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Triaxial Hartree-Fock-Bogolyubov calculations with $D1$ effective interaction

M. Girod
Service de Physique Neutronique et Nucléaire, Centre d'Etudes de Bruyères-le-Châtel, 92542 Montrouge Cedex, France

B. Grammaticos*
Service de Physique Théorique, Centre de Recherches Nucléaires, 67037 Strasbourg, France
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The Hartree-Fock and Hartree-Fock-Bogolyubov methods are used for the description of nuclei with triaxial (i.e., ellipsoidal) shapes. The Gogny $D1$ finite range density dependent interaction is employed. A comparison between various prescriptions for the calculation of pairing correlations in nuclei indicates the necessity for the self-consistent treatment of pairing. Using this last method we obtain results concerning nuclear shapes and deformation energy surfaces for nuclei ranging from the lightest ones to the fission barrier of ^{240}Pu.

[NUCLEAR STRUCTURE Density-dependent Hartree-Fock-Bogolyubov approximation applied to the description of nuclei with triaxial shapes: pairing correlation, comparison HFB-HFBCS, potential energy surface, density distributions.]

I. INTRODUCTION

The Hartree-Fock (HF) method has met with a great success, this last decade, in the description of the structure of the nucleus. This can be mainly attributed to the use of density dependent interactions which has made possible simultaneously a satisfactory description of nuclear binding energies, sizes, and also detailed level structure. The two main components of this approach are the following. First, an assumption is made that the many-body wave function of the nucleus is a single Slater determinant. This, of course, amounts to neglecting all correlations due to the nuclear interactions, localizing the center of mass position as well as the orientation of the (deformed) nucleus, while fixing the deformation of a soft nucleus to the ground state one. This approximation can nevertheless be adequate in certain cases, especially for closed-shell or light $N=Z$ nuclei. The second assumption is related to the effective interaction. In most modern Hartree-Fock calculations the interaction used has been a variant of the Skyrme force.[1] The technical advantages of this zero range velocity dependent interaction have made possible the use of large oscillator bases, necessary for the precise description of the single particle orbitals, or even the solution of HF equations in configuration space, as the HF Hamiltonian for the Skyrme interaction is a local one. On a more fundamental level this interaction presents the advantage of having been derived[2] (or rather *a posteriori* justified) through a short range (on nonlocality) expansion of the one-body density matrix. However, due to its specific form, the Skyrme interaction does not exhibit good pairing properties, which are of crucial importance when it comes to describing nonmagic, $N\neq Z$ nuclei.

The Hartree-Fock-Bogolyubov approach, first substantiated by the work of Gogny,[3] was the natural extension of the HF approach as it allows a correct description of the pairing correlations in nuclei. This was made possible by the determination, by Gogny, of the effective interaction $D1$ with good pairing properties,[4] together with the separation method[5] which makes feasible the computation of matrix elements in an oscillator basis, with speed competitive to the ones achieved by the Skyrme interaction. Moreover, although the $D1$ interaction is purely phenomenological, it exhibits a more realistic behavior than the more fundamentally derived Skyrme force, as it closely follows the behavior of realistic g matrices on each particular S-T subspace in nuclear matter. Results obtained with the Gogny $D1$ interaction have been presented in previous publications concerning spherical nuclei,[6] giant resonances on magic nuclei,[7] charge and matter densities of the latter,[8] axially deformed nuclei,[9] and two center calculations of extremely deformed systems.[10]

In this paper we will focus our attention on the triaxial degree of freedom in nuclei. The importance of the inclusion of the ellipsoidal degree in studies of the nuclear shapes is well established. First of all, some nuclei indeed present a departure from the axial symmetry in their ground state.[11] Also, in a nucleus with an axial ground state, there might exist a low lying triaxial isomer state.[12] In some cases a saddle-point deformation, as a fission barrier,[10] can be triaxial. Next, a fact already known from the Jacobi instability of a rotating liquid drop, a nucleus can adopt a triaxial shape when it is cranked to high angular momenta.[13] But the triaxiality has a still greater impact on the dynamics of the nucleus. In the low frequency regime the importance of the γ degree on the quadrupole motion of the nucleus has been demonstrated in the works of Kumar and Baranger.[14] In the giant resonance regime the nonaxial vibration is the source of (experimentally observed) splitting of the giant quadrupole resonance.[15] Moreover, the nonaxial component is the one which incorporates the largest part of the energy weighted quadrupole sum rule.[16] Finally, in a different domain, the triaxial degree of freedom has been found to be of the utmost importance for the correct description of heavy-ion fusion[17] in the framework of the time dependent Hartree-Fock method. In this work we will limit ourselves to a study of the static aspect only of the triaxiality in nuclei. This paper is organized as follows. In Sec. II the triaxial symmetries are presented in detail. The particular form the Hartree-Fock Hamiltonian assumes under these symmetries is also given, while the technical details are relegated to an appendix. The Hartree-Fock-Bogolyubov equations are next presented together with their approximation: the self-consistent HF plus BCS scheme. Our results are given in Sec. III, while Sec. IV briefly presents our conclusions.

II. HARTREE-FOCK AND HARTREE-BOGOLYUBOV EQUATIONS IN THE PRESENCE OF TRIAXIAL SYMMETRIES

A. Hartree-Fock equations

We limit ourselves to a sketchy presentation of the derivation of the HF equations existing in standard textbooks. The HF method is based on the assumption of a determinantal wave function,

$$|\Psi\rangle=\frac{1}{\sqrt{A!}}\det\{\varphi_\lambda(r_i)\}\ ,$$

where A is the nucleon number and φ_λ are the single particle orbitals. The Hartree-Fock equations are obtained through minimization of the total energy (with respect to normalized Ψ's)

$$E=\langle\Psi|H|\Psi\rangle=\sum_{\lambda\in F}\langle\lambda|t|\lambda\rangle+\tfrac{1}{2}\sum_{\lambda,\mu\in F}\langle\lambda\mu|V|\widetilde{\lambda\mu}\rangle\ ,$$

where H is the nuclear Hamiltonian, containing a kinetic t and a potential V part. The symbol $\lambda\in F$ denotes an occupied orbital. As a consequence of the application of the variational principle, the Hartree-Fock orbitals are solutions of the equation

$$h_{\rm HF}|\lambda\rangle=e_\lambda|\lambda\rangle\ , \tag{2.1}$$

where $h_{\rm HF}$ is a single particle Hamiltonian (the Hartree-Fock Hamiltonian), and the quantities e_λ are interpreted as the energies of the HF orbitals. The Hartree-Fock Hamiltonian can be most easily given through its matrix elements on a basis of arbitrary states $\alpha,\beta,\gamma,\ldots$,

$$\langle\alpha|h_{\rm HF}|\gamma\rangle=\langle\alpha|t|\gamma\rangle+\sum_{\lambda\in F}\langle\alpha\lambda|V|\widetilde{\gamma\lambda}\rangle\ .$$

The dependence of the Hartree-Fock Hamiltonian on the occupied states, besides the fact that it makes Eq. (2.1) a nonlinear one to be solved in an iterative way until self-consistency is achieved, has particular consequences as far as the symmetries of $h_{\rm HF}$ are concerned.

B. Triaxial self-consistent symmetries

As is well known, the symmetries of the Hartree-Fock Hamiltonian, i.e., the self-consistent symmetries, are not those of the nuclear Hamiltonian. Actually the following theorem holds true.[18] If U is a unitary operator which commutes with the nuclear Hamiltonian and leaves invariant the space spanned by the occupied orbitals, then U commutes with the Hartree-Fock Hamiltonian, i.e., U is a self-consistent symmetry.

In the following study we will be interested in the triaxial shapes in even-even nuclei. It then seems reasonable to choose as self-consistent symmetries the symmetries of the ellipsoid or triaxial symmetries, i.e., reflections with respect to the planes yz,zx,xy, and time reversal.[19,20]

We denote by Π_1,Π_2,Π_3 the unitary operators associated to the three reflections

$$\Pi_j=PR_j(\pi)=\Pi_j^x(-i\sigma_j)\ ,$$

where P is the parity operator, $R_j(\pi)$ a rotation of π around the j axis, Π_j^x a space reflection operator ($x_j\rightarrow -x_j$), and σ_j a Pauli matrix, the latter form being due to the fact that we are dealing with spin $\frac{1}{2}$ particles.

The three reflection operators do not commute with one another, so one can form a complete system of operators including two out of the reflection operators, or, preferably, two combinations of them, namely:

$$P=-\Pi_1\Pi_2\Pi_3 ,$$

$$\Pi_{12}=-i\Pi_1\Pi_2=\Pi_1^x\Pi_2^x\sigma_3 .$$

So the Hartree-Fock orbitals will be characterized by two good quantum numbers p,q associated to the operators P and Π_{12}.

The fact that the time-reversal operator K commutes with the Hartree-Fock Hamiltonian can be used in order to deduce reality properties of the single-particle wave function. We actually know that the phase of the eigenstates of a unitary antilinear operator (such as K) can be chosen in such a way as to make the eigenvalue equal to one.

For spin $\frac{1}{2}$ particles a set of commuting observables is $\vec{R},\vec{S}^2,S_3$ and the corresponding basis is $|\vec{r}\rangle|\frac{1}{2}\sigma\rangle$. The standard choice of phase is then

$$K|\vec{r}\rangle=|\vec{r}\rangle ,$$

$$R_2(\pi)K|\tfrac{1}{2}\sigma\rangle=|\tfrac{1}{2}\sigma\rangle .$$

For the set of observables $H,\Pi_{12},P,\vec{S}^2$ we are interested in, we can introduce a basis $|nqp\frac{1}{2}\rangle$ characterized by the quantum numbers of the operators of the set. One can readily show that the operator Π_2K commutes with the operators of the set. The operator Π_2K being antiunitary, we can choose the phase of the wave function $|nqp\frac{1}{2}\rangle$ such as

$$\Pi_2K|nqp\tfrac{1}{2}\rangle=|nqp\tfrac{1}{2}\rangle . \tag{2.2}$$

We expand now on the basis $|\vec{r}\rangle|\frac{1}{2}\sigma\rangle$ and get

$$|nqp\tfrac{1}{2}\rangle=\int d^3r\sum_\sigma f_{nqp\sigma}(\vec{r})|\vec{r}\rangle|\tfrac{1}{2}\sigma\rangle .$$

It can be shown easily that the application of (2.2) leads to

$$f_{nqp\sigma}(\vec{r})=f^*_{nqp\sigma}(\Pi_2\vec{r}) . \tag{2.3}$$

We can further exploit this relation by writing f as a sum of functions even and odd with respect to Π_2:

$$f_{nqp\sigma}\equiv f^+_{nqp\sigma}+f^-_{nqp\sigma} .$$

The relation (2.3) gives then

$$\mathrm{Im}f^+_{nqp\sigma}=0 ,$$

$$\mathrm{Re}f^-_{nqp\sigma}=0 .$$

We can now write the wave function of a state $i\equiv(nqp)$ as

$$\Phi_i(\vec{r},\sigma)=\sum_{\sigma=\pm\frac{1}{2}}(f^+_{i\sigma}(\vec{r})+if^-_{i\sigma}(\vec{r}))\chi(\sigma) ,$$

where the functions $f^\pm_{i\sigma}$ are assumed to be real.

One can further show that Φ, as defined above, is an eigenstate of Π_{12} with eigenvalue q, and that the state $K\Phi$ is also an eigenstate with eigenvalue $-q$. These two states are degenerate in energy (Kramer's degeneracy).

Let us make a final remark on isospin. We do not allow for any isospin mixing in the Hartree-Fock wave functions which are thus eigenstates of the isospin component:

$$\Phi_i(\vec{r},\sigma,\tau)=\chi_{\tau i}(\tau)\sum_{\sigma=\pm\frac{1}{2}}(f^+_{i\sigma}(\vec{r})+if^-_{i\sigma}(\vec{r}))\chi(\sigma) .$$

C. Cartesian oscillator basis

The basis on which we expand the Hartree-Fock wave functions is the basis formed by wave functions of a three-dimensional harmonic oscillator in Cartesian coordinates:

$$\langle\vec{r}|n_xn_yn_z\rangle=(i)^{n_y}\psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z) ,$$

where $\psi_{n_x}(x)$ is a normalized oscillator function in the x direction

$$\psi_{n_x}(x)=\sqrt{\alpha_x}e^{-(1/2)\xi^2}h_{n_x}(\xi) .$$

We have made use of the usual definition $\xi=\alpha_x x$, where $\alpha_x=(m\omega_x/\hbar)^{1/2}$, with ω_x the frequency of the oscillator and m the mass of the particle. The normalized Hermite polynomial is given by

$$h_{n_x}(\xi)=\frac{1}{(\sqrt{\pi}2^{n_x}n_x!)^{1/2}}H_{n_x}(\xi) ,$$

where $H_{n_x}(\xi)$ is the usual Hermite polynomial

$$H_n(\xi)=(-1)^ne^{\xi^2}\frac{d^n}{d\xi^n}e^{-\xi^2} .$$

For a spin $\frac{1}{2}$ particle the wave function is a spinor, and the basis functions become

$$\langle\sigma|\langle\vec{r}|n_xn_yn_z\sigma\rangle=(i)^{n_y}\Psi_{n_x}(x)\Psi_{n_y}(y)\Psi_{n_z}(z)\chi(\sigma_z) ,$$

with $\chi(\frac{1}{2})=\binom{1}{0}$ and $\chi(-\frac{1}{2})=\binom{0}{1}$.

The phase $(i)^{n_y}$ is consistent with the phase choice (2.2) and can be shown to lead to real matrix elements for the Hartree-Fock Hamiltonian.

The quantum numbers p and q can be expressed in a very simple way on the basis:

$$P\,|\,n_x n_y n_z \sigma_z\rangle=(-1)^{n_x+n_y+n_z}\,|\,n_x n_y n_z \sigma_z\rangle\ ,$$

$$\Pi_{12}\,|\,n_x n_y n_z \sigma_z\rangle=(-1)^{n_x+n_y}\sigma_z\,|\,n_x n_y n_z \sigma_z\rangle\ ,$$

and

$$p=(-1)^{n_x+n_y+n_z}\ ,$$

$$q=(-1)^{n_x+n_y}\sigma_z\ .$$

In what follows we will make use of the time reversal properties of the basis. Let us denote by (α) the quantum numbers $(n_x,n_y,n_z;\sigma)$. The following relations hold for the basis wave functions under time reversal:

$$|\,\bar{\alpha}\rangle\equiv K\,|\,\alpha\rangle=(-1)^{n_y^\alpha}\sigma_\alpha\,|\,\underline{\alpha}\rangle\ ,$$

where

$$(\underline{\alpha})=(n_x n_y n_z;-\sigma)\ .$$

Let us consider the expansion

$$|\,\lambda\rangle=\sum_\alpha C_\alpha^\lambda\,|\,\alpha\rangle$$

of the Hartree-Fock wave function on the basis functions. The application of K on both members of the expansion gives

$$C_{\bar{\alpha}}^{\bar{\lambda}}=C_\alpha^\lambda\ ,$$

$$C_{\underline{\alpha}}^{\bar{\lambda}}=(-1)^{n_y^\alpha}\sigma_\alpha C_\alpha^\lambda\ .$$

The density matrix

$$\rho_{\beta\delta}=\sum_\lambda C_\beta^\lambda C_\delta^\lambda\ ,$$

where the sum runs over occupied states, obeys the following relations:

$$\begin{aligned}\bar{\rho}_{\bar{\beta}\bar{\delta}}&=\rho_{\beta\delta}\ ,\\ \bar{\rho}_{\underline{\beta}\underline{\delta}}&=(-1)^{n_y^\beta+n_y^\delta}\sigma_\beta\sigma_\delta\rho_{\beta\delta}\ ,\end{aligned}\tag{2.4}$$

where $\bar{\rho}$ denotes the density matrix for the time reversed states. The relations (2.4) for the density matrix will be useful for the calculation of the Hartree-Fock Hamiltonian.

D. Hartree-Fock Hamiltonian

In what follows we present the results for the direct and exchange parts of the Hartree-Fock potential for a general finite range interaction:

$$V_0=(W+BP_\sigma-HP_\tau-MP_\sigma P_\tau)V(\,|\,\vec{r}_1-\vec{r}_2\,|\,)\ ,$$

where P_σ,P_τ are spin and isospin exchange operators.

A somewhat more detailed derivation can be found in the Appendices, together with the final expressions used in the numerical computation. The matrix elements of the Hartree-Fock field are given by

$$\langle\alpha\,|\,V_{\rm HF}\,|\,\gamma\rangle=\sum_{\beta\delta}\langle\alpha\beta\,|\,V_0\,|\,\widetilde{\gamma\delta}\rangle\rho_{\beta\delta}\ ,$$

where the tilde denotes antisymmetrized matrix elements.

Restricting ourselves to the mean field for one species of particles, and using the notation

$$V_1=(W+BP_\sigma)V,\quad V_2=-(H+MP_\sigma)V$$

we get

$$\begin{aligned}\langle\alpha\,|\,V_{\rm HF}^\tau\,|\,\gamma\rangle=\sum_{\beta\delta}\{&\langle\alpha\beta\,|\,V_1\,|\,\gamma\delta\rangle(\rho_{\beta\delta}^p+\rho_{\beta\delta}^n)-\langle\alpha\beta\,|\,V_1\,|\,\delta\gamma\rangle\rho_{\beta\delta}^\tau\\&+\langle\alpha\beta\,|\,V_2\,|\,\gamma\delta\rangle\rho_{\beta\delta}^\tau-\langle\alpha\beta\,|\,V_2\,|\,\delta\gamma\rangle(\rho_{\beta\delta}^p+\rho_{\beta\delta}^n)\}\ .\end{aligned}$$

By making the spin dependence of the matrix elements explicit we obtain

$$\begin{aligned}\langle\alpha\,|\,V_{\rm HF}^\tau\,|\,\gamma\rangle=\sum_{\beta\delta}\{&\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle(\rho_{\beta\delta}^p+\rho_{\beta\delta}^n)(W\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}+B\delta_{\sigma_\alpha\sigma_\delta}\delta_{\sigma_\beta\sigma_\gamma})\\&-\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle\rho_{\beta\delta}^\tau(W\delta_{\sigma_\alpha\sigma_\delta}\delta_{\sigma_\beta\sigma_\gamma}+B\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta})\\&+\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle\rho_{\beta\delta}^\tau(-H\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}-M\delta_{\sigma_\alpha\sigma_\delta}\delta_{\sigma_\beta\sigma_\gamma})\\&-\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle(\rho_{\beta\delta}^p+\rho_{\beta\delta}^n)(-H\delta_{\sigma_\alpha\sigma_\delta}\delta_{\sigma_\beta\sigma_\gamma}-M\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta})\}\ .\end{aligned}$$

We readily distinguish the different structure of the space-direct and exchange terms. The general form of the direct term is

$$\Gamma_{\alpha\gamma}{}^{1}=\sum_{\beta\delta}\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}\,,$$
$$\Gamma_{\alpha\gamma}{}^{2}=\sum_{\beta\delta}\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\delta}\delta_{\sigma_\beta\sigma_\gamma}\,. \tag{2.5}$$

For the exchange potential we have

$$G_{\alpha\gamma}{}^{1}=\sum_{\beta\delta}\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\delta}\delta_{\sigma_\beta\sigma_\gamma}\,,$$
$$G_{\alpha\gamma}{}^{2}=\sum_{\beta\delta}\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}\,.$$

When the effective interaction includes zero range parts, as is the case of the Gogny interaction,[4,5] the Hartree-Fock potential associated to the latter can be calculated by using the standard techniques developed for the treatment of the Skyrme interaction[2] involving the calculation of various densities.[1]

The treatment of the Coulomb interaction follows the method sketched above, the only difference residing in the evaluation of the matrix element $\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle$. In the numerical calculations we have performed, only the direct part of the Coulomb potential was considered.

E. Self-consistent Hartree-Fock plus BCS and HFB theories

Let us introduce the creation and annihilation operator of one nucleon in a Hartree-Fock orbital λ, $\eta_\lambda^\dagger,\eta_\lambda$. The relation between these operators and the operators corresponding to the basis states $a_\alpha^\dagger$ is simply

$$\eta_\lambda^\dagger=\sum_\alpha C_\alpha^\lambda a_\alpha^\dagger\,. \tag{2.6}$$

The transformation C being unitary we can inverse relation (2.6) and find

$$a_\alpha^\dagger=\sum_\lambda C_\alpha^\lambda\eta_\lambda^\dagger\,.$$

The phase convention, under time-reversal, for the Hartree-Fock states amounts to

$$K^{-1}\eta_\lambda^\dagger K=\eta_{\bar\lambda}^\dagger\,.$$

The BCS transformation u_λ,v_λ transforms the particles $\eta_\lambda^\dagger$ into quasiparticles $\xi_\lambda^\dagger$ which are obtained as linear combinations of a particle state and the time-reversed hole state:

$$\eta_\lambda^\dagger=u_\lambda\xi_\lambda^\dagger+v_\lambda\xi_{\bar\lambda}\,.$$

The convention for the u_λ,v_λ coefficients is the following:

$$u_{\bar\lambda}=u_\lambda\,,$$
$$v_{\bar\lambda}=-v_\lambda\,,$$

and we have

$$u_\lambda{}^2+v_\lambda{}^2=1\,.$$

The $v_\lambda{}^2$ will subsequently be interpreted as the probability of occupation of the state λ. The Hartree-Fock plus BCS transformation can now be written as

$$a_\alpha^\dagger=\sum_\lambda C_\alpha^\lambda u_\lambda\xi_\lambda^\dagger+C_\alpha^\lambda v_\lambda\xi_{\bar\lambda}\,. \tag{2.7}$$

The wave function of the nucleus is a wave function of independent quasiparticles $|\tilde 0\rangle=\Pi_\lambda\xi_\lambda\,|\,0\rangle$, where $|\,0\rangle$ is the true particle vacuum.

In order to simplify our expressions we introduce the following convention. The base states are characterized by the quantum number q. All states with $q>0$ correspond to the same block of the Hartree-Fock Hamiltonians and are referred to as states q. The time reversed of the former states are referred to as states $\bar q$ and correspond to $q<0$.

The density matrix for a BCS state is

$$\rho_{\beta\delta}=\langle\tilde 0\,|\,a_\delta^\dagger a_\beta\,|\,\tilde 0\rangle=\sum_{\lambda\mu}C_\beta^\lambda v_\lambda C_\delta^\mu v_\mu\langle\tilde 0\,|\,\xi_{\bar\lambda}\xi_{\bar\mu}^\dagger\,|\,\tilde 0\rangle$$
$$=\sum_\lambda C_\beta^\lambda C_\delta^\lambda v_\lambda{}^2\,. \tag{2.8}$$

Its properties are the same as in the Hartree-Fock case:

$$\rho_{\beta\delta}=\rho_{\delta\beta}\,,$$
$$\rho_{\beta\delta}=\bar\rho_{\bar\beta\bar\delta}\,. \tag{2.9}$$

Contrary to the Hartree-Fock case there exists another nonzero contraction, the pairing tensor

$$\kappa_{\beta\delta}=\langle\tilde 0\,|\,a_\delta a_\beta\,|\,\tilde 0\rangle$$
$$=\langle\tilde 0\,|\,a_\beta^\dagger a_{\bar\delta}^\dagger\,|\,\tilde 0\rangle$$
$$=\sum_{\lambda\in q}C_\beta^\lambda C_{\bar\delta}^{\bar\lambda}u_\lambda v_\lambda\,.$$

The notation $\lambda\in q$ means that λ belongs to the block q. Consequently, $\bar\lambda$ belongs to the block $\bar q$, and $\bar\delta$ is a state of this block. A correct notation for κ is then $\kappa_{\beta\bar\delta}$.

The symmetry relations for κ are better understood with the aid of Fig. 1 which represents the blocks $q,\bar q$. The big symmetry relates $\kappa_{\beta\bar\delta}$ and $\kappa_{\bar\delta\beta}$, while β and $\bar\delta$ remain in their initial blocks. We find

$$\kappa_{\bar\delta\beta}=-\kappa_{\beta\bar\delta}\,.$$

The small symmetry is a relation between $\kappa_{\beta\bar\delta}$ and $\kappa_{\delta\bar\beta}$, where δ and β swap blocks:

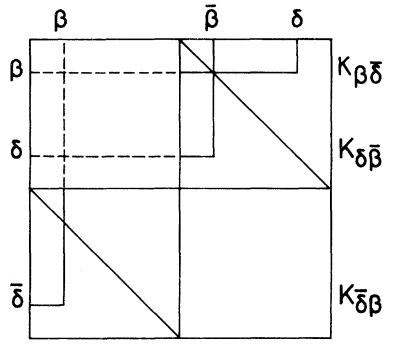

FIG. 1. The symmetry relations of the pairing tensor.

$$\kappa_{\beta\bar{\delta}}=\kappa_{\delta\bar{\beta}} .$$

The total energy for a BCS wave function is given by

$$\langle\tilde{0}\,|\,H\,|\,\tilde{0}\rangle=\sum_{\alpha\gamma}\langle\alpha\,|\,t\,|\,\gamma\rangle\rho_{\alpha\gamma}+\frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta\,|\,V\,|\,\widetilde{\gamma\delta}\rangle\rho_{\beta\delta}\rho_{\alpha\gamma}+\frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\bar{\gamma}\,|\,V\,|\,\widetilde{\beta\bar{\delta}}\rangle\kappa_{\bar{\delta}\beta}\kappa_{\alpha\bar{\gamma}} .$$

The last term on the right-hand side is the pairing energy. We can thus introduce the pairing field, whose matrix elements are given by

$$\Delta_{\alpha\bar{\gamma}}=\frac{1}{2}\sum_{\beta\bar{\delta}}\langle\alpha\bar{\gamma}\,|\,V\,|\,\widetilde{\beta\bar{\delta}}\rangle\kappa_{\bar{\delta}\beta}=\frac{1}{2}\sum_{\mu}\langle\alpha\bar{\gamma}\,|\,V\,|\,\widetilde{\mu\bar{\mu}}\rangle u_{\bar{\mu}}v_{\mu} .$$

The detailed calculation of the pairing potential is given in an appendix. The pairing energy is now given simply by

$$E_p=\frac{1}{2}\mathrm{Tr}(\Delta\kappa)=\frac{1}{2}\sum_{\alpha\bar{\gamma}}\Delta_{\bar{\gamma}\alpha}\kappa_{\alpha\bar{\gamma}} .$$

The BCS approximation relies upon the hypothesis that the pairing field is diagonal in the Hartree-Fock basis. This means that only matrix elements of the type

$$\Delta_{\lambda\bar{\lambda}}=\frac{1}{2}\sum_{\mu}\langle\lambda\bar{\lambda}\,|\,V\,|\,\widetilde{\mu\bar{\mu}}\rangle u_{\bar{\mu}}v_{\mu}$$

exist while

$$\Delta_{\lambda\bar{\nu}}=\frac{1}{2}\sum_{\mu}\langle\lambda\bar{\nu}\,|\,V\,|\,\widetilde{\mu\bar{\mu}}\rangle u_{\bar{\mu}}v_{\mu}$$

for $\lambda\neq\nu$ are zero. In practice this approximation is well justified: The off-diagonal matrix elements of Δ are in fact smaller than the diagonal ones by two or three orders of magnitude. Once this approximation of the pseudodiagonalization of Δ has been made, the application of the variational principle becomes straightforward.

The Hartree-Fock-Bogolyubov (HFB) theory allows one to get rid of the simplifying assumptions about the pairing potential that one makes in the Hartree-Fock plus BCS case. In this theory we start with the most general Bogolyubov transformation on the nucleon creation operators:

$$\xi_{\lambda}^{\dagger}=\sum_{\alpha}U_{\alpha}^{\lambda}a_{\alpha}^{\dagger}+V_{\alpha}^{\lambda}a_{\alpha} .$$

Again in the HFB case the wave function of the nucleus is a wave function of independent quasiparticles, the expression for the total energy is the same as in the BCS case, and ρ and κ are defined as:

$$\rho_{\delta\beta}=\langle\tilde{0}\,|\,a_{\beta}^{\dagger}a_{\delta}\,|\,\tilde{0}\rangle=\sum_{\lambda}V_{\beta}^{\lambda}V_{\delta}^{\lambda} ,$$

$$\kappa_{\bar{\delta}\beta}=\langle\tilde{0}\,|\,a_{\delta}a_{\beta}\,|\,\tilde{0}\rangle=\sum_{\lambda}U_{\delta}^{\bar{\lambda}}V_{\beta}^{\lambda} .$$

The application of the variational principle on $\langle\tilde{0}\,|\,H\,|\,\tilde{0}\rangle$, with the constraint $-\lambda N$ for the mean particle number to be conserved, leads to the HFB equations. We write, in matrix notation,

$$\begin{pmatrix}\epsilon_{\alpha\gamma} & \Delta_{\alpha\bar{\gamma}}\\ -\Delta_{\bar{\alpha}\gamma} & -\epsilon_{\bar{\alpha}\bar{\gamma}}\end{pmatrix}\begin{pmatrix}U_{\gamma}\\ \bar{V}_{\gamma}\end{pmatrix}=e_{\alpha}\begin{pmatrix}U_{\alpha}\\ \bar{V}_{\alpha}\end{pmatrix} ,$$

where

$$\epsilon_{\alpha\gamma}=t_{\alpha\gamma}-\lambda\delta_{\alpha\gamma}+\Gamma_{\alpha\gamma} ,$$

with $\Gamma_{\alpha\gamma}$ being the Hartree-Fock potential (direct and exchange). The matrix $\epsilon_{\alpha\gamma}$ is evidently symmetric. This eigenvalue problem can be transformed into an eigenvalue problem for a symmetric matrix, using the properties of Γ and Δ.

III. RESULTS

A. Choice of the oscillator parameters: Optimization of the oscillator basis

The parameters of the oscillator basis are variational parameters of the problem. The total energy must be minimized with respect to these parameters. This is particularly important as the basis of the oscillator is truncated according to the prescription

$$n_x+n_y+n_z\leq N_0 ,$$

where n_i is the number of quanta on each direction. However, the exact minimization being prohibitively long for large bases, for which the dependence of the energy on the oscillator parameters is not absolutely crucial, the following method for an optimal choice of these parameters has been introduced. We as-

similate the nucleus to an ellipsoidal liquid drop whose axes are given by

$$R_x=R_0\left[1+\left[\frac{5}{4\pi}\right]^{1/2}\beta\cos\left[\gamma-\frac{2\pi}{3}\right]\right],$$
$$R_y=R_0\left[1+\left[\frac{5}{4\pi}\right]^{1/2}\beta\cos\left[\gamma+\frac{2\pi}{3}\right]\right], \quad (3.1)$$
$$R_z=R_0\left[1+\left[\frac{5}{4\pi}\right]^{1/2}\beta\cos\gamma\right],$$

where β,γ are the usual Bohr-Mottelson parameters. If one wishes to employ a prescription which is volume conserving to all orders, then one should use the Hill-Wheeler prescription

$$R_x=R_0\exp\left[\left[\frac{5}{4\pi}\right]^{1/2}\beta\cos\left[\gamma-\frac{2\pi}{3}\right]\right],$$

etc. We present our analysis solely for the first prescription, the extension being evident.

The β,γ parameters are related to the quadrupole moments Q_0,Q_2 through

$$\beta=\left[\frac{\pi}{5}\right]^{1/2}\frac{(Q_0^2+3Q_2^2)^{1/2}}{ZR_P^2+NR_N^2},$$
$$Q_0=2AR^2\beta\left[\frac{5}{4\pi}\right]^{1/2}\cos\gamma,$$
$$\gamma=\arctan\frac{\sqrt{3}Q_2}{Q_0},$$
$$Q_2=2AR^2\beta\left[\frac{5}{4\pi}\right]^{1/2}\sin\gamma/\sqrt{3},$$

where

$$Q_0=\int\rho(\vec{r})(2z^2-x^2-y^2)d^3r,$$
$$Q_2=\int\rho(\vec{r})(x^2-y^2)d^3r,$$

and $R_{P(N)}^2$ is the mean square radius of protons (neutrons). We introduce the parameters p,q of the deformation of the basis through

$$q=\frac{\alpha_x^2}{\alpha_z^2},\quad p=\frac{\alpha_x^2}{\alpha_y^2}.$$

We make the following choice for p and q: We suppose that they are fixed by the shape of the nucleus, i.e.,

$$q=\frac{R_z}{R_x},\quad p=\frac{R_y}{R_x}. \quad (3.2)$$

If one chooses to constrain the values of β and γ, the p and q can be directly calculated starting from (3.2) using (3.1). In order to obtain the volume parameter of the oscillator,

$$\omega=(\omega_x\omega_y\omega_z)^{1/3},$$

we start by calculating the radius

$$R^2=R_x^2+R_y^2+R_z^2=R_x^2(1+q^2+p^2).$$

For volume conservation we introduce R_0 through

$$\left[\frac{R_0}{\sqrt{3}}\right]^3=R_xR_yR_z=R_x^3pq,$$

and finally

$$R=\frac{R_0}{(pq)^{1/3}}\left[\frac{1+p^2+q^2}{3}\right]^{1/2}.$$

Here R_0 is the real rms radius calculated, through an exact minimization with respect to $\hbar\omega_0$, at the spherical point $p=q=1$. The volume parameter of the oscillator basis $\hbar\omega$ can then be calculated through a scaling on the radius:

$$\hbar\omega=\hbar\omega_0\frac{3(pq)^{2/3}}{1+p^2+q^2}.$$

However, this prescription is not always good, the Hartree-Fock energy depending crucially on this parameter. The best solution to this problem is to explicitly minimize with respect to $\hbar\omega_\beta$ at each axial point ($\gamma=0$), and estimate the $\hbar\omega$ for the same β at $\gamma\neq0$ through

$$\hbar\omega=\hbar\omega_\beta\frac{3p^{2/3}}{2+p^2}.$$

We have verified in certain cases, through an explicit minimization with respect to the oscillator parameters, that the above prescription for the latter is very successful, leading to an error in the binding energy of the order of $\Delta E\leq200$ keV.

Note that this error concerns the basis effects. The numerical accuracy of the calculations is of the order of $\Delta E\sim100$ keV. This has been checked through the comparison of results of the spherical, axial, and triaxial codes.

B. Comparison between HF Bogolyubov, HFBCS, and HF plus schematic pairing calculations

As we have previously seen, the treatment of pairing correlations in nuclei can be performed in the framework of the full Hartree-Fock-Bogolyubov approach or the HF plus BCS approximation. The latter can be carried through either in a self-consistent way, as described in Sec. II (and will be hereafter denoted as HFBCS), or at a more schemat-

ic level using a constant gap Δ (denoted by HF Δ). Let us focus first on the HFBCS and HF Δ comparison. The constant gap is in most practical calculations chosen equal to the experimental one. Of course once the HFBCS calculation result, at a fixed deformation, is known, the constant gap Δ can be chosen equal to the "mean" HFBCS gap, in which case the total energies calculated by the two methods coincide for this deformation. The main difference between the two approaches lies in the deformation dependence of the gap. This may result in quite different potential-energy surfaces. A particularly striking example is offered by the nuclei ^{74}Ge and ^{76}Se, for which we present the energy as a function of the axial quadrupole moment in Figs. 2(a) and (b). The HF Δ calculation predicts a deformed, oblate and prolate, respectively, shape while a full HFBCS treatment leads to a spherical minimum. In general, for the nuclei we examined, the HFBCS calculation has led to a substantial gain in energy for the spherical shape, and thus a reduction of the spherical barrier.

For the comparison of the HFB and HFBCS methods we have calculated the energy as a function of the axial deformation for the nucleus ^{152}Sm. In Fig. 3 we present the result together with the HF Δ one. The HFB and HFBCS energy surfaces are indistinguishable, their difference being smaller than

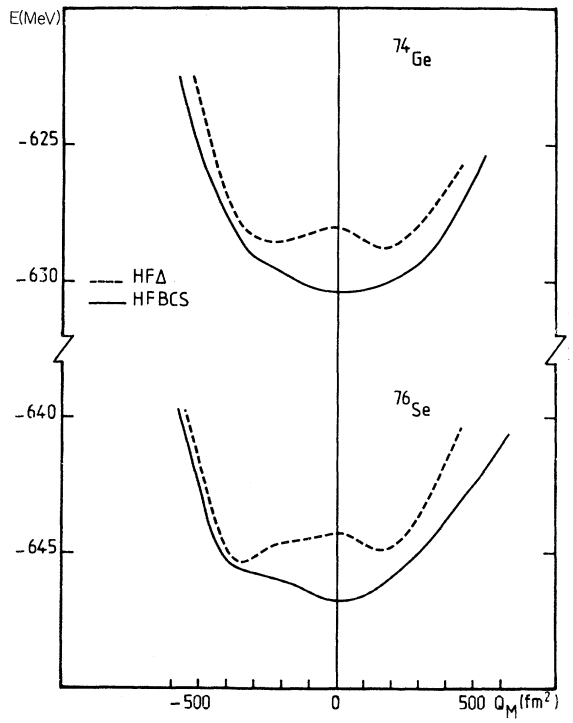

FIG. 2. The potential energy surface (PES) of ^{74}Ge and ^{76}Se obtained by restricted HFB calculation (HFBCS) and the constant gap prescription (HF Δ).

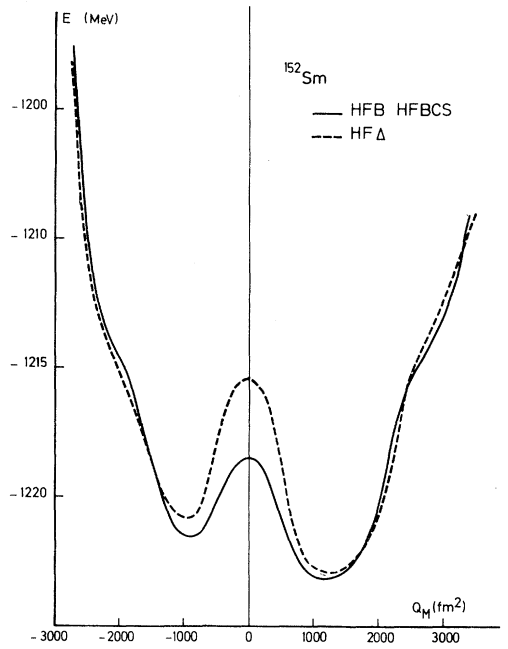

FIG. 3. The potential energy surface of ^{152}Sm obtained by full HFB calculation (HFB), restricted HFB calculation (HFBCS), and constant gap prescription (HF Δ).

the line thickness. Other quantities of physical interest are the gap (which is materialized in our calculation by the minimum quasiparticle energy, which explains why the "constant gap" we represent graphically is not constant) and the pairing energy. Their variation as a function of the quadrupole moment is shown in Figs. 4(a) and (b). The difference of the various quantities is indeed minute, far smaller than the accuracy with which these quantities are usually calculated. The same applies to the calculation of other quantities as, for example, collective inertia parameters, which can influence the dynamics of the nucleus.

The above conclusions hold provided that one uses the same space for the HFB and HFBCS calculations with no cutoff whatsoever. This is possible solely thanks to the finite range of the interaction. It would be impossible to perform an analogous calculation with a velocity dependent, Skyrme-type force, even if the latter had good pairing properties. So, to conclude this subsection, we may state that the HFB and self-consistent HFBCS methods are equivalent for the study of the statics of the nucleus, and, leading to the same inertia parameters, for the dynamics as well.[21]

C. Alpha particle structure of light nuclei

One of the most important characteristics of the $D1$ interaction is its alpha-clustering property which

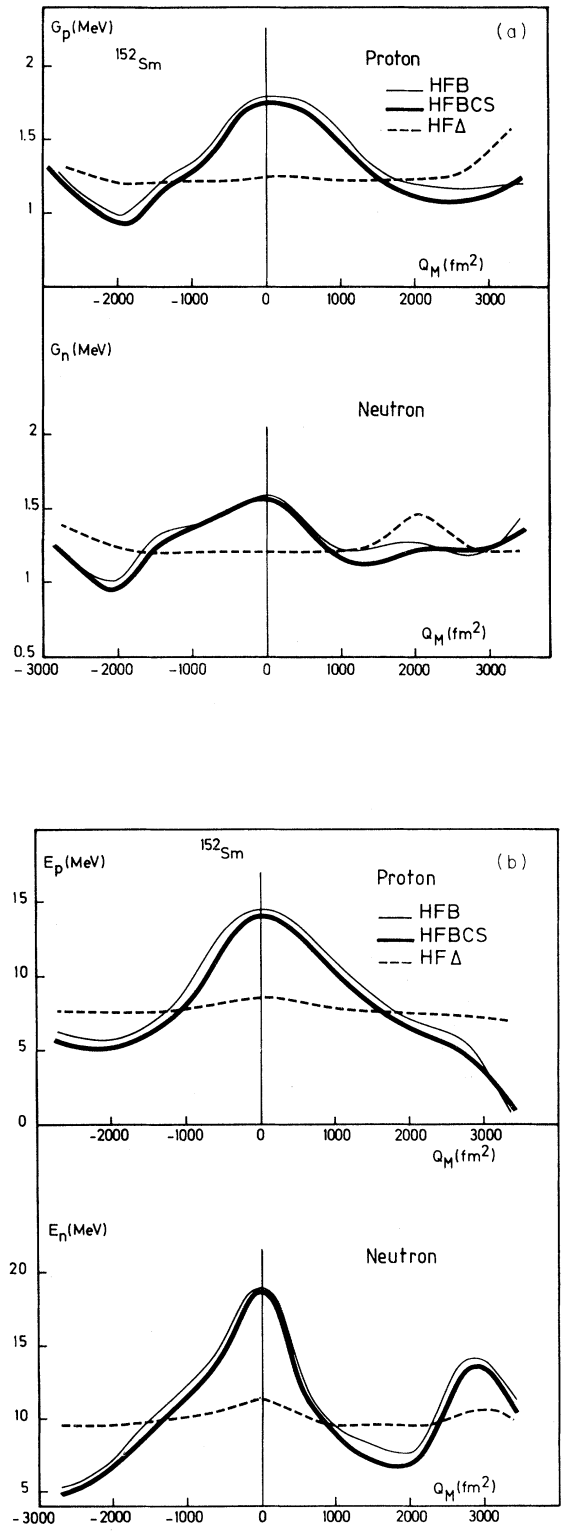

FIG. 4. Neutron and proton gaps (a), pairing energy (b), as function of the deformation of ^{152}Sm for several pairing prescriptions (HFB, HFBCS, HF Δ).

manifests itself in the light nuclei domain. As a matter of fact, most currently used density dependent interactions do not lead to appreciable α clustering.[22] The Skyrme forces typically belong to this class. The only variants of the Skyrme interaction which lead to some clustering[23] achieve that at the expense of an unphysically large binding for the α particle. This is not the case for the $D1$ interaction, with which the α-particle binding energy is quite satisfactory, 28.4 MeV.

Lacking detailed α-particle model calculations for light nuclei with the $D1$ interaction, we present here the HFB predictions for two selected structures: the aligned (4p-4h) configuration in ^{12}C and the diamond (4p-4h) configuration in ^{16}O. The energy curve of the former, together with the density corresponding to the prolate well-deformed minimum at $Q=188$ fm^2 exhibiting pronounced clusterization, is given in Figs. 5(a) and (b). However, this is not a proof for the existence of the α structure. As a matter of fact, detailed α-model calculations[24] indicate that the 4p-4h state is probably a mixture of various triangular configurations. Such configurations are unfortunately not compatible with the symmetries adopted in our code. For the ^{16}O case we present a similar curve as a function of the quadrupole moment [Fig. 6(a)]. The diamond configuration being a triaxial one, we have considered triaxial shapes as well. They lead, in fact, to an energy gain. The situation becomes even more interesting when the spurious rotational energy is subtracted from the potential energy surface. This is done according to the prescriptions of Ref. 25, and from a physical point of view corresponds to an angular momentum projection. Thus, the spherical point stays at its position while a large energy gain is observed for deformed shapes. The triaxial minimum of the energy curve around $Q_0=150$ fm^2 (which corresponds to a γ of 10°) is thus brought down to ~ 10 MeV. This point is to be associated with the band head at 6 MeV. An exact projection would tend to make the agreement even better, but, anyhow, the agreement is far better than the one observed with the various Skyrme interactions.[19] The density associated to this 4p-4h state is also shown in Fig. 6(b) and apparently exhibits cluster structure.

D. Contour maps of the potential energy surfaces

The knowledge of the ground state energy and deformation of the nucleus does not suffice in order to characterize its properties. One cannot form a clear picture concerning its behavior with respect to collective motion on this data alone. A far more clear picture is offered by the potential energy surface.

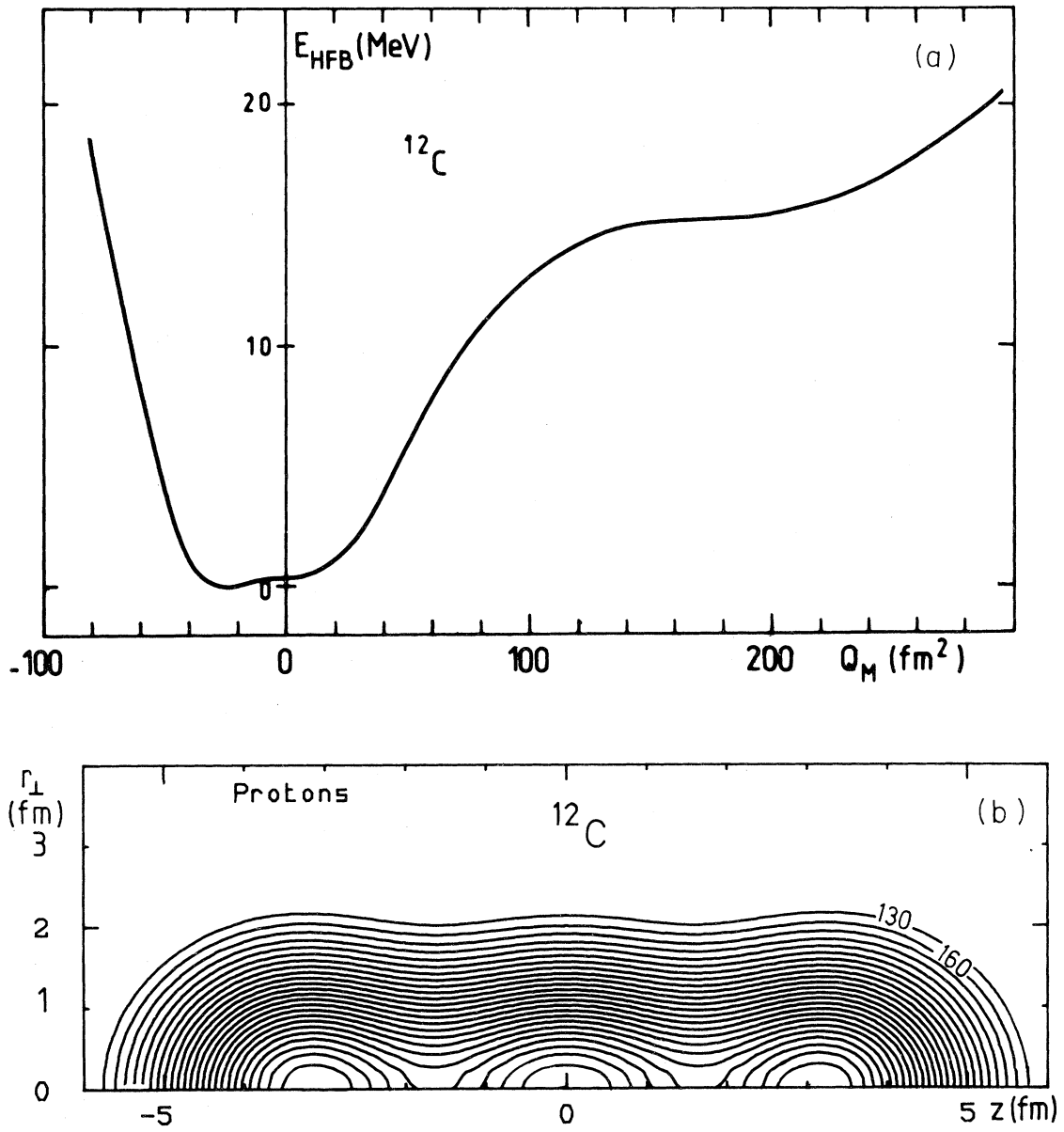

FIG. 5. ^{12}C: the potential energy surface (a), proton density contour plot for the 4p-4h configuration (b).

The latter is given by the energy of the nucleus as a function of deformation, and, as can be shown in theories of collective motion, coincides with the potential to be injected in the collective Hamiltonian.

A notion which is particularly useful in characterizing the potential energy surface is the softness with respect to a particular direction. If the nucleus is easily deformable this would mean that its description in terms of a single Slater determinant (or HFB wave function) is not adequate. This is especially important in the case of γ deformations, for which the great majority of nuclei are soft.

The potential energy surfaces we are going to display were obtained through a constrained Hartree-Fock-Bogolyubov calculation. Two constraints, on the deformation parameters β and γ, are used. The constraints are linear with respect to the parameters β and γ. The convergence on the constrained value of the deformation is achieved through the iterative readjustment of the Lagrange multiplier and density matrix as explained in Ref. 9. The bases used corresponded to $N_0=4$ for s-d shell nuclei, $N_0=6$ for Ni and Ge, and $N_0=8$ for the heavier nuclei.

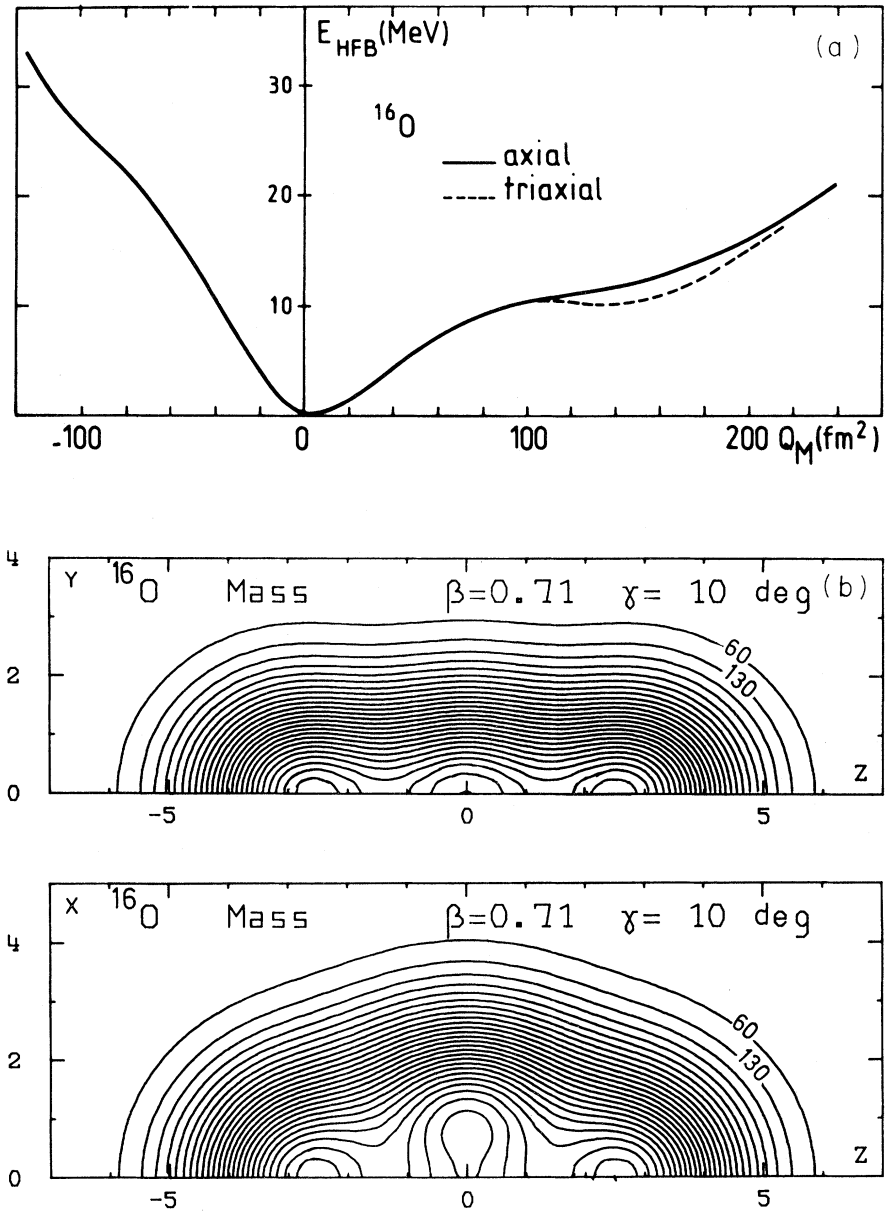

FIG. 6. ^{16}O: the potential energy surface with axial and triaxial symmetry (a), nuclear density contour plots for 4p-4h configuration of ^{16}O in units of 10^{-4} fm^{-3} (b). The lengths are expressed in fermis. The density is plotted in two planes through the nuclear center: $x=0$ on the top, $y=0$ on the bottom.

In Fig. 7 we present the energy surface for ^{24}Mg, which in the traditional s-d shell studies [SU(3) or deformed oscillator] is a typical triaxial nucleus. We observe that in our HFB calculation the ^{24}Mg has an axially symmetric prolate shape. This is a feature already observed in calculations with Skyrme interactions and is due to the spin-orbit interaction.[26] The ^{32}S case is shown next (Fig. 8). This map is particularly interesting as the oblate and prolate minima of the energy surface are very close in energy. Thus the ^{32}S is a γ-unstable nucleus, at least around the ground state deformation, and the full dynamics of the collective motion must be considered in this case.

Next we focus our interest on the transition families of Ni and Ge. The nickel nuclei are particularly soft ones already in the β direction. Starting with ^{56}Ni, which is a doubly magic spherical nucleus, the isotopes we examined are centered around a spherical shape. Although some deformation sets in by

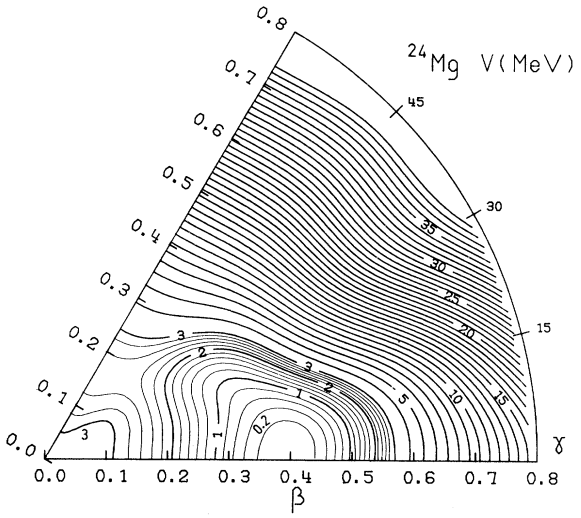

FIG. 7. Contour map for the collective potential $V(\beta,\gamma)$ for ^{24}Mg as it results from a constrained HFB calculation.

the time we reach ^{62}Ni, namely an oblate one with $\beta=0.2$, the extreme softness is the mean characteristic of this family [Figs. 9(a)—(c)].

In the case of the germanium isotopes, we follow the transition from oblate shapes for ^{68}Ge to spherical ^{72}Ge and finally prolate for ^{76}Ge. This transition is in agreement with the experimentally deduced one[27] which operates around neutron numbers of $N=40$—42. Although no statically triaxial shapes are obtained in this study, the γ softness of the germanium isotopes is expected to lead to an appreciable dynamical triaxiality [Figs. 10(a)—(e)].

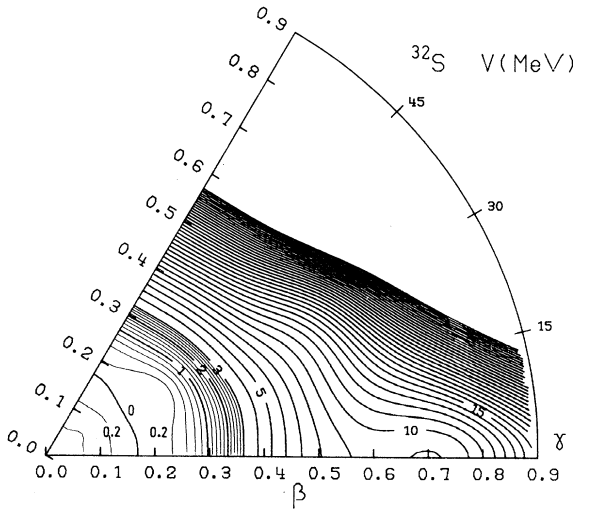

FIG. 8. Contour map for the collective potential $V(\beta,\gamma)$ for ^{32}S.

Further examples of soft nuclei are offered by the maps of ^{110}Pd and ^{134}Ce [Figs. 11(a) and (b)]. In both cases a small equilibrium β deformation is obtained, with ^{110}Pd being axial. But even in this case the energy surface is extremely soft in the γ direction, leading, undoubtedly, to a dynamic triaxiality.

Finally, we present the potential energy surfaces for ^{150}Sm and ^{152}Sm. The spherical-deformed shape transition in the samarium isotopes is well established[28] experimentally and has been theoretically studied.[9] In this case the energy surface allows a better assessment of the importance of the triaxiality in the dynamics of the collective motion [Figs. 12(a) and (b)].

This, in fact, is a general conclusion to be drawn from the study of the potential energy surfaces in this subsection. Qualitatively they allow us to understand the behavior of the nucleus better than the simple data of its static deformation. Quantitatively these energy surfaces can be injected in a collective Hamiltonian and produce the excitation spectrum of the nucleus.

E. Electron scattering and ground states densities

Electron scattering experiments, used in conjunction with model-independent analyses, have proven extremely useful in determining the ground state densities of nuclei. In view of what we have previously stated concerning the softness of nuclei, it is clear a simple, rotational model based, treatment of either the ground state or of the transition density, may be inadequate. Calculations which include the dynamical correlations in the ground state,[29] or the transition density, have indeed been attempted. Such a complete treatment is of course beyond the scope of this paper, and will be presented elsewhere.[30] In what follows we will limit ourselves to considering ground state densities obtained from a simple rotational model assumption. However, in order to account for the effect of dynamics in some crude way, we can choose as a ground state deformation not the one resulting from static calculations, but the one corresponding to the mean dynamic deformation, as obtained in Ref. 21.

In Figs. 13 and 14 we present the results for the ground state spherical densities for the nuclei ^{24}Mg and ^{58}Ni. These experimental results have been deduced from a model independent analysis of data obtained from electron scattering up to very high transfer.[31] The results from our HFB calculation are presented at both deformations corresponding to the static and dynamic equilibriums. It is to be remarked that the consideration of the dynamic deformation suffices in order to smooth the density os-

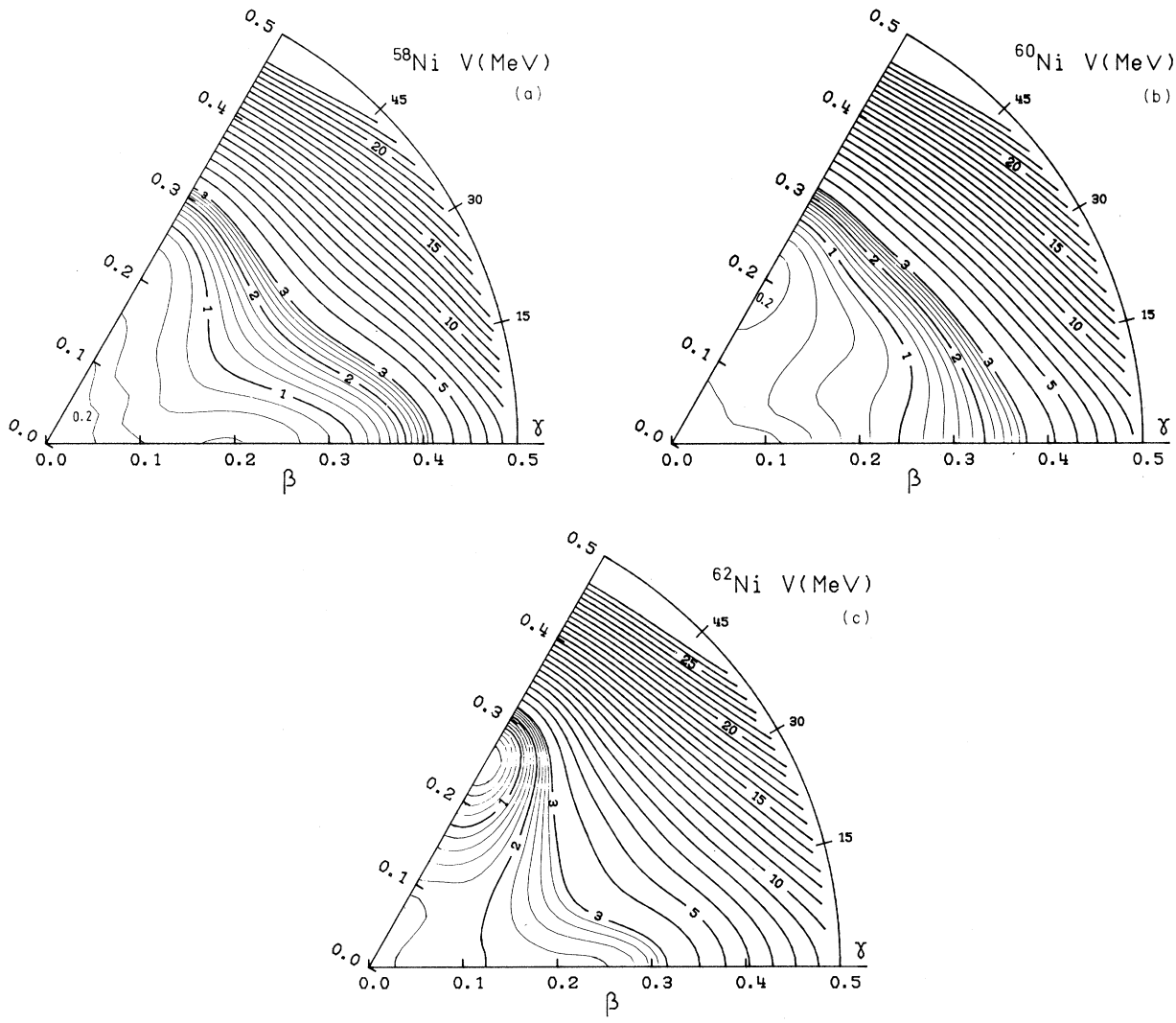

FIG. 9. Contour maps for the collective potential $V(\beta,\gamma)$ for ^{58}Ni (a), ^{60}Ni (b), ^{62}Ni (c).

cillations in the interior of the nucleus, thus bringing the calculation closer to the experimental result. In the case of ^{24}Mg the effect is small due to the rigidity of the nucleus, and some disagreement persists at small radii.

F. The fission barrier of ^{240}Pu

The importance of the triaxial degree of freedom in the fission barrier of the actinides has already been established in the framework of Strutinsky calculations. In a detailed study[32] Larsson and Leander have shown that the height of the first barrier in most actinides can be diminished by 1–2 MeV when we allow for a finite triaxiality 5–20 deg. In our case systematic study is out of the question, one HFB iteration on an IBM 3033 computer necessitating $\sim$10 min for a basis of 11 major oscillator shells (the strict minimal basis for a fission barrier calculation). So, we have limited ourselves to the case of ^{240}Pu, which is the test case of self-consistent fission barrier calculations.[33,34]

In Fig. 15 we present a part of the ^{240}Pu fission barrier as obtained by Berger and one of us (M.G.). The effect of the triaxiality, solely on the first barrier, is also displayed. We readily remark that a substantial decrease of the barrier height results, corresponding to a triaxiality of 7 deg. This result is in fair agreement with the Larsson-Leander calculation.

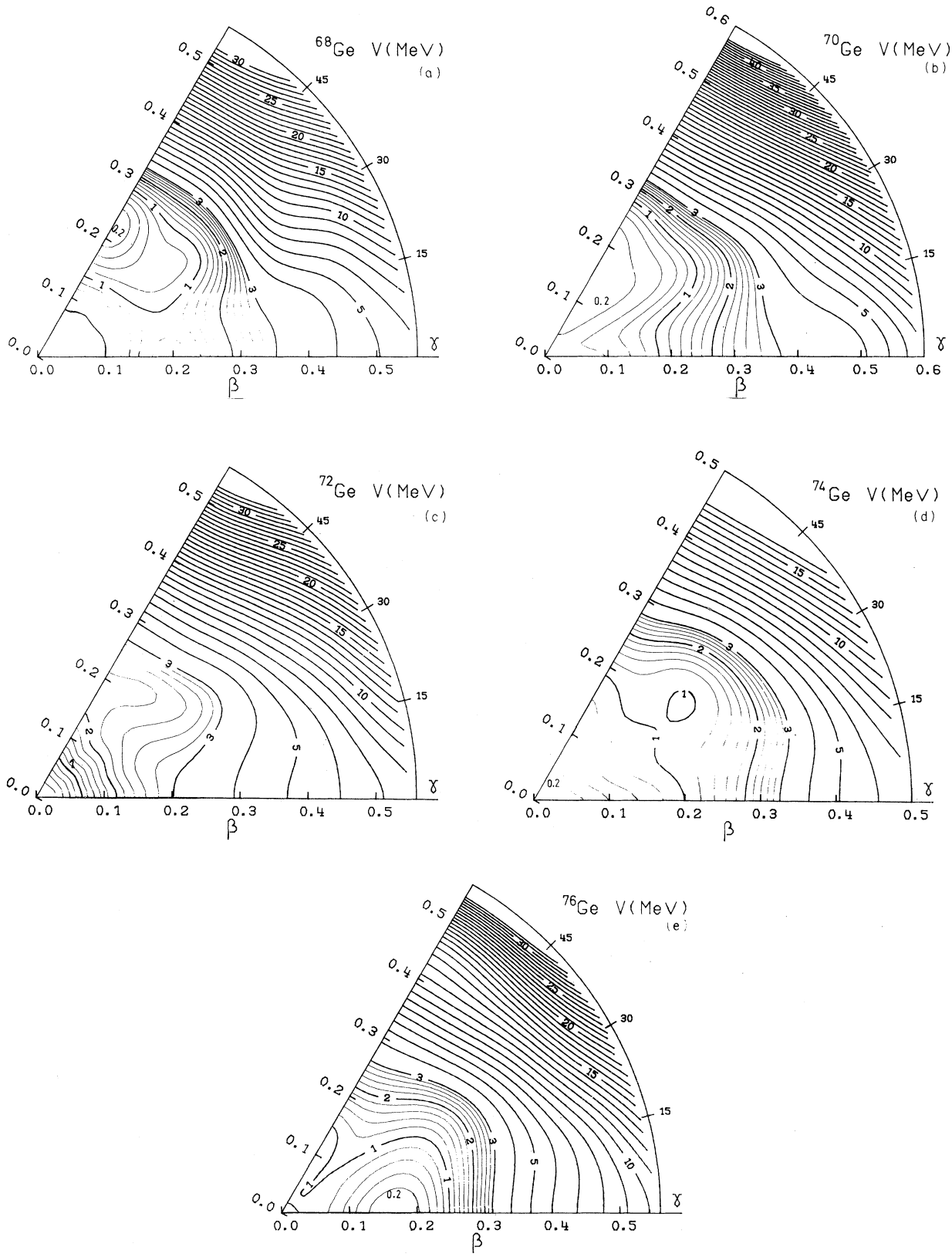

FIG. 10. Contour maps for the collective potential $V(\beta,\gamma)$ for ^{68}Ge (a), ^{70}Ge (b), ^{72}Ge (c), ^{74}Ge (d), ^{76}Ge (e).

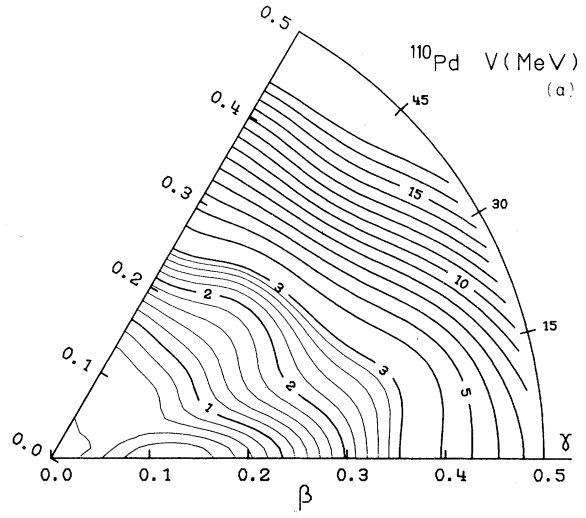

FIG. 11. Contour maps for the collective potential $V(\beta,\gamma)$ for ^{110}Pd (a), ^{134}Ce (b).

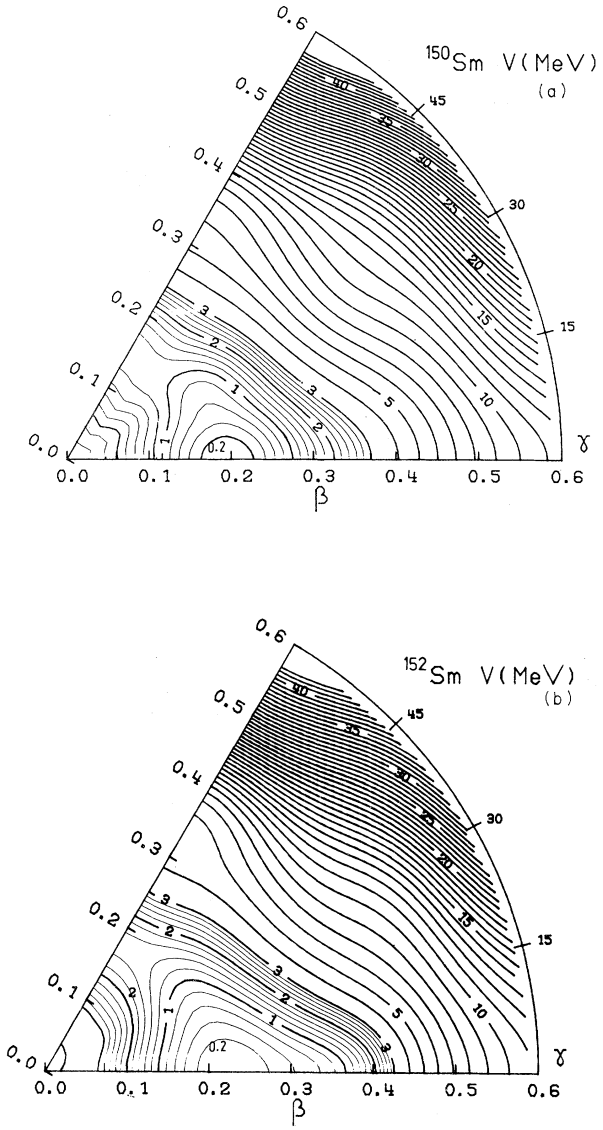

FIG. 12. Contour maps for the collective potential $V(\beta,\gamma)$ for ^{150}Sm (a), ^{152}Sm (b).

IV. CONCLUSION

In this paper we have presented Hartree-Fock-Bogolyubov calculations obtained with a finite range interaction, with triaxial self-consistent symmetries. In our treatment we have been able to handle up to very heavy nuclei with no assumption whatsoever about inert core nucleons. Moreover, large oscillator bases were considered throughout in order to ensure a fair convergence of the results. This has been achieved through an extensive use of the Gogny separation procedure for the interaction while taking full advantage of the symmetries of the problem. The formalism and details of the calculation have been presented in Sec. II and in an appendix.

From the point of view of the results, we have here investigated just the static aspect of triaxiality by looking into the effect of the γ degree of freedom on the ground or isomer states of nuclei, or in the fission barriers. However, the most important result

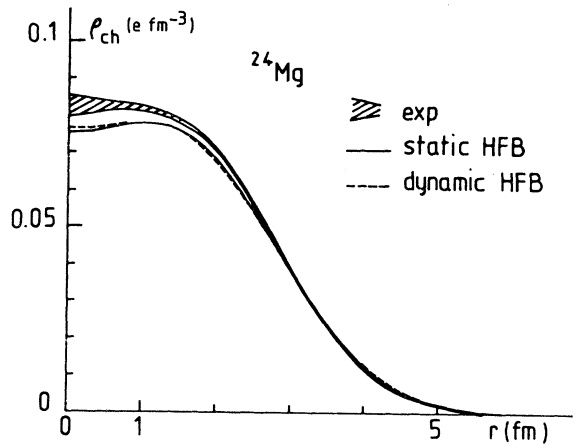

FIG. 13. Static HFB, dynamic HFB, and experimental charge densities of ^{24}Mg.

of this work is the estimation of the γ polarizability, as represented by the potential energy maps. The latter confirm the alleged γ softness of nuclei and thus render imperative a full dynamical treatment of the quadrupole collective motion in nuclei, while at the same time constituting the most important ingredient of the collective Hamiltonian. Such work is currently in progress and will be presented in a future publication.

In the following appendices we present the necessary formal development which can lead to the construction of a HF or HFB code with triaxial symmetries. Our approach is quite general and as such it encompasses the case of the Gogny $D1$ interaction. The latter comprises, apart from the finite range part, zero range density dependent and spin-orbit parts. The technology for the treatment of these zero range parts being standard, we will not enter into any detail as far as these terms are concerned.

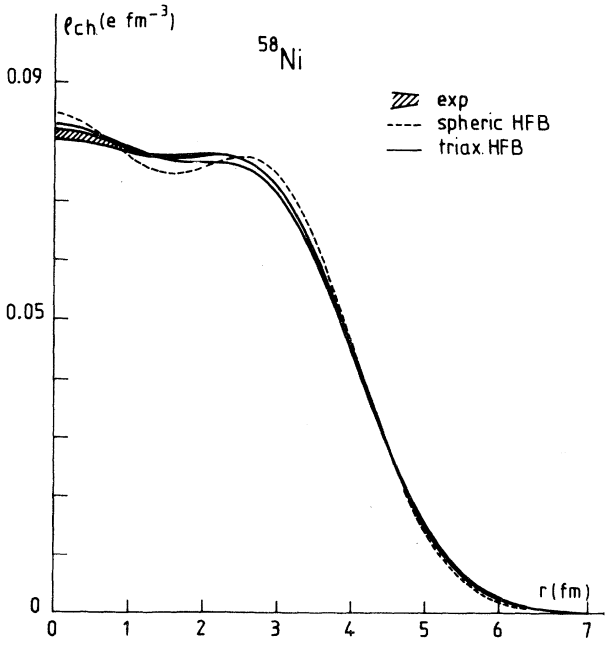

FIG. 14. Spherical HFB, triaxial HFB, and experimental charge densities of ^{58}Ni.

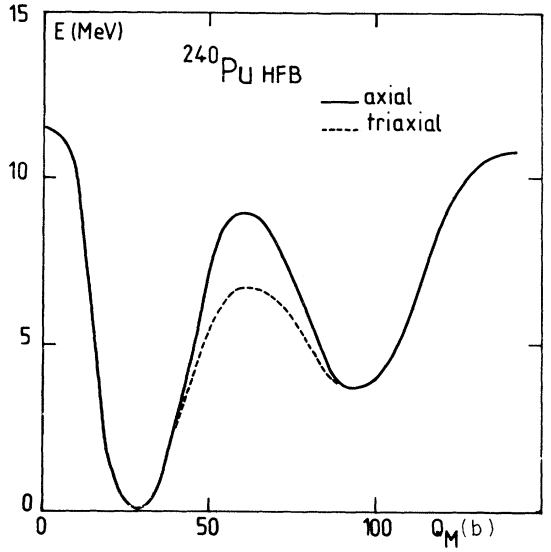

FIG. 15. Potential energy surface of the ^{240}Pu in axial and triaxial HFB calculation.

APPENDIX A: BRIEF RECALL OF THE GOGNY SEPARATION METHOD

We recall briefly the application of the Gogny separation method to the calculation of the matrix element

$$\langle\alpha\beta|V|\gamma\delta\rangle = \int\int \varphi_\alpha^*(x_1)\varphi_\beta^*(x_2)V(x_1-x_2)\varphi_\gamma(x_1)\varphi_\delta(x_2) \times dx_1 dx_2 ,$$

and for simplicity we limit ourselves to the one-dimensional case. The essential property of the basis functions which allows the application of the separation method is a general property of every family of orthogonal polynomials, namely that we can express the product of two functions as a product of one weight function times a finite sum of functions of the same family. In the case of oscillator wave functions ($\xi=\alpha x$),

$$\varphi_\alpha(x)=e^{-\xi^2/2}\left[\frac{\alpha}{\sqrt{\pi}2^{n_\alpha}n_\alpha!}\right]^{1/2}H_{n_\alpha}(\xi) .$$

We have

$$\varphi_\alpha(x)\varphi_\gamma(x)=e^{-\xi^2/2}\sum_\mu \left[\frac{\alpha}{\sqrt{\pi}2^\mu\mu!}\right]^{1/2} I_{ac\mu}\varphi_\mu(x) , \tag{A1}$$

where

$$I_{ac\mu}=\frac{\mu!(n_\alpha!n_\gamma!2^\mu)^{1/2}}{\left[\frac{n_\alpha+\mu-n_\gamma}{2}\right]!\left[\frac{n_\gamma+\mu-n_\alpha}{2}\right]!\left[\frac{n_\alpha+n_\gamma-\mu}{2}\right]!} .$$

Using the transformation (A1) we can rewrite the matrix element

$$\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle=\sum_{\mu\nu} I_{\alpha\gamma\mu}I_{\beta\delta\nu}\int\int \varphi_\mu(x_1)e^{-\alpha^2x_1^2/2}V(\,|x_1-x_2|\,)e^{-\alpha^2x_2^2/2}\varphi_\nu(x_2)dx_1dx_2 . \tag{A2}$$

We can verify that the integral in expression (A2) remains unchanged if we replace $V(x)$ by

$$\mathscr{V}(x)=\sum_\mu \left[\int V(x)e^{-\alpha^2x_1^2/2}\varphi_\mu(x_1)dx_1\right]e^{-\alpha^2x_1^2/2}\varphi_\mu^*(x_1) .$$

We set

$$\mathscr{V}(x)=\sum_\mu f_\mu(x_2)\hat{\varphi}_\mu(x_1) ,$$

where

$$\hat{\varphi}_\mu(x_1)=e^{-\alpha^2x_1^2/2}\varphi_\mu(x_1)$$

and

$$f_\mu(x_2)=\int e^{-\alpha^2x_1^2/2}V(x)\varphi_\mu(x_1)dx_1 .$$

We thus obtain a representation of the potential $\mathscr{V}(x)$ by a sum of terms separable in coordinates 1 and 2. The two potentials $\mathscr{V}(x)$ and $V(x)$ are perfectly equivalent as far as the computation of matrix elements is concerned:

$$\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle=\langle\alpha\beta\,|\,\mathscr{V}\,|\,\gamma\delta\rangle=\sum_\mu \langle\alpha\,|\,\hat{\varphi}_\mu(x_1)\,|\,\gamma\rangle\langle\beta\,|\,f_\mu(x_2)\,|\,\delta\rangle .$$

For the calculation of the two terms we proceed thus. Using relation (A1) we can calculate the matrix element

$$\langle\alpha\,|\,\hat{\varphi}_\mu(x_1)\,|\,\gamma\rangle=\left[\frac{\alpha}{\sqrt{\pi}2^\mu\mu!}\right]^{1/2} I_{\alpha\gamma\mu} . \tag{A3}$$

But $I_{\alpha\gamma\mu}$ exists only if the factorials in the denominator make sense. This gives the following restrictions on n_α,n_γ:

$$|\,n_\alpha-n_\gamma\,|\le\mu\le n_\alpha+n_\gamma .$$

We remark that due to the presence of the term (A3) the sum comprises a finite number of terms. We now examine the second term $J_\mu^{\beta\delta}=\langle\beta\,|\,f_\mu\,|\,\delta\rangle$. Applying relation (A1) we get

$$\langle\beta\,|\,f_\mu\,|\,\delta\rangle=\left[\frac{\alpha}{\sqrt{\pi}}\right]^{1/2}\sum_{\nu=|\beta-\delta|}^{\beta+\delta}\frac{I_{\beta\delta\nu}}{\sqrt{2^\nu\nu!}}\int\int e^{-\alpha^2x_2^2/2}\varphi_\nu(x_2)\varphi_\mu(x_1)V(x_1-x_2)e^{-\alpha^2x_1^2/2}dx_1dx_2 .$$

We perform now a Moshinsky transformation,

$$x=\frac{x_1-x_2}{\sqrt{2}} , \quad X=\frac{x_1+x_2}{\sqrt{2}} ;$$

$$\varphi_\mu(x_1)\varphi_\nu(x_2)=\sum_s M_s^{\mu\nu}\varphi_s(X)\varphi_{\mu+\nu-s}(x) ,$$

where the coefficients $M_s^{\mu\nu}$ are the Moshinsky coefficients. We thus get

$$\langle\beta|f_\mu|\delta\rangle=\left[\frac{\alpha}{\sqrt{\pi}}\right]^{1/2}\sum_{\nu=|\beta-\delta|}^{\beta+\delta}\frac{I_{\beta\delta\nu}}{\sqrt{2^\nu\nu!}}\sum_s M_s^{\mu\nu}\int\int e^{-\alpha^2(x^2+X^2)/2}\varphi_\nu(X)\varphi_{\mu+\nu-s}(x)V(\sqrt{2}x)dx\,dX\ .$$

The integration on X can be readily carried through

$$\left[\frac{\alpha}{\sqrt{\pi}}\right]^{1/2}\int e^{-\alpha^2X^2/2}\varphi_s(X)dX=\delta_{s0}\ .$$

Thus $s=0$ and

$$\langle\beta|f_\mu|\delta\rangle=\sum_{\nu=|\beta-\delta|}^{\beta+\delta}\frac{I_{\beta\delta\nu}}{\sqrt{2^\nu\nu!}}M_0^{\mu\nu}\int\varphi_{\mu+\nu}(x)\,e^{-\alpha^2x^2/2}V(\sqrt{2}x)dx$$

with

$$M_0^{\mu\nu}=(-1)^\mu\left[\frac{(\mu+\nu)!}{2^{\mu+\nu}\mu!\nu!}\right]^{1/2}\ .$$

So, for a given interaction V we must calculate the integral

$$\Theta_\lambda=\int\varphi_\lambda(x)e^{-\alpha^2x^2/2}V(\sqrt{2}x)dx\ . \tag{A4}$$

In the case of a Gaussian interaction, integral (A4) can be performed analytically. For $V=e^{-(x_1-x_2)^2/\mu^2}$ we get

$$\Theta_\lambda=\mu\left[\frac{\alpha\sqrt{\pi}}{2+\alpha^2\mu^2}\right]^{1/2}\frac{\sqrt{(2k)!}}{k!}\left[\frac{-1}{2+\alpha^2\mu^2}\right]^k,\quad\lambda=2k\ ,$$

$$=0\ ,\quad\lambda=2k+1\ .$$

The extension of the separation method to three spatial dimensions is straightforward. In general we obtain an expression of the type

$$\langle\alpha\beta|V|\gamma\delta\rangle=\sum_\nu I_\nu^{\alpha\gamma}J_\nu^{\beta\delta}\ ,$$

where the sum is finite and $I_\nu^{\alpha\gamma}$ depends only on the indices α,γ,ν and $J_\nu^{\beta\delta}$ incorporates the two-body interaction. Such a representation allows a simple, rapid, and numerically precise computation of matrix elements.

APPENDIX B: CALCULATION OF THE DIRECT AND EXCHANGE HARTREE-FOCK POTENTIALS

A. Direct potential

We start with the expression of the direct term (2.5),

$$\Gamma_{\alpha\gamma}{}^1=\sum_{\beta\delta}\langle\alpha\beta|V|\gamma\delta\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}\ ,\quad\Gamma_{\alpha\gamma}{}^2=\sum_{\beta\delta}\langle\alpha\beta|V|\gamma\delta\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\delta}\delta_{\sigma_\beta\sigma_\gamma}\ .$$

The summation $\beta\delta$ is carried out over all occupied states. However, we can limit the summation over half of the states (states with $q>0$ where q is the quantum number defined in Sec. II B) and calculate the contribution of the time reversed states.

We use relation (2.4) on the density matrix

$$\bar{\rho}_{\bar{\beta}\bar{\delta}}=\rho_{\beta\delta}(-1)^{n_y^\beta+n_y^\delta}\sigma_\beta\sigma_\delta$$

as well as the relation

$$\langle\alpha\beta|V|\gamma\delta\rangle=\langle\alpha\bar{\beta}|V|\gamma\bar{\delta}\rangle$$

between spatial matrix elements. Limiting the summations over states with $q=+1$ we get

$$\Gamma_{\alpha\gamma}{}^{1}=\sum_{\beta\delta>0}\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}[1+(-1)^{n_y^\beta+n_y^\delta}\sigma_\beta\sigma_\delta]\ ,$$

$$\Gamma_{\alpha\gamma}{}^{2}=\sum_{\beta\delta>0}\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle\rho_{\beta\delta}[\delta_{\sigma_\alpha\sigma_\delta}\delta_{\sigma_\beta\sigma_\gamma}+(-1)^{n_y^\beta+n_y^\delta}\sigma_\beta\sigma_\delta(1-\delta_{\sigma_\alpha\sigma_\delta})(1-\delta_{\sigma_\beta\sigma_\gamma})]\ .$$

We distinguish $\sigma_\alpha=\sigma_\gamma$ and $\sigma_\alpha=-\sigma_\gamma$ in the second term:

$$\Gamma_{\alpha\gamma}{}^{2}=\sum_{\beta\delta>0}\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}[\delta_{\sigma_\alpha\sigma_\delta}+(-1)^{n_y^\beta+n_y^\delta}(1-\delta_{\sigma_\alpha\sigma_\delta})]$$
$$+\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle\rho_{\beta\delta}(1-\delta_{\sigma_\alpha\sigma_\gamma})[\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\gamma}-(-1)^{n_y^\beta+n_y^\delta}(1-\delta_{\sigma_\alpha\sigma_\delta})(1-\delta_{\sigma_\beta\sigma_\gamma})]\ .$$

Using the symmetry property of the density matrix $\rho_{\beta\delta}=\rho_{\delta\beta}$ we can limit the summation to $\beta\leq\delta$:

$$\Gamma_{\alpha\gamma}{}^{1}=\sum_{\beta\leq\delta}\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}(1+(-1)^{n_y^\beta+n_y^\delta})(1+(-1)^{n_y^\beta-n_y^\delta})(1-\tfrac{1}{2}\delta_{\beta\delta})\ ,$$

$$\Gamma_{\alpha\gamma}{}^{2}=\sum_{\beta\leq\delta}\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}[\delta_{\sigma_\alpha\sigma_\delta}+(1-\delta_{\sigma_\alpha\sigma_\delta})(-1)^{n_y^\beta+n_y^\delta}](1+(-1)^{n_y^\beta-n_y^\delta})(1-\tfrac{1}{2}\delta_{\beta\delta})\ .$$

The contribution with $\sigma_\alpha=-\sigma_\gamma$ is identically zero. We distinguish at last the case $n_y^\beta+n_y^\delta=$even:

$$\Gamma_{\alpha\gamma}{}^{1}=\sum_{\beta\leq\delta}\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle 2\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}(2-\delta_{\beta\delta})\ ,$$

$$\Gamma_{\alpha\gamma}{}^{2}=\sum_{\beta\leq\delta}\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}(2-\delta_{\beta\delta})\ .$$

For $n_y^\beta+n_y^\delta=$odd there exist no contributions to the direct potential.

B. Exchange potential

For the exchange field we have

$$G_{\alpha\gamma}{}^{1}=\sum_{\beta\delta}\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\delta}\delta_{\sigma_\beta\delta_\gamma}\ ,$$

$$G_{\alpha\gamma}{}^{2}=\sum_{\beta\delta}\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}\ .$$

The summation over the time-reversed states gives

$$G_{\alpha\gamma}{}^{1}=\sum_{\beta\delta>0}\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle\rho_{\beta\delta}[\delta_{\sigma_\alpha\sigma_\delta}\delta_{\sigma_\beta\sigma_\gamma}+(-1)^{n_y^\beta+n_y^\delta}\sigma_\beta\sigma_\delta(1-\delta_{\sigma_\alpha\sigma_\delta})(1-\delta_{\sigma_\beta\sigma_\gamma})]\ ,$$

$$G_{\alpha\gamma}{}^{2}=\sum_{\beta\delta>0}\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}(1+(-1)^{n_y^\beta+n_y^\delta})\ .$$

We distinguish $\sigma_\alpha=\sigma_\gamma$ and $\sigma_\alpha=-\sigma_\gamma$:

$$G_{\alpha\gamma}{}^{2}=\sum_{\beta\delta}\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}(1+(-1)^{n_y^\beta+n_y^\delta})\ ,$$

$$G_{\alpha\gamma}{}^{1}=\sum_{\beta\delta}\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}[\delta_{\sigma_\alpha\sigma_\delta}+(-1)^{n_y^\beta+n_y^\delta}(1-\delta_{\sigma_\alpha\sigma_\delta})]\ ,$$

$$G_{\alpha\gamma}{}^{1}=\sum_{\beta\delta}\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle\rho_{\beta\delta}(1-\delta_{\sigma_\alpha\sigma_\gamma})(1-\delta_{\sigma_\beta\sigma_\delta})[\delta_{\sigma_\alpha\sigma_\delta}-(-1)^{n_y^\beta+n_y^\delta}(1-\delta_{\sigma_\alpha\sigma_\delta})]\ .$$

We use the symmetry $\rho_{\beta\delta}=\rho_{\delta\beta}$ to limit the summations to $\beta\leq\delta$:

$$G_{\alpha\gamma}{}^{2}=\sum_{\beta\leq\delta}\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}[\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle+\langle\alpha\delta\,|\,V\,|\,\beta\gamma\rangle](1+(-1)^{n_y^\beta+n_y^\delta})\ ,$$

$$G_{\alpha\gamma}{}^{1}=\sum_{\beta\le\delta}\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}[\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle+\langle\alpha\delta\,|\,V\,|\,\beta\gamma\rangle][\delta_{\sigma_\alpha\sigma_\delta}+(-1)^{n_y^\beta+n_y^\delta}(1-\delta_{\sigma_\alpha\sigma_\delta})]\ ,$$

$$G_{\alpha\gamma}{}^{1}=\sum_{\beta\le\delta}\rho_{\beta\delta}(1-\delta_{\sigma_\alpha\sigma_\gamma})(1-\delta_{\sigma_\beta\sigma_\delta})[\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle-(-1)^{n_y^\beta+n_y^\delta}\langle\alpha\delta\,|\,V\,|\,\beta\gamma\rangle][\delta_{\sigma_\alpha\sigma_\delta}-(-1)^{n_y^\beta+n_y^\delta}(1-\delta_{\sigma_\alpha\sigma_\delta})]\ .$$

We distinguish $n_y^\beta+n_y^\delta=$even

$$\left.\begin{aligned}G_{\alpha\gamma}{}^{2}&=\sum_{\beta\le\delta}[\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle+\langle\alpha\delta\,|\,V\,|\,\beta\gamma\rangle]2\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}\\ G_{\alpha\gamma}{}^{1}&=\sum_{\beta\le\delta}[\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle+\langle\alpha\delta\,|\,V\,|\,\beta\gamma\rangle]\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}\end{aligned}\right\}\ \text{(field 0)}\ ,$$

$$G_{\alpha\gamma}{}^{1}=\sum_{\beta\le\delta}[\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle-\langle\alpha\delta\,|\,V\,|\,\beta\gamma\rangle]\rho_{\beta\delta}(1-\delta_{\sigma_\alpha\sigma_\gamma})(1-\delta_{\sigma_\beta\sigma_\delta})(2\delta_{\sigma_\alpha\sigma_\delta}-1)\ \text{(field 1)}\ ,$$

and $n_y^\beta+n_y^\delta=$odd,

$$G_{\alpha\gamma}{}^{1}=\sum_{\beta\le\delta}[\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle+\langle\alpha\delta\,|\,V\,|\,\beta\gamma\rangle]\rho_{\beta\delta}(1-\delta_{\sigma_\alpha\sigma_\gamma})(1-\delta_{\sigma_\beta\sigma_\delta})\ \text{(field 2)}\ ,$$

$$G_{\alpha\gamma}{}^{1}=\sum_{\beta\le\delta}[\langle\alpha\beta\,|\,V\,|\,\delta\gamma\rangle+\langle\alpha\delta\,|\,V\,|\,\beta\gamma\rangle]\rho_{\beta\delta}\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}(2\delta_{\sigma_\alpha\sigma_\delta}-1)\ \text{(field 3)}\ .$$

For the actual computation of fields 1 and 3 it is preferable to use the property

$$2\delta\sigma_\alpha\sigma_\delta-1=\sigma_\alpha\sigma_\delta\ .$$

Field 0 must be multiplied by $(1-\frac{1}{2}\delta_{\beta\delta})$ to avoid a double counting.

APPENDIX C: TREATMENT OF THE COULOMB INTERACTION

For the calculation of the mean field due to the electrostatic repulsion between protons we again use the separation method. Actually we use the identity

$$\frac{1}{|\vec{r}-\vec{r}'|}=\frac{2}{\sqrt{\pi}}\int_0^\infty e^{-(\vec{r}-\vec{r}')^2/\mu^2}\frac{d\mu}{\mu^2}\ .$$

The calculation of the Θ integrals (A4) is now straightforward and we find

$$\Theta_{\lambda_x\lambda_y\lambda_z}=\frac{2}{\sqrt{\pi}}\left[\frac{\pi^{3/2}\alpha_x\alpha_y\alpha_z\lambda_x!\lambda_y!\lambda_z!}{(\lambda_x/2)!(\lambda_y/2)!(\lambda_z/2)!}\right]^{1/2}(-1)^{(\lambda_x+\lambda_y+\lambda_z)/2}$$
$$\times\tfrac{1}{2}\int_0^\infty\frac{dt}{(2+\alpha_x{}^2t)^{(\lambda_x+1)/2}(2+\alpha_y{}^2t)^{(\lambda_y+1)/2}(2+\alpha_z{}^2t)^{(\lambda_z+1)/2}}\ ,$$

where we have set $t=\mu^2$ and $\lambda_x,\lambda_y,\lambda_z$ are always even.

The complication of the Coulomb interaction stems from the fact that the integration over the range couples the directions x,y,z and the three summations are no longer independent. A second difficulty is related to the integration over t, the calculation of which using recursion relations may become unstable for certain values of the deformation. We sketch the method we have adopted for a very precise numerical calculation of the integral

$$\Theta=\int_0^\infty\frac{dt}{(2+\alpha_1t)^{N_1+1/2}(2+\alpha_2t)^{N_2+1/2}(2+\alpha_3t)^{N_3+1/2}}\ .$$

We set

$$u^2=\frac{2}{2+\alpha t}\ \text{and}\ \frac{\alpha_i}{\alpha}=\beta_i\ .$$

$$\Theta=\frac{\sqrt{2}}{\alpha}\int_0^1\frac{(u^2/2)^{N_1+N_2+N_3}du}{(\beta_1+(1-\beta_1)u^2)^{N_1+1/2}(\beta_2+(1-\beta_2)u^2)^{N_2+1/2}(\beta_3+(1-\beta_3)u^2)^{N_3+1/2}}\ .$$

The optimum choice of α is to take it equal to the maximum of $(\alpha_1,\alpha_2,\alpha_3)$. The resulting integral can be calculated numerically with a Gauss-Legendre method. The above treatment has actually been limited to the case of the direct Coulomb potential. The treatment of the exchange contribution, although possible, would have been prohibitively long numerically. We have preferred to include, in a perturbative way, the contribution of the Coulomb exchange energy in the Slater approximation:

$$E_{c,\mathrm{ex}}=-\tfrac{3}{4}e^2\left[\frac{3}{\pi}\right]^{1/3}\int\rho_p^{4/3}d^3r\ .$$

APPENDIX D: CALCULATION OF THE PAIRING POTENTIAL

Before calculating the pairing field

$$\Delta_{\alpha\bar{\gamma}}=\tfrac{1}{2}\sum_{\beta\delta}\langle\alpha\bar{\gamma}\,|\,V\,|\,\widetilde{\beta\delta}\rangle\kappa_{\bar{\delta}\beta}\ , \tag{D1}$$

we consider the isospin quantum number. We assume pairing between proton-proton or neutron-neutron only. It follows that all four states $\alpha,\beta,\gamma,\delta$ must possess the same isospin projection. A two body force of the type

$$W+BP_\sigma-HP_\tau-MP_\sigma P_\tau$$

can be replaced by $(W-H)+(B-M)P_\sigma$. In the following we are going to work with a force of the type $W+BP_\sigma$ keeping in mind that the correct expression is $(W-H)+(B-M)P_\sigma$.

We can rewrite expression (D1) of the pairing potential as

$$\Delta_{\alpha\bar{\gamma}}=\tfrac{1}{2}\left[\sum_{\beta\delta\in q}\langle\alpha\bar{\gamma}\,|\,V\,|\,\beta\bar{\delta}\rangle\kappa_{\bar{\delta}\beta}-\langle\alpha\bar{\gamma}\,|\,V\,|\,\bar{\delta}\beta\rangle\kappa_{\bar{\delta}\beta}+\sum_{\bar{\beta}\bar{\delta}\in q}\langle\alpha\bar{\gamma}\,|\,V\,|\,\bar{\beta}\delta\rangle\kappa_{\delta\bar{\beta}}-\langle\alpha\bar{\gamma}\,|\,V\,|\,\delta\bar{\beta}\rangle\kappa_{\delta\bar{\beta}}\right].$$

By permutation of β and δ after the second summation and using the fact that $\kappa_{\bar{\delta}\beta}=-\kappa_{\beta\bar{\delta}}$ we get

$$\Delta_{\alpha\bar{\gamma}}=\sum_{\beta\delta\in q}\langle\alpha\bar{\gamma}\,|\,V\,|\,\widetilde{\beta\delta}\rangle\kappa_{\bar{\delta}\beta}\ .$$

We remark that β,δ can in fact be limited in a single block q and that the states of the block $\bar{q}$ contribute by a simple factor of 2.

Using the expression of $V=W+BP_\sigma$ we obtain

$$\begin{aligned}\Delta_{\alpha\bar{\gamma}}=\sum_{\beta\delta}\kappa_{\bar{\delta}\beta}[&\langle\alpha\bar{\gamma}\,|\,W\,|\,\beta\bar{\delta}\rangle\delta_{\sigma_\alpha\sigma_\beta}\delta_{\sigma_\gamma\sigma_{\bar{\delta}}}+\langle\alpha\bar{\gamma}\,|\,B\,|\,\beta\bar{\delta}\rangle\delta_{\sigma_\alpha\sigma_{\bar{\delta}}}\delta_{\sigma_\gamma\sigma_\beta}\\&-\langle\alpha\bar{\gamma}\,|\,W\,|\,\bar{\delta}\beta\rangle\delta_{\sigma_\alpha\sigma_{\bar{\delta}}}\delta_{\sigma_\gamma\sigma_\beta}-\langle\alpha\bar{\gamma}\,|\,B\,|\,\bar{\delta}\beta\rangle\delta_{\sigma_\alpha\sigma_\beta}\delta_{\sigma_\gamma\sigma_{\bar{\delta}}}]\ .\end{aligned}$$

We use the following relations between matrix elements:

$$\begin{aligned}&\langle\alpha\bar{\gamma}\,|\,V\,|\,\beta\bar{\delta}\rangle=\sigma_\gamma\sigma_\delta\langle\alpha\underline{\delta}\,|\,V\,|\,\beta\underline{\gamma}\rangle=(-1)^{n_y^\gamma+n_y^\delta}\sigma_\gamma\sigma_\delta\langle\alpha\underline{\gamma}\,|\,V\,|\,\beta\underline{\delta}\rangle\ ,\\&\langle\alpha\bar{\gamma}\,|\,V\,|\,\bar{\delta}\beta\rangle=(-1)^{n_y^\delta+n_y^\beta}\sigma_\gamma\sigma_\delta\langle\alpha\beta\,|\,V\,|\,\underline{\delta}\underline{\gamma}\rangle\ ,\\&\langle\alpha\beta\,|\,V\,|\,\gamma\delta\rangle=\langle\bar{\alpha}\bar{\beta}\,|\,V\,|\,\bar{\gamma}\bar{\delta}\rangle\ ,\end{aligned}\tag{D2}$$

and find

$$\begin{aligned}\Delta_{\alpha\bar{\gamma}}=\sigma_\gamma\sum_{\beta\delta}\sigma_\delta\kappa_{\bar{\delta}\beta}\{&[\langle\alpha\delta\,|\,W\,|\,\beta\gamma\rangle-\langle\alpha\beta\,|\,B\,|\,\delta\gamma\rangle(-1)^{n_y^\beta+n_y^\delta}]\delta_{\sigma_\alpha\sigma_\beta}\delta_{\sigma_\gamma\sigma_\delta}\\&+[\langle\alpha\delta\,|\,B\,|\,\beta\gamma\rangle-\langle\alpha\beta\,|\,W\,|\,\delta\gamma\rangle(-1)^{n_y^\beta+n_y^\delta}]\delta_{\sigma_\alpha\sigma_{\bar{\delta}}}\delta_{\sigma_\beta\sigma_{\bar{\gamma}}}\}\ .\end{aligned}$$

We distinguish, as in the case of the Hartree-Fock potential, $\sigma_\alpha=\sigma_\gamma$ and $\sigma_\alpha=\sigma_{\bar{\gamma}}$.

We limit the summations to $\beta\leq\delta$, using the small symmetry $\kappa_{\bar{\beta}\bar{\delta}}=\kappa_{\bar{\delta}\beta}$, and we finally obtain for $n_y^\beta+n_y^\delta=$even,

$$\Delta_{\alpha\bar{\gamma}}=\sigma_\gamma\sum_{\beta\le\delta}\sigma_\delta\kappa_{\bar{\delta}\beta}[\langle\alpha\delta\,|\,W-B\,|\,\beta\gamma\rangle+\langle\alpha\beta\,|\,W-B\,|\,\delta\gamma\rangle]\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}(2\delta_{\sigma_\alpha\sigma_\beta}-1)\quad\text{(field 0)}\,,$$

$$\Delta_{\alpha\bar{\gamma}}=\sigma_\gamma\sum_{\beta\le\delta}\sigma_\delta\kappa_{\bar{\delta}\beta}[\langle\alpha\delta\,|\,W+B\,|\,\beta\gamma\rangle-\langle\alpha\beta\,|\,W+B\,|\,\delta\gamma\rangle]\delta_{\sigma_\alpha\sigma_{\bar{\gamma}}}\delta_{\sigma_\beta\sigma_{\bar{\delta}}}\quad\text{(field 1)}\,,$$

and for $n_y^\beta+n_y^\delta=\text{odd}$,

$$\Delta_{\alpha\bar{\gamma}}=\sigma_\gamma\sum_{\beta\le\delta}\sigma_\delta\kappa_{\bar{\delta}\beta}[\langle\alpha\delta\,|\,W+B\,|\,\beta\gamma\rangle+\langle\alpha\beta\,|\,W+B\,|\,\delta\gamma\rangle]\delta_{\sigma_\alpha\sigma_{\bar{\gamma}}}\delta_{\sigma_\beta\sigma_{\bar{\delta}}}(2\delta_{\sigma_\alpha\sigma_\beta}-1)\quad\text{(field 2)}\,,$$

$$\Delta_{\alpha\bar{\gamma}}=\sigma_\gamma\sum_{\beta\le\delta}\sigma_\delta\kappa_{\bar{\delta}\beta}[\langle\alpha\delta\,|\,W+B\,|\,\beta\gamma\rangle+\langle\alpha\beta\,|\,W+B\,|\,\delta\gamma\rangle]\delta_{\sigma_\alpha\sigma_\gamma}\delta_{\sigma_\beta\sigma_\delta}\quad\text{(field 3)}\,.$$

These expressions can be further reduced using the identity $2\delta\sigma_\alpha\sigma_\beta-1=\sigma_\alpha\sigma_\beta$. We remark that the fields $\Delta_{0,1,2,3}$ are identical to the exchange fields $G_{0,1,2,3}$ provided one replaces ρ by κ, and allows for the multiplicative factors $W+B$. This is of a great practical importance as it allows the use of the same algorithm for the calculation of the exchange and pairing potentials. Another remark concerns the $W\pm B$ factor. For Gogny's interaction the only appreciable combination is the factor $W-B$ of the field 0. This field is the singlet one, which, as expected, leads to strong pairing.

For a density dependent δ interaction of the form $V=t(1+P_\sigma)\rho^\alpha\delta$ the pairing field is zero. As a matter of fact, the action of the antisymmetrization operator $(1-P_xP_\sigma P_\tau)$ reduces to $(1-P_\sigma)$, which combined to $(1+P_\sigma)$ from the force gives

$$(1+P_\sigma)(1-P_\sigma)=1-P_\sigma{}^2=0\,.$$

For the evaluation of the spin orbit pairing field one can calculate the associated densities. However, a large number of densities results, and motivated by the fact that their contribution, in the limit of axial deformations, has proven to be negligibly small, we have preferred to omit the spin orbit contribution to the pairing potential altogether. The same applies to the pairing Coulomb potential, the calculation of which is of the same degree of complication as the Hartree-Fock exchange Coulomb field.

*Present address: Department of Mathematics, Centre National d'Etudes des Télécommunications, 92131 Issy les Moulineaux, France.

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