E_{so} would vanish identically if the radial wave functions of the two members of the doublet were identical. For interaction II it is found that $E_{\mathrm{so}}=-0.6$ MeV for oxygen-16 and -0.9 MeV for calcium-40. For spin-unsaturated nuclei, however, one can get a significant contribution of the two-body spin-orbit force to the total binding energy. Indeed, we find with interaction II that $E_{\mathrm{so}}=-26.6$ MeV for calcium-48, -33.9 MeV for zirconium-90, and -76.8 MeV for lead-208. Table III shows that the two sets of parameters I and II give very similar results. Binding energies calculated with the parameter Set I are consistently larger than those calculated with Set II. This difference can easily be understood by looking at the input values for ^{16}O and nuclear matter used to determine the parameters (Table II). Both interactions I and II give better binding energies than the calculations[7,8] made with realistic forces using the local-density approximation.

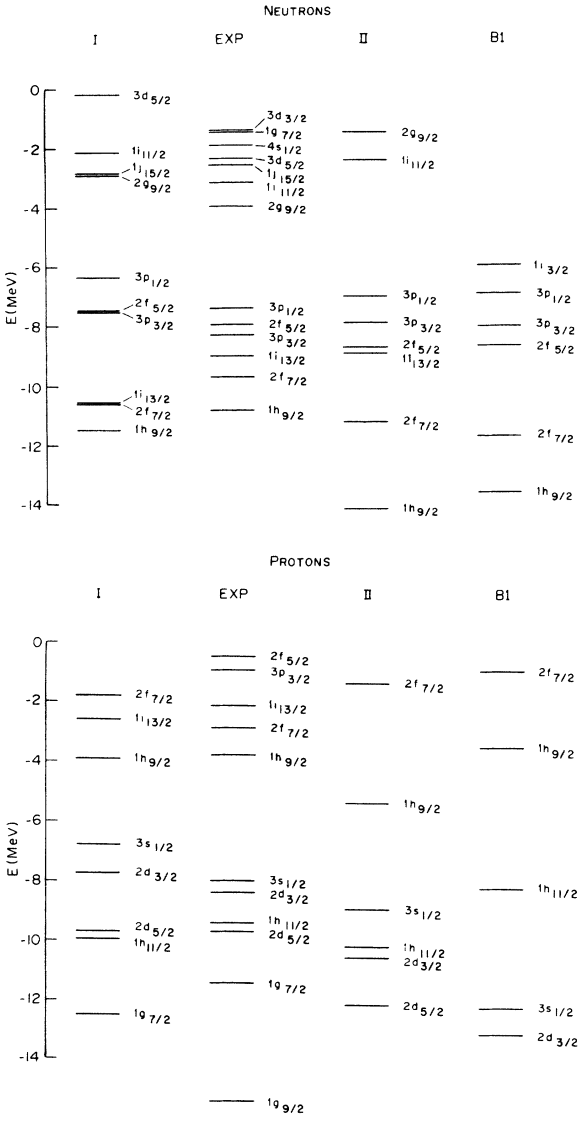

FIG. 7. Single-particle states of ^{208}Pb near the Fermi level. The results obtained with the modified Skyrme interaction are compared with the experimental values and with the spectrum calculated in Ref. 23.

C. Single-Particle Energies

Single-particle energies were defined in Eq. (19) as the Lagrange multipliers associated with the constraints $\langle\phi_i|\phi_i\rangle=1$. However, the relevant quantities to compare with experimental data are rather the removal energies which are given by the mass differences $E(A)-E_i(A-1)$. If we assume that there is no polarization of the core of the mass-A nucleus by the hole created in the state i, i.e., if one assumes the single-particle wave functions of the A and $A-1$ systems to be identical, then the mass difference calculated from Eq. (10) is

$$\begin{aligned} E(A)-E_i(A-1) &= \left\langle i\left|\frac{p^2}{2m}\right|i\right\rangle+\sum_j\langle ij|\bar{v}_{12}|ij\rangle \\ &\quad+\tfrac{1}{2}\sum_{jk}\langle ijk|\bar{v}_{123}|ijk\rangle\,, \end{aligned} \tag{40}$$

where the sums in Eq. (40) run over all occupied single-particle states. Evaluating the right-hand side of Eq. (40) and comparing the result with Eq. (20) one obtains the result (see Appendix A) that the Lagrange multipliers e_i are exactly equal to the removal energies (40), as in Hartree-Fock calculations using two-body forces. Table IV shows the single-particle energies calculated with both sets of parameters and Fig. 7 compares the calculated single-particle energies of states near the Fermi level in ^{208}Pb with experimental values. The order of the levels in this nucleus is found to be correct, the spacings are reasonably good, and the binding energy of the last nucleon is near the experimental value. In contrast, as was mentioned in Sec. I, all published calculations made with density-independent forces[23,24] give too large level spacings. As an example the spectrum calculated in Ref. 23 has been plotted in Fig. 7. One can see that in the latter case the order of the single-particle levels is almost correct, but that the density of levels is much too small.

Whereas, the results concerning binding energies and densities are very close for interactions I and II, the corresponding spectra exhibit some differences, especially in the binding energy of the deepest single-particle states. The calculated 1*s* proton levels for interaction I are always too weakly bound; whereas, they are much closer to experimental values[28] for interaction II. For instance, the binding energy of a 1*s* proton in calcium-40 is only 32 MeV in the case of interaction I. For interaction II it is 48 MeV, in much better agreement with the experimental value of 50 ± 11 MeV.[28]

To investigate the origin of this difference we have graphed in Figs. 8 and 9 the neutron and proton potentials defined by Eq. (22), and the neutron and proton effective masses m^*/m [Eq. (21)] in the case of lead-208. This figure shows that for interaction I the radius dependence of the effective mass is practically negligible so that the Hartree-Fock potential is nearly local. In contrast, the effective mass in the case of interaction II is of the order of 0.6 inside the nucleus, therefore leading to important nonlocality effects. Let us notice that since the density of lead-208 inside the nucleus is very close to the nuclear-matter density, the value of the parameter $3t_1+5t_2$ determines quite accurately the average effective mass in the interior of lead-208, and therefore the nonlocality of the Hartree-Fock potential. This remark elucidates the statement we made in Sec. III concerning the importance of the parameter $3t_1+5t_2$ for single-particle energy levels.

Figures 10–12 show the Hartree-Fock single-particle potentials $U_n(r)$, $U_p(r)$ for neutrons and protons and the effective masses $m_n^*(r)$, $m_p^*(r)$ calculated with the interaction parameters II for the nuclei ^{16}O, ^{40}Ca, and ^{48}Ca. The proton single-particle potential $U_p(r)$ does not include the Coulomb term $V_C(r)$ [Eq. (13)]. The single-particle potentials $U_n(r)$ and $U_p(r)$ are not of Woods-Saxon shape, but have irregularities associated with the shell structure of the corresponding nuclei. Charge symmetry would require that $U_n=U_p$ and $m_n^*=m_p^*$ in the self-conjugate nuclei ^{16}O and ^{40}Ca. The small differences between U_n and U_p, and m_n^* and m_p^* show the charge-symmetry-violating effects introduced by the Coulomb interaction which have been discussed in Ref. 16.

Charge symmetry does not require any special relations between U_n, U_p and m_n^*, m_p^* for the non-self-conjugate nucleus ^{48}Ca, and Fig. 12 shows

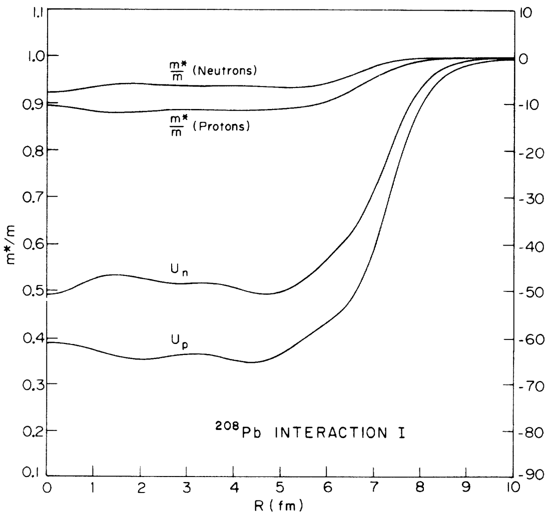

FIG. 8. Effective mass m^*/m and potential U calculated in ^{208}Pb with interaction I. The Coulomb term (13) is not included in U.

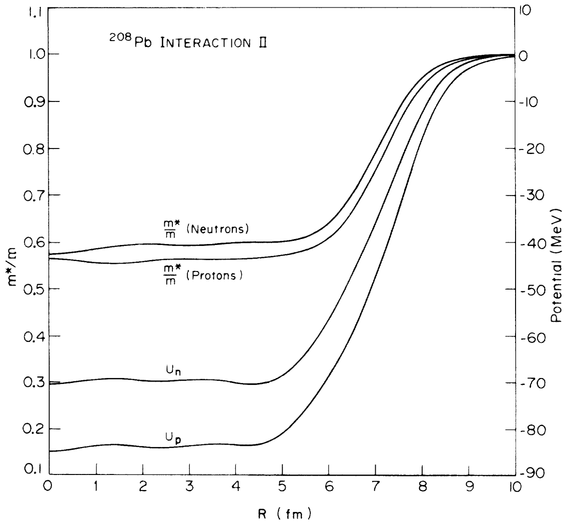

FIG. 9. Effective mass m^*/m and potential U calculated in ^{208}Pb with interaction II.

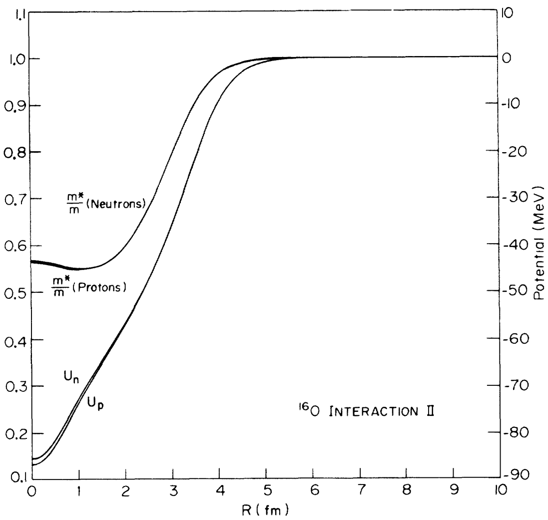

FIG. 10. Effective mass m^*/m and potential U calculated in ^{16}O with interaction II.

that there are considerable differences. A careful comparison of Figs. 11 and 12 shows that $U_n(r)$ is almost unchanged in going from ^{40}Ca to ^{48}Ca. On the other hand, there is a considerable change in the strength and the range of the proton single-particle potential $U_p(r)$. In this case adding neutrons to ^{40}Ca changes U_p much more than U_n. The same effect shows up in the neutron and proton single-particle energies of ^{40}Ca and ^{48}Ca. Table IV shows that the neutron single-particle levels are not changed much between ^{40}Ca and ^{48}Ca. On the other hand, the proton single-particle binding energies are increased by about 6 MeV. These theoretical results agree with the experimental trends.

D. Spin-Orbit Splittings

The two-body spin-orbit term in Skyrme's interaction contains only one parameter. As mentioned earlier, this parameter has been adjusted to reproduce approximately the experimental splitting of the $1p$ levels in oxygen-16. Both interactions I and II give similar splittings throughout the Periodic Table. However there are some small differences in lead-208. For instance, the splitting of the $3p$-neutron levels in this nucleus is 1.14 MeV for interaction I; whereas, it is only 0.92 MeV for interaction II (versus 0.87 MeV experimentally). This difference is perhaps related to the smaller radii and surface thicknesses obtained in the case of interaction I.

An important difference with other Hartree-Fock calculations[4, 5, 23, 24] concerns the position of unnatural-parity states in lead-208 ($1i_{13/2}n$ and $1h_{11/2}p$). Whereas, in most Hartree-Fock calculations these levels are much too high, they come out quite well in the present one. However, even though part of this difference arises from the much better level density obtained here – which is reflected by a much better distribution for the barycenters of the various spin-orbit doublets – the agreement is only apparent. One reason is that we have omitted in numerical applications the one-body spin-orbit term

$$\tfrac{1}{8}(t_1 - t_2)\frac{1}{r}J_q(r)\vec{l}\cdot\vec{\sigma} \qquad (41)$$

produced by the central force [see Eq. (32)]. Including this term in perturbation theory actually shifts the $1i_{13/2}$-neutron level up by 0.41 MeV (0.60 MeV) and the $1h_{11/2}$-proton level up by 0.27 MeV (0.41 MeV) in the case of interaction I (II). Anoth-

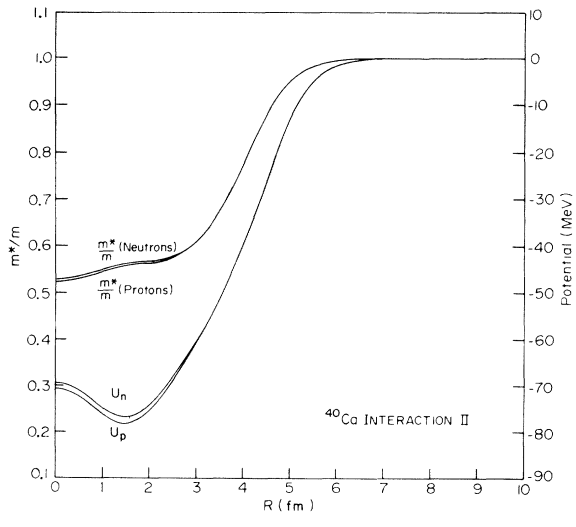

FIG. 11. Effective mass m^*/m and potential U calculated in ^{40}Ca with interaction II.

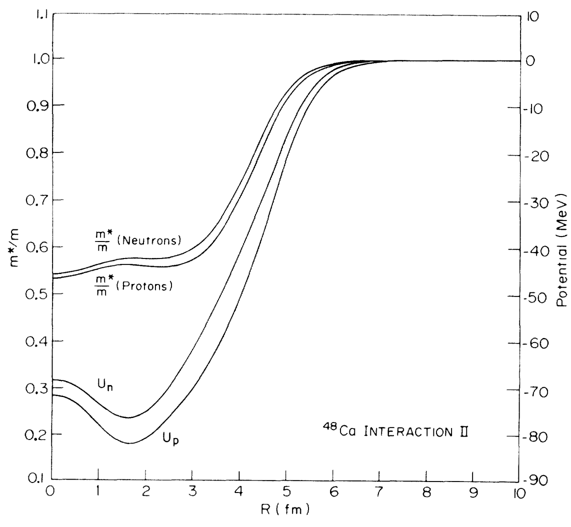

FIG. 12. Effective mass m^*/m and potential U calculated in ^{48}Ca with interaction II.

er, and probably more important effect through the tensor force,[24,29] should also alter this agreement. For instance, in Ref. 24 the spin-orbit splitting of the $1h$-neutron levels in ^{208}Pb due to the $\vec{L}\cdot\vec{S}$ force alone (5.88 MeV) is reduced by 1.49 MeV by the central force and by 2.79 MeV by the tensor force.

The spin-orbit splittings we obtain for the $1d$-levels decrease slightly from ^{40}Ca to ^{48}Ca by roughly the same amount for neutron and proton states. In the case of interaction I (II) this decrease is $\Delta n = 0.99$ MeV (0.82 MeV) for neutron states, while $\Delta p = 0.68$ MeV (0.58 MeV) for proton states. On the other hand, if the term (41) is included in perturbation theory, the situation becomes rather different for neutron and proton states. Indeed, in this case, the previous numbers are changed into $\Delta n = 1.91$ MeV (2.22 MeV) and $\Delta p = 0.61$ MeV (0.55 MeV) for interaction I (II). The origin of this difference can be readily understood by noticing that since calcium-40 is spin-saturated, $J_n(^{40}\text{Ca}) \simeq J_p(^{40}\text{Ca}) \simeq 0$; whereas, due to the presence of an $f_{7/2}$ spin-unsaturated neutron shell in calcium-48, $J_p(^{48}\text{Ca}) \simeq 0$, and $J_n(^{48}\text{Ca}) > 0$. The effect of the one-body spin-orbit potential (41) is therefore to decrease spin-orbit splittings of neutron states in calcium-48. Unfortunately experimental information on $1d_{5/2}$ levels is too scarce to allow any comparison with the previous numbers. Also, the tensor force would probably play a dominant role in the previous discussion.[29]

E. Superheavy Nuclei

Results of Hartree-Fock calculations with interaction I in the superheavy region have already been presented and discussed in Ref. 18. Therefore we will restrict ourselves here to a brief comparison of the results obtained with forces I and II for the superheavy element $^{298}114$, whose single-particle energies were given in Table IV. Even though interaction II gives a slightly better description of the properties of doubly-closed nuclei the results in both cases are very similar. Such a comparison is then very instructive as far as it indicates the sensitivity of the extrapolation to the superheavy region with respect to a small change in the two-body force. For interaction I a proton gap of 2.16 MeV is found at $Z = 114$, while at $N = 184$ the neutron gap turns out to be only 0.85 MeV. In the case of interaction II the proton gap at $Z = 114$ is 0.9 MeV, while at $N = 184$ the neutron gap is 1.5 MeV. This difference modifies slightly the conclusion we draw in Ref. 18, since in the latter case the proton gap at $Z = 114$ disappears, while a small neutron gap is obtained at $N = 184$.

This difference also shows that any small change in the fit to the properties of doubly-closed-shell nuclei becomes drastically amplified in the superheavy region. Since interaction II gives a better (and remarkable) fit to electron scattering data than interaction I, it is expected to give a better description of surface effects. Also, since it reproduces much more satisfactorily the deep proton levels of oxygen-16 and calcium-40, it should give a better description of the density dependence of the effective mass, i.e., of the nonlocality of the average nuclear field. These two remarks would make it worthwhile to perform a new calculation of the superheavy elements we investigated in Ref. 18. A part of this program has already been carried out by Flocard,[30] who made in particular a calculation of the nucleus $^{362}114$ with interaction II. His result indicates that our outstanding conclusion in Ref. 18, namely, the existence of a strong shell effect at $N = 228$, remains unchanged.

VIII. CONCLUSIONS

We have seen that the density dependence of Skyrme's interaction allows a remarkable description of ground-state properties of doubly-closed-shell nuclei. Over all, these results are even in better agreement with experiment than any Hartree-Fock calculations made with density-dependent effective forces derived from Brueckner's theory in the local-density approximation.[7,8] They show that Skyrme's interaction provides, with only five parameters, a very simple parametrization of the nuclear effective interaction, which already contains all the ingredients necessary to give a good description of the average nuclear field. The quality of the agreement we have obtained raises in fact the question of the existence of a relation between the parameters of Skyrme's interaction and those of more realistic forces, such as the G matrices of Refs. 7 and 8.

Another outstanding feature of Skyrme's interaction is the great simplicity of the calculations involved. In particular, from the algebraic relation between the average nuclear field and the densities we have been able to work out the physical significance of the parameters. Also, due to the minimal amount of numerical work necessary to solve the Hartree-Fock equations it becomes possible to carry out the systematic studies in the superheavy region we made in Ref. 18. Let us finally mention that the simple structure of the Hartree-Fock equations for Skyrme's force makes it possible to perform deformed calculations with a very large deformed-harmonic-oscillator basis, therefore allowing a study of heavy deformed nuclei in the Hartree-Fock approximation. Such calculations will be described in a forthcoming paper.

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APPENDIX A. HAMILTONIAN DENSITY FOR THE CENTRAL TERM

In all calculations we assume that the subspace of occupied states is invariant under time reversal. In other words we assume that if a single-particle state $|i\rangle$ is occupied, the time-reversed state $|\bar{i}\rangle = K|i\rangle$ is also occupied. Since the time-reversal operator in the case of a spin-$\frac{1}{2}$ particle can be written as $K = -i\sigma_y K_0$, where K_0 denotes the complex-conjugation operator associated with the space representation, the wave function of the time-reversed state is just

$$\begin{aligned}\phi_{\bar{i}}(\vec{r},\sigma,q) &= -i\sum_{\sigma'}\langle\sigma|\sigma_y|\sigma'\rangle\,\phi_i^*(\vec{r},\sigma',q)\\ &= -2\sigma\phi_i^*(\vec{r},-\sigma,q)\,.\end{aligned}\tag{A1}$$

Here $\vec{r}$ is the nucleon coordinate, σ $(=\pm\frac{1}{2})$ is the spin, and q is the isospin ($q = +\frac{1}{2}$ for a proton, $-\frac{1}{2}$ for a neutron). In what follows, the sum

$$\sum_i \phi_i^*(\vec{r},\sigma_1,q)\phi_i(\vec{r},\sigma_2,q)$$

will occur frequently in our calculations. From our assumption it is equal to

$$\tfrac{1}{2}\sum_i[\phi_i^*(\vec{r},\sigma_1,q)\phi_i(\vec{r},\sigma_2,q) + 4\sigma_1\sigma_2\phi_i(\vec{r},-\sigma_1,q)\phi_i^*(\vec{r},-\sigma_2,q)]\,.$$

If $\sigma_1 = -\sigma_2$ it vanishes identically; whereas, if $\sigma_1 = \sigma_2$ it is

$$\tfrac{1}{2}\sum_{i,\sigma}|\phi_i(\vec{r},\sigma,q)|^2 = \tfrac{1}{2}\rho_q(\vec{r})\,.$$

We have therefore

$$\sum_i \phi_i^*(\vec{r},\sigma_1,q)\phi_i(\vec{r},\sigma_2,q) = \tfrac{1}{2}\delta_{\sigma_1,\sigma_2}\,\rho_q(\vec{r})\,. \tag{A2}$$

Because of the fact that the trace of the Pauli spin matrices is zero, this equation implies that

$$\sum_{i,\sigma_1,\sigma_2}\phi_i^*(\vec{r},\sigma_1,q)\langle\sigma_1|\vec{\sigma}|\sigma_2\rangle\,\phi_i(\vec{r},\sigma_2,q) = 0\,,$$

which will be written in spinor notation as

$$\sum_i \phi_i^*(\vec{r})\vec{\sigma}\phi_i(\vec{r}) = 0\,, \tag{A3}$$

where $\phi_i(\vec{r})$ is a four-component spinor in the spin and isospin space.

The contribution V_0 to the potential energy arising from the term proportional to t_0 in the Skyrme interaction is

$$V_0 = \tfrac{1}{2}\sum_{ij}\langle ij|\,t_0\delta(\vec{r}_1-\vec{r}_2)(1+x_0P_\sigma)(1-P_MP_\sigma P_\tau)|ij\rangle\,. \tag{A4}$$

Using the fact that a δ force acts only in S waves, one can replace P_M by 1 in Eq. (A4). Also, we assume that there is no charge mixing of the Hartree-Fock states, so that the effect of the isospin-exchange operator is just to introduce a factor δ_{q_i,q_j}, where q_i denotes the charge of the single-particle state i. Since the spin-exchange operator is $P_\sigma = \frac{1}{2}(1+\vec{\sigma}_1\cdot\vec{\sigma}_2)$, V_0 can be written as

$$V_0 = \tfrac{1}{2}\sum_{ij}\langle ij|\,t_0\delta(\vec{r}_1-\vec{r}_2)[1-x_0\delta_{q_i,q_j}+\tfrac{1}{2}(1+\vec{\sigma}_1\cdot\vec{\sigma}_2)(x_0-\delta_{q_i,q_j})]|ij\rangle\,. \tag{A5}$$

Because of Eq. (A3), the terms containing Pauli matrices do not contribute and one is left finally with the following expression:

$$V_0 = \tfrac{1}{2}t_0\sum_{ij}\int d^3r\,[\phi_i^*(\vec{r})\phi_i(\vec{r})][\phi_j^*(\vec{r})\phi_j(\vec{r})][1+\tfrac{1}{2}x_0-\delta_{q_i,q_j}(x_0+\tfrac{1}{2})]\,, \tag{A6}$$

which means that the contribution to the energy density is

$$H_0 = \tfrac{1}{2}t_0[(1+\tfrac{1}{2}x_0)\rho^2-(x_0+\tfrac{1}{2})(\rho_n^2+\rho_p^2)]\,. \tag{A7}$$

For the term proportional to t_1, the contribution V_1 to the potential energy including the exchange term is

$$V_1 = -\tfrac{1}{16} t_1 \sum_{ij} \langle ij|\,\delta(\vec{r}_1-\vec{r}_2)(\nabla_1^2+\nabla_2^2-2\vec{\nabla}_1\cdot\vec{\nabla}_2)(1-\tfrac{1}{2}\delta_{q_i,q_j}-\tfrac{1}{2}\vec{\sigma}_1\cdot\vec{\sigma}_2\delta_{q_i,q_j})|ij\rangle + \text{H.c.}, \tag{A8}$$

where H.c. in Eq. (A8) denotes the Hermitian conjugate of the first term. Here again, the terms containing Pauli matrices will not contribute when combined with ∇_1^2 or ∇_2^2 because of Eq. (A3). The expression for V_1 therefore reduces to

$$V_1 = -\tfrac{1}{16} t_1 \sum_{ij} \langle ij|\,\delta(\vec{r}_1-\vec{r}_2)(\nabla_1^2+\nabla_2^2-2\vec{\nabla}_1\cdot\vec{\nabla}_2)|ij\rangle(1-\tfrac{1}{2}\delta_{q_i,q_j}) - \tfrac{1}{16} t_1 \sum_{ij} \langle ij|\,\delta(\vec{r}_1-\vec{r}_2)(\vec{\nabla}_1\cdot\vec{\nabla}_2)(\vec{\sigma}_1\cdot\vec{\sigma}_2)|ij\rangle\,\delta_{q_i,q_j} + \text{H.c.} \tag{A9}$$

The first term in Eq. (A9) can be easily evaluated by using Eq. (28) and noting that, owing to time-reversal invariance

$$\sum_i \phi_i^*(\vec{r})\vec{\nabla}\varphi_i(\vec{r}) = \tfrac{1}{2}\sum_{i,\sigma,q}[\phi_i^*(\vec{r},\sigma,q)\vec{\nabla}\phi_i(\vec{r},\sigma,q)+\phi_i(\vec{r},-\sigma,q)\nabla\phi_i^*(\vec{r},-\sigma,q)] = \tfrac{1}{2}\vec{\nabla}\rho\,. \tag{A10}$$

The result is given by the following expression:

$$-\tfrac{1}{16} t_1 \int d^3r\{\rho\nabla^2\rho - 2\tau - \tfrac{1}{2}(\vec{\nabla}\rho)^2 - \tfrac{1}{2}\sum_q[\rho_q\nabla^2\rho_q - 2\tau_q - \tfrac{1}{2}(\nabla\rho_q)^2]\}. \tag{A11}$$

Integrating by parts, expression (A11) finally reduces to

$$\tfrac{1}{16} t_1 \int d^3r(2\rho\tau - \rho_n\tau_n - \rho_p\tau_p - \tfrac{3}{2}\rho\nabla^2\rho + \tfrac{3}{4}\rho_n\nabla^2\rho_n + \tfrac{3}{4}\rho_p\nabla^2\rho_p). \tag{A12}$$

To evaluate the second term in Eq. (A9) we use the identity[31]

$$(\vec{\nabla}_1\cdot\vec{\nabla}_2)(\vec{\sigma}_1\cdot\vec{\sigma}_2) = \tfrac{1}{3}(\vec{\nabla}_1\cdot\vec{\sigma}_1)(\vec{\nabla}_2\cdot\vec{\sigma}_2) + \tfrac{1}{2}(\vec{\nabla}_1\times\vec{\sigma}_1)\cdot(\vec{\nabla}_2\times\vec{\sigma}_2) + (\vec{\nabla}_1\times\vec{\sigma}_1)^{(2)}\cdot(\vec{\nabla}_2\times\vec{\sigma}_2)^{(2)}. \tag{A13}$$

Assuming axial symmetry in addition to time-reversal invariance, one can see, by writing explicitly the dependence of the wave functions on the azimuthal variable, that the quantities $\sum_i\phi_i^*(\vec{r})(\vec{\nabla}\cdot\vec{\sigma})\phi_i(\vec{r})$ and $\sum_i\phi_i^*(\vec{r})(\vec{\nabla}\times\vec{\sigma})^{(2)}\phi_i(\vec{r})$ vanish identically. The second term in Eq. (A9) therefore reduces to

$$-\tfrac{1}{32} t_1 \sum_{ij}\langle ij|\,\delta(\vec{r}_1-\vec{r}_2)(\vec{\nabla}_1\cdot\vec{\sigma}_1)(\vec{\nabla}_2\cdot\vec{\sigma}_2)|ij\rangle\,\delta_{q_i,q_j} = \tfrac{1}{32} t_1 \int d^3r[\vec{J}_n^{\,2}(\vec{r}) + \vec{J}_p^{\,2}(\vec{r})]. \tag{A14}$$

Collecting all the previous terms and adding their Hermitian conjugates, one obtains the result that the contribution H_1 to the energy density is given by

$$H_1 = \tfrac{1}{16} t_1(4\rho\tau - 2\rho_n\tau_n - 2\rho_p\tau_p - 3\rho\nabla^2\rho + \tfrac{3}{2}\rho_n\nabla^2\rho_n + \tfrac{3}{2}\rho_p\nabla^2\rho_p + \vec{J}_n^{\,2} + \vec{J}_p^{\,2}). \tag{A15}$$

The calculation of the contribution V_2 to the potential energy arising from the t_2 term is very similar. The only difference is that since this term acts in P waves, the Majorana exchange operator P_M has to be replaced by -1 in evaluating the exchange term. Using an obvious symmetry between the indices 1 and 2 one gets

$$V_2 = \tfrac{1}{4} t_2 \sum_{ij}\langle ij|[\vec{\nabla}_1'\cdot\delta(\vec{r}_1-\vec{r}_2)\vec{\nabla}_1 - \vec{\nabla}_2'\cdot\delta(\vec{r}_1-\vec{r}_2)\vec{\nabla}_1](1-P_MP_\sigma P_\tau)|ij\rangle, \tag{A16}$$

where the primes indicate that the gradient operator is acting on the left. Carrying out an integration by part this expression becomes

$$V_2 = \tfrac{1}{4} t_2 \sum_{ij}\langle ij|[2\vec{\nabla}_1'\cdot\delta(\vec{r}_1-\vec{r}_2)\vec{\nabla}_1 + \delta(\vec{r}_1-\vec{r}_2)(\nabla_1^2+\vec{\nabla}_1\cdot\vec{\nabla}_2)](1+P_\sigma\delta_{q_i,q_j})|ij\rangle. \tag{A17}$$

Replacing P_σ by $\frac{1}{2}(1+\vec{\sigma}_1\cdot\vec{\sigma}_2)$ the $\vec{\sigma}_1\cdot\vec{\sigma}_2$ term will contribute only when combined with $\vec{\nabla}_1\cdot\vec{\nabla}_2$ because of Eq. (A3). Thus,

$$\begin{aligned} V_2 = {} & \tfrac{1}{4} t_2 \sum_{ij}\langle ij|[2\vec{\nabla}_1'\cdot\delta(\vec{r}_1-\vec{r}_2)\vec{\nabla}_1 + \delta(\vec{r}_1-\vec{r}_2)(\nabla_1^2+\vec{\nabla}_1\cdot\vec{\nabla}_2)]\,|ij\rangle(1+\tfrac{1}{2}\delta_{q_i,q_j}) \\ & + \tfrac{1}{8} t_2 \sum_{ij}\langle ij|\,\delta(\vec{r}_1-\vec{r}_2)(\vec{\nabla}_1\cdot\vec{\nabla}_2)(\vec{\sigma}_1\cdot\vec{\sigma}_2)|ij\rangle\,\delta_{q_i,q_j}. \end{aligned} \tag{A18}$$

Using Eqs. (28), (A10), and the result (A14) for the second term yields, after an integration by parts of

$(\vec{\nabla}\rho)^2$, the following expression for the contribution H_2 to the potential-energy density:

$$H_2=\tfrac{1}{16}t_2(4\rho\tau+2\rho_n\tau_n+2\rho_p\tau_p+\rho\nabla^2\rho+\tfrac{1}{2}\rho_n\nabla^2\rho_n+\tfrac{1}{2}\rho_p\nabla^2\rho_p-\vec{J}_n^{\,2}-\vec{J}_p^{\,2})\,. \tag{A19}$$

The evaluation of the contribution to the potential energy coming from the three-body force

$$V_3=\tfrac{1}{6}\sum_{ijk}\langle ijk|\tilde{v}_{123}|ijk\rangle \tag{A20}$$

is also straightforward. In the previous expression there are five exchange terms, which can be included formally by means of exchange operators. Because of the presence of two δ functions in the three-body force, the Majorana exchange operator acting on any pair of particles can be replaced by 1. Thus, all the exchange terms in Eq. (A20) can be included by writing

$$\begin{aligned}\tilde{v}_{123}=t_3\delta(\vec{r}_1-\vec{r}_2)\delta(\vec{r}_2-\vec{r}_3)[1&+P_\sigma(12)P_\sigma(23)P_\tau(12)P_\tau(23)\\&+P_\sigma(13)P_\sigma(23)P_\tau(13)P_\tau(23)-P_\sigma(12)P_\tau(12)-P_\sigma(23)P_\tau(23)-P_\sigma(31)P_\tau(31)]\,.\end{aligned} \tag{A21}$$

By relabeling the indices in Eq. (A20) one can see that the second and third terms in Eq. (A21) give the same contribution to the potential energy, and that the same holds for the last three terms. Expression (A21) can then be written as

$$\tilde{v}_{123}=t_3\delta(\vec{r}_1-\vec{r}_2)\delta(\vec{r}_2-\vec{r}_3)[1+2P_\sigma(12)P_\sigma(23)P_\tau(12)P_\tau(23)-3P_\sigma(12)P_\tau(12)]\,. \tag{A22}$$

Substituting the expression of the spin-exchange operators in terms of Pauli matrices, one gets

$$\tilde{v}_{123}=t_3\delta(\vec{r}_1-\vec{r}_2)\delta(\vec{r}_2-\vec{r}_3)[1+\tfrac{1}{2}P_\tau(12)P_\tau(23)-\tfrac{3}{2}P_\tau(12)]\,, \tag{A23}$$

since, because of Eq. (A3), terms containing $\vec{\sigma}$ matrices do not contribute to the energy. Equation (A23) immediately gives the following expression for V_3:

$$V_3=\tfrac{1}{6}t_3\sum_{ijk}\int d^3r(\phi_i^*\phi_i)(\phi_j^*\phi_j)(\phi_k^*\phi_k)(1+\tfrac{1}{2}\delta_{q_i,q_j}\delta_{q_j,q_k}-\tfrac{3}{2}\delta_{q_i,q_j})\,. \tag{A24}$$

The contribution of the three-body force to the energy density is therefore

$$H_3=\tfrac{1}{6}t_3[\rho^3+\tfrac{1}{2}(\rho_n^{\,3}+\rho_p^{\,3})-\tfrac{3}{2}\rho(\rho_n^{\,2}+\rho_p^{\,2})]=\tfrac{1}{4}t_3\rho_n(\vec{r})\rho_p(\vec{r})\rho(\vec{r})\,. \tag{A25}$$

Collecting all the previous expressions for H_0, H_1, H_2, H_3 [Eqs. (A7), (A15), (A19), (A25)] one gets the following result for the Hamiltonian density:

$$\begin{aligned}H(\vec{r})=\tfrac{1}{2}t_0[(1+\tfrac{1}{2}x_0)\rho^2-(x_0+\tfrac{1}{2})(\rho_n^{\,2}+\rho_p^{\,2})]&+\tfrac{1}{4}(t_1+t_2)\rho\tau+\tfrac{1}{8}(t_2-t_1)(\rho_n\tau_n+\rho_p\tau_p)+\tfrac{1}{16}(t_2-3t_1)\rho\nabla^2\rho\\&+\tfrac{1}{32}(3t_1+t_2)(\rho_n\nabla^2\rho_n+\rho_p\nabla^2\rho_p)+\tfrac{1}{16}(t_1-t_2)(\vec{J}_n^{\,2}+\vec{J}_p^{\,2})+\tfrac{1}{4}t_3\rho_n\rho_p\rho\,.\end{aligned} \tag{A26}$$

Before closing this section we will prove that the Lagrange multipliers e_i defined in Eq. (19) are equal to the single-particle removal energies $\tilde{e}_i$, provided that the single-particle wave functions of the A and $A-1$ systems are identical. For this purpose we consider a system of $A-1$ particles obtained by creating a hole in the single-particle state i. The binding-energy difference is

$$\begin{aligned}\tilde{e}_i&=E(A)-E_i(A-1)\\&=\left\langle i\left|\frac{p^2}{2m}\right|i\right\rangle+\sum_{j=1}^{A}\langle ij|\tilde{v}_{12}|ij\rangle+\tfrac{1}{2}\sum_{j,k=1}^{A}\langle ijk|\tilde{v}_{123}|ijk\rangle\,.\end{aligned} \tag{A27}$$

Since the equivalence between e_i and $\tilde{e}_i$ is known to hold for the one- and two-body terms, it is sufficient to check it for the three-body term

$$\tilde{e}_i(3)=\tfrac{1}{2}\sum_{j,k=1}^{A}\langle ijk|\tilde{v}_{123}|ijk\rangle\,. \tag{A28}$$

In Eq. (A21) for $\tilde{v}_{123}$ one can see that the second and third terms will give the same contribution to the removal energy, and that the same is true for the fourth and sixth terms. Here also, because of Eq. (A3), the spin-exchange operators can be replaced by a factor $\frac{1}{2}$. Thus,

$$\tilde{e}_i(3)=\tfrac{1}{2}t_3\sum_{j,k=1}^{A}\langle ijk|\,\delta(\vec{r}_1-\vec{r}_2)\delta(\vec{r}_2-\vec{r}_3)|ijk\rangle(1+\tfrac{1}{2}\delta_{q_i,q_j}\delta_{q_j,q_k}-\delta_{q_i,q_j}-\tfrac{1}{2}\delta_{q_j,q_k})\,. \tag{A29}$$

Using the definition (11) for the density, one gets

$$\tilde{e}_i(3)=\tfrac{1}{2}t_3\int d^3r(\phi_i^*\phi_i)(\rho^2+\tfrac{1}{2}\rho_{q_i}{}^2-\rho_{q_i}\rho-\tfrac{1}{2}\rho_n{}^2-\tfrac{1}{2}\rho_p{}^2)=\tfrac{1}{4}t_3\int d^3r(\phi_i^*\phi_i)(\rho^2-\rho_{q_i}{}^2). \tag{A30}$$

Since the contribution of the three-body force to the average nuclear field is $\frac{1}{4}t_3(\rho^2-\rho_{q_i}{}^2)$, Eq. (A30) shows that $e_i(3)=\tilde{e}_i(3)$.

APPENDIX B. HAMILTONIAN DENSITY FOR THE SPIN-ORBIT FORCE

The two-body spin-orbit interaction we use can be written as

$$V_{LS}=\tfrac{1}{4}iW_0(\vec{\sigma}_1+\vec{\sigma}_2)\cdot[(\vec{\nabla}_1'-\vec{\nabla}_2')\times\delta(\vec{r}_1-\vec{r}_2)(\vec{\nabla}_1-\vec{\nabla}_2)], \tag{B1}$$

where the primes indicate that the corresponding gradient operators have to act on the left. This force acts in triplet-P states only and therefore in calculating the exchange contribution to the binding energy one can replace the Majorana exchange operator by −1 and the spin-exchange operator by 1. The contribution E_{so} of the two-body spin-orbit force to the potential energy is thus

$$\begin{aligned}E_{so}&=\tfrac{1}{2}\sum_{ij}\langle ij|V_{LS}(1-P_MP_\sigma P_\tau)|ij\rangle\\&=\tfrac{1}{2}\sum_{ij}\langle ij|V_{LS}|ij\rangle(1+\delta_{q_iq_j}).\end{aligned} \tag{B2}$$

Expanding expression (B1) gives a sum of eight terms. However, when calculating the potential energy (B2), one can use an obvious symmetry between the indices 1 and 2 and write

$$V_{LS}=\tfrac{1}{2}iW_0[(\vec{\nabla}_1'\times\vec{\nabla}_1)\cdot\vec{\sigma}_2+\vec{\nabla}_1'\cdot(\vec{\nabla}_1\times\vec{\sigma}_1)-(\vec{\nabla}_1'\times\vec{\nabla}_2)\cdot\vec{\sigma}_1-\vec{\nabla}_2'\cdot(\vec{\nabla}_1\times\vec{\sigma}_1)]. \tag{B3}$$

In Eq. (B3), for more simplicity, we have not written the δ functions explicitly. The first term in Eq. (B3) will not contribute, because of Eq. (A3). Also, carrying out an integration by parts in Eq. (B2), one can replace the term $-(\vec{\nabla}_1'\times\vec{\nabla}_2)\cdot\vec{\sigma}_1$ in expression (B3) by

$$(\vec{\nabla}_2'\times\vec{\nabla}_2)\cdot\vec{\sigma}_1+(\vec{\nabla}_1\times\vec{\nabla}_2)\cdot\vec{\sigma}_1+(\vec{\nabla}_2\times\vec{\nabla}_2)\cdot\vec{\sigma}_1. \tag{B4}$$

Here again, because of Eq. (A3), the only nonzero contribution will be obtained from the second term and expression (B4) therefore reduces to $-\vec{\nabla}_2\cdot(\vec{\nabla}_1\times\vec{\sigma}_1)$. Because of time-reversal invariance this result is also equivalent to $-\vec{\nabla}_2'\cdot(\vec{\nabla}_1\times\vec{\sigma}_1)$. In a similar way one can also show that the term $\vec{\nabla}_1'\cdot(\vec{\nabla}_1\times\vec{\sigma}_1)$ can be replaced by $-2\vec{\nabla}_2\cdot(\vec{\nabla}_1\times\vec{\sigma}_1)$, so that the expression for V_{LS} finally reduces to

$$V_{LS}=-2iW_0\vec{\nabla}_2\cdot\delta(\vec{r}_1-\vec{r}_2)(\vec{\nabla}_1\times\vec{\sigma}_1), \tag{B5}$$

when calculating the potential energy. Inserting this value into Eq. (B2) yields the following expression for E_{so}:

$$E_{so}=-iW_0\sum_{jk}\int d^3r[\phi_j^*(\vec{\nabla}\times\vec{\sigma})\phi_j]\cdot(\phi_k^*\vec{\nabla}\phi_k)(1+\delta_{q_jq_k}). \tag{B6}$$

Using Eq. (A10) and the definition (11) of the spin density, this last equation becomes

$$E_{so}=\tfrac{1}{2}W_0\int d^3r(\vec{\nabla}\rho\cdot\vec{J}+\vec{\nabla}\rho_n\cdot\vec{J}_n+\vec{\nabla}\rho_p\cdot\vec{J}_p). \tag{B7}$$

Integrating by parts, this gives the following expression for the Hamiltonian density H_{so} arising from the two-body spin-orbit force:

$$H_{so}=-\tfrac{1}{2}W_0(\rho\vec{\nabla}\cdot\vec{J}+\rho_n\vec{\nabla}\cdot\vec{J}_n+\rho_p\vec{\nabla}\cdot\vec{J}_p). \tag{B8}$$

APPENDIX C. APPLICATION OF THE VARIATIONAL PRINCIPLE

From Eqs. (A26) and (B8) the binding-energy difference

$$\delta E=E(\phi_i+\delta\phi_i)-E(\phi_i) \tag{C1}$$

can be written, after integration by parts, as

$$\delta E=\sum_{q=(n,p)}\int d^3r\left[\frac{\hbar^2}{2m_q^*}\delta\tau_q(\vec{r})+U_q(\vec{r})\delta\rho_q(\vec{r})+\vec{W}_q(\vec{r})\cdot\delta\vec{J}_q(\vec{r})\right]. \tag{C2}$$

In the case of neutrons, the coefficients of the variations in Eq. (C2) are given by

$$\frac{\hbar^2}{2m_n^*(\vec{r})}=\frac{\hbar^2}{2m}+\tfrac{1}{4}(t_1+t_2)\rho(\vec{r})+\tfrac{1}{8}(t_2-t_1)\rho_n(\vec{r}), \tag{C3}$$

$$\begin{aligned}U_n(\vec{r})&=t_0[(1+\tfrac{1}{2}x_0)\rho-(x_0+\tfrac{1}{2})\rho_n]-\tfrac{1}{8}(3t_1-t_2)\nabla^2\rho+\tfrac{1}{16}(3t_1+t_2)\nabla^2\rho_n\\&\quad+\tfrac{1}{4}(t_1+t_2)\tau+\tfrac{1}{8}(t_2-t_1)\tau_n+\tfrac{1}{4}t_3\rho_p(\rho+\rho_n)-\tfrac{1}{2}W_0(\vec{\nabla}\cdot\vec{J}+\vec{\nabla}\cdot\vec{J}_n),\\ \vec{W}_n(\vec{r})&=\tfrac{1}{2}W_0(\vec{\nabla}\rho+\vec{\nabla}\rho_n)+\tfrac{1}{8}(t_1-t_2)\vec{J}_n.\end{aligned} \tag{C4}$$

The corresponding formulas for protons are obtained from the previous ones by interchanging the indices n and p. Since we require time-reversal invariance, we will allow only variations such that $\delta\phi_{\bar{i}}(r,\sigma,q)=-2\sigma\delta\phi_i^*(r,-\sigma,q)$. In such case the expressions for the variations of the densities can be reduced to

$$\begin{aligned}\delta\rho_q(\vec{r})&=2\sum_{i,\sigma}\delta\phi_i^*(\vec{r},\sigma,q)\phi_i(\vec{r},\sigma,q),\\ \delta\tau_q(\vec{r})&=2\sum_{i,\sigma}[\vec{\nabla}\delta\phi_i^*(\vec{r},\sigma,q)]\cdot\vec{\nabla}\phi_i(\vec{r},\sigma,q),\\ \delta\vec{J}_q(\vec{r})&=-2i\sum_{i,\sigma_1,\sigma_2}\delta\phi_i^*(\vec{r},\sigma_1,q)\vec{\nabla}\phi_i(\vec{r},\sigma_2,q)\times\langle\sigma_1|\vec{\sigma}|\sigma_2\rangle.\end{aligned} \tag{C5}$$

Inserting these expressions into Eq. (C2) and integrating the $\delta\tau$ term by parts yields the following result for the binding-energy difference:

$$\delta E=2\sum_{i=1}^{A}\int d^3r\,\delta\phi_i^*(\vec{r})\Big\}-\vec{\nabla}\cdot\left(\frac{\hbar^2}{2m_{q_i}^*}\vec{\nabla}\phi_i\right)+[U_{q_i}+\vec{W}_{q_i}\cdot(-i)(\vec{\nabla}\times\vec{\sigma})]\,\phi_i\Big\{, \tag{C6}$$

where we have used the spinor notation for more simplicity. The condition that the total energy be stationary,

$$\delta\left[E-\sum_i e_i\int d^3r\,\phi_i^*(\vec{r})\phi_i(\vec{r})\right]=0, \tag{C7}$$

therefore requires that

$$-\vec{\nabla}\cdot\left(\frac{\hbar^2}{2m_{q_i}^*}\vec{\nabla}\phi_i\right)+[U_{q_i}(\vec{r})+\vec{W}_{q_i}\cdot(-i)(\vec{\nabla}\times\vec{\sigma})]\phi_i=e_i\phi_i. \tag{C8}$$

APPENDIX D. EVALUATION OF THE SPIN DENSITY FOR SPHERICAL NUCLEI

The evaluation of the spin density for spherical nuclei can be simplified by noticing that, in using the relation

$$\vec{\nabla}f(r)Y_{lm}(\Omega)=\frac{\vec{r}}{r}\frac{\partial f}{\partial r}Y_{lm}(\Omega)+f(r)\vec{\nabla}Y_{lm}(\Omega), \tag{D1}$$

the contribution of the first term vanishes, since it is proportional to the radial derivative of the left-hand side of Eq. (A3). Using the notation of Sec. IV, one is therefore left with the following expression for $\vec{J}$:

$$\vec{J}(\vec{r})=(-i)\sum_\alpha\frac{R_\alpha^2(r)}{r^2}\sum_{m_l m_l'}\sum_{m m_s m_s'}\langle l\tfrac{1}{2}m_l m_s|jm\rangle\langle l\tfrac{1}{2}m_l'm_s'|jm\rangle Y_{lm_l}^*(\Omega)[\vec{\nabla}Y_{lm_l'}(\Omega)]\times\langle m_s|\vec{\sigma}|m_s'\rangle. \tag{D2}$$

In the orthonormal basis $\{\vec{e}_\mu\}$ defined as

$$\vec{e}_0=\vec{e}_z,\quad \vec{e}\pm1=\mp\frac{1}{\sqrt{2}}(\vec{e}_x\pm i\vec{e}_y), \tag{D3}$$

the components of the outer product of two vectors $\vec{A}$ and $\vec{B}$ are

$$(\vec{A}\times\vec{B})_\mu=-i\sqrt{2}\sum_{\mu_1\mu_2}\langle 11\mu_1\mu_2|1\mu\rangle A_{\mu_1}B_{\mu_2}. \tag{D4}$$

Using Wigner-Eckart's theorem and carrying out the sum over the indices m, m_s, m_s' by means of standard formulas for 3-j symbols[32] yields the following result for the components of the spin density:

$$J_\mu(\vec{r})=6\sum_\alpha(2j_\alpha+1)\frac{R_\alpha{}^2(r)}{r^2}\sum_{m_l m_l'}\sum_{\mu_1\mu_2}(-1)^{j-1/2+\mu+m_l'}\begin{pmatrix}1 & 1 & 1\\ \mu_1 & \mu_2 & -\mu\end{pmatrix}\begin{pmatrix}l & l & 1\\ m_l & -m_l' & \mu_2\end{pmatrix}\begin{Bmatrix}l & l & 1\\ \frac{1}{2} & \frac{1}{2} & j\end{Bmatrix}Y^*_{l m_l}(\Omega)\nabla_{\mu_1}Y_{l m_l'}(\Omega)\,. \tag{D5}$$

The components of the gradient operator acting on a spherical harmonic can be obtained from the so-called gradient formula,[31] which gives

$$\nabla_{\mu_1}Y_{l m_l'}(\Omega)=\sum_{LM}f(l,L)\langle l1m_l'\mu_1|LM\rangle Y_{LM}(\Omega)\,, \tag{D6}$$

where the function $f(l,L)$ is $-l[(l+1)/(2l+3)]^{1/2}$ if $L=l+1$, $-(l+1)[l/(2l-1)]^{1/2}$ if $L=l-1$, and 0 otherwise. Inserting expression (D6) into Eq. (D5), one can carry out, again by means of the same relation for 3-j symbols,[32] the sum over the indices μ_1, μ_2, and m_l'. The result is

$$J_\mu(\vec{r})=6\sum_\alpha(2j_\alpha+1)\frac{R_\alpha{}^2(r)}{r^3}\sum_L\sum_{Mm_l}(-1)^{j+1/2+M}(2L+1)^{1/2}f(l,L)\begin{Bmatrix}l & l & 1\\ \frac{1}{2} & \frac{1}{2} & j\end{Bmatrix}\begin{Bmatrix}L & l & 1\\ 1 & 1 & l\end{Bmatrix}\begin{pmatrix}L & l & 1\\ M & -m_l & -\mu\end{pmatrix}Y^*_{l m_l}(\Omega)Y_{LM}(\Omega)\,. \tag{D7}$$

Finally, one can recouple in Eq. (D7) the product of the two spherical harmonics by summing over the indices m_l and M, so that the components of $\vec{J}$ can be expressed as

$$J_\mu(\vec{r})=2\sqrt{3}\sum_\alpha(2j_\alpha+1)\frac{R_\alpha{}^2(r)}{r^3}\sum_L(-1)^{j+1/2}(2L+1)\left(\frac{2l+1}{4\pi}\right)^{1/2}f(l,L)\begin{Bmatrix}l & l & 1\\ \frac{1}{2} & \frac{1}{2} & j\end{Bmatrix}\begin{Bmatrix}L & l & 1\\ 1 & 1 & l\end{Bmatrix}\begin{pmatrix}l & L & 1\\ 0 & 0 & 0\end{pmatrix}Y_{1\mu}(\Omega)\,. \tag{D8}$$

Since the components of $\vec{r}/r$ in the basis $\{\vec{e}_\mu\}$ are $(\frac{4}{3}\pi)^{1/2}Y_{1\mu}(\Omega)$, Eq. (D8) shows that the spin density $\vec{J}$ for a doubly-closed-shell nucleus is proportional to $\vec{r}$. Furthermore, using the explicit values of the 3-j and 6-j symbols allows one to carry out the sum over L

$$\sum_L(2L+1)f(l,L)\begin{Bmatrix}L & l & 1\\ 1 & 1 & l\end{Bmatrix}\begin{pmatrix}l & L & 1\\ 0 & 0 & 0\end{pmatrix}=\frac{1}{\sqrt{6}}(-1)^l[l(l+1)]^{1/2}\,. \tag{D9}$$

The final result is

$$\vec{J}(\vec{r})=\frac{\vec{r}}{4\pi r^4}\sum_\alpha(2j_\alpha+1)[j_\alpha(j_\alpha+1)-l_\alpha(l_\alpha+1)-\tfrac{3}{4}]R_\alpha{}^2(r)\,. \tag{D10}$$

APPENDIX E. NUMERICAL SOLUTION OF THE RADIAL SCHRÖDINGER EQUATION

For more convenience we will write the radial Schrödinger Eq. (35) in the form

$$R''(r)=\alpha(r,E)R(r)+\beta(r)R'(r)\,. \tag{E1}$$

For a given energy E we denote by $R_i(r)$ the solution of Eq. (E1) such that $R_i(0)=0$, and $R_o(r)$ the solution of Eq. (E1) satisfying $R_o(\infty)=0$. For a given matching radius ρ we also define the logarithmic derivatives

$$L_i(E,\rho)=\frac{R_i'(\rho)}{R_i(\rho)}\,,\quad L_o(E,\rho)=\frac{R_o'(\rho)}{R_o(\rho)}\,. \tag{E2}$$

In this notation the eigenvalue E we are looking for is a solution of the equation

$$F(E)=L_o(E,\rho)-L_i(E,\rho)=0\,. \tag{E3}$$

In our calculation the solution of Eq. (E3) has been obtained by the Newton-Raphson method; i.e., starting from a first approximation E_0 to the exact eigenvalue E, we have calculated a new approximation E_1

$$E_1=E_0-\frac{F(E_0)}{F'(E_0)}\,, \tag{E4}$$

and so on until convergence was reached. The calculation of $F'(E_0)$ can be carried out by considering two neighboring values of the energy. Another way is to use the differential Eq. (E1) as follows. Let us consider, for a given solution $R(r)$ corresponding to an energy-independent boundary condition, the function

$$f(r)=R^2(r)\frac{\partial L(E,r)}{\partial E}=R\frac{\partial R'}{\partial E}-R'\frac{\partial R}{\partial E}\,. \tag{E5}$$

Using the differential Eq. (E1), one finds that $f(r)$ has to satisfy the differential equation

$$f'(r)=R^2(r)\frac{\partial\alpha(r,E)}{\partial E}+\beta(r)f(r)\,. \tag{E6}$$

Noticing that

$$\beta(r) = -\frac{\partial}{\partial r}\ln\left[\frac{\hbar^2}{2m^*(r)}\right], \quad \frac{\partial\alpha(r,E)}{\partial E} = -\frac{2m^*(r)}{\hbar^2},$$

one can write the general solution of Eq. (E6) as

$$f(r) = -\frac{2m^*(r)}{\hbar^2}\left[\int_0^r R^2(\xi)d\xi + C\right], \tag{E7}$$

where C is a constant. Applying this relation to the solutions $R_i(r)$ and $R_o(r)$ we find that

$$F'(E) = \frac{2m^*(\rho)}{\hbar^2 R_o{}^2(\rho)}\int_\mu^\infty R_o{}^2(r)dr + \frac{2m^*(\rho)}{\hbar^2 R_i{}^2(\rho)}\int_0^\rho R_i{}^2(r)dr. \tag{E8}$$

In practice we have proceeded as follows. Starting from a first approximation E_0 to the eigenvalue E, Eq. (E1) was integrated outwards from 0 to some matching radius ρ by the Runge-Kutta method to obtain $R_i(r)$, and then from 25 fm to ρ inwards to get $R_o(r)$. A new approximation E_1 to E was next calculated by means of Eqs. (E4) and (E8), and so on. We have not investigated the problem of adjusting the matching radius to get the best rate of convergence. We have rather choosen ρ, as in the usual case of a local Schrödinger equation, to be the last extremum of the radial wave function, therefore varying it from iteration to iteration.

For an improper choice of E_0 the previous iteration procedure may converge to a solution with the undesired number of nodes. To avoid such solutions a simple and efficient prescription[33] is to multiply the initial guess for E at each step of the iteration procedure by a factor of 0.9 if the number of nodes is too small, and by 1.2 if the number of nodes is too large.

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