Particle number Auctuations in the moment of inertia

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The nonphysical effects due to the false components introduced by the nonconservation of the particle number in the BCS states are eliminated in the theoretical values of the moment of inertia calculated by the microscopic cranking model. The states of the system are obtained by successive projections of the BCS states in the occupation number space. The moment of inertia appears then as a limit of a rapidly convergent sequence. The errors due to this false component have been numerically estimated and appear to be important both in the BCS states and in the matrix elements of the angular momentum. The predicted values of the moment of inertia satisfactorily reproduce the experimental data over a large number of nuclei within rare-earth and actinide regions with discrepancies ranging from 0.1% to 8% .

I. INTRODUCTION

Within the framework of the BCS theory, the pairing correlation effects, which are thoroughly taken into account, play a major role in the understanding of the different types of collective motion of the nucleus. Since the early works of Belyaev¹ on the moment of inertia for the rotation and of Bes^2 on the inertia parameters associated to the vibrations, the cranking model proposed by Inglis³ has had a major impact for such a description. Since then, many corrections to the cranking model related to the moment of inertia have been proposed. The effect of the interaction between quasiparticles has been studied following Migdal's⁴ theory for finite Fermi systems. With a formalism based on Green's functions, this approach allows the calculation of the moment of inertia while taking into account the reaction of the moment to the mean field to the collective rotational motion. This can be done by the introduction of the effective mass arising from the dependence of the speed of the singleparticle model. Similar results have been rederived by Belyaev using the formalism of self-consistent field⁵ and confirmed numerically using the generalized Nilsson potential. 6 The shortcomings of the cranking model have been revealed by Thouless and Valatin using the Hartree-Fock self-consistent method.⁷ However, the high number of matrix elements of the two-body interaction to be evaluated for the number of particles of the system makes such a calculation very impractical and expensive, particularly for nonlight nuclei. This method has been reviewed and generalized by Kunz and Nix^8 and the general equation of the cranking model, taking into account the linear term of the collective motion, has been obtained from a perturbative treatment of the dependent Hartree-Pock model.

However, the systematic study of moments of inertia using this method can only be done with the help of a very involved computation. Recently, Schaaser and Brink⁹ developed a new analytical formalism of the moment of inertia of the β and γ bands by using the intrinsic states of the interacting boson model (IBM). This model, very close to that of Bohr and Mottelson, 10 has been applied with success by Mishra and Mantri¹¹ to the numerical calculation of the moment of the inertia of the ground states of many rare-earth and actinide nuclei. However, this method is not free from phenomenology, and the good agreement obtained seems to be due to a rather excessive parametrization of the Hamiltonian of the model.

The different alternatives to the cranking model have not yet given the expected results for the moment of inertia, as the disagreements between theory and experiments remain important despite the different attempts to reduce them. Indeed, the theoretical values calculated since the cranking model has been developed¹² for the ground states of the rare-earth and actinide nuclei are systematically smaller than the experimental values by a factor of 10–40%. Moreover, neither the use of a realistic mean field as that of Woods and Saxon combined with a pairing strength which depends on the density of states in the vicinity of the Fermi sea^{13} nor the use of Nilsson's mean field with a pairing strength which depends on the isospin and which may or may not be a function of the parameter describing the deformation of the nucleus^{14,15} can reduce the disagreement between theory and experiment. This disagreement is certainly due to the nonconservation of the number of particles in the BCS wave functions. In fact, it has been shown that this nonconservation implies some nonphysical effects such as the existence of a critical value for the pairing strength under which there exist only trivial solutions of the BCS equations¹⁶ and the reversal of the energy spectrum in the calculations of the Hartree-Fock-Bogoliubov (HFB) type with a projection on the eigenstates of the moment of inertia.^{17,18} As is well established, the fluctuations of the number of particles affect the electromagnetic¹⁹ and beta²⁰ transitions, which are strongly dependent on the wave functions. In parallel, the moment of inertia is very sensitive to the wave functions, and as a result may also be affected by the fIuctuations of the number of particles. Up to recently, very few authors have taken into account the conserthe conservation of the number of particles in the calculations of the moment of inertia. By using Bayman's wave functions, 21 which are generated from BCS wave functions, Rich²² has evaluated the moment of inertia of five rare-earth nuclei. This method allows the approximate cancellation of the major fluctuations in the number of particles and is reduced, in its simplest form, to the usual BCS approximation. In a later development, Frauen d orf²³ studied the Coriolis antipairing effect in even-even rare-earth nuclei. By cancellation of the fluctuation in the number of particles, Frauendorf confirmed the experimental results on the back bending of the moment of inertia. He also established that only the cancellation of the nonphysical components of the BCS wave functions allows one to predict the angular momentum value for which the nucleus makes a transition from superfluid to normal one.

In this paper we propose an analytical and numerical study of the effects of nonconservation of the number of particles in the BCS wave functions on the moment of inertia. The method of projection of the BCS states on the occupation number space²⁴ is recalled in Sec. II; the projected states are then calculated and their corresponding energies evaluated. Since the projection destroys the orthonormalization of the BCS states, a new basis of orthonormal states which conserves the number of particles and which may represent the states of the system is built in Sec. III. Furthermore, the moment of inertia is also given. Section IV deals with the numerical results obtained. A comparison of these results with both the experimental and numerical ones obtained by different methods is also given.

II. STRICT CONSERVATION OF THE NUMBER OF PARTICLES

For the sake of coherence, we briefly recall the principle of the projection method previously developed.²⁴ In particular, expressions for the projected states and their energies are derived.

A. Projected wave functions

In the usual BCS theory, the intrinsic motion of 2P paired particles (neutrons or protons) is described by the intrinsic Hamiltonian

$$
H = \sum_{\nu > 0} \varepsilon_{\nu} (a_{\nu}^{\dagger} a_{\nu} + a_{\bar{\nu}}^{\dagger} a_{\bar{\nu}}) - G \sum_{\nu, \mu > 0} a_{\nu}^{\dagger} a_{\bar{\nu}}^{\dagger} a_{\mu} a_{\mu} , \qquad (1)
$$

where the pairing strength G is supposed to be constant and the state $|\tilde{v}\rangle = a^{\dagger}_{\tilde{v}}|0\rangle$ is the time reverse of the state $|v\rangle = a_v^{\dagger} |0\rangle$ and of energy ε_v . In Eq. (1) the time-reversal invariance of H is taken into account, which implies that $\epsilon_v = \epsilon_v$. In BCS theory the fundamental state is given by

$$
|\psi\rangle = \prod_{\nu>0} (u_{\nu} + v_{\nu} a_{\nu}^{\dagger} a_{\bar{\nu}}^{\dagger})|0\rangle , \qquad (2)
$$

where the parameters u_v and v_v represent the occupation and in occupation amplitudes of the state $|v\rangle$.

In the quasiparticle representation, defined with the help of the Bogoliubov-Valatin transformation, the state (2) represents the quasiparticle vacuum whose the creation and annihilation operators α_v^{\dagger} and α_v are such that $\alpha_{y}|\psi\rangle = 0$ for any v. The excited states of the system are described by an even number of quasiparticles. However, these BCS states are not eigenstates of particlenumber operator,

$$
N = \sum_{\nu > 0} \left(a_{\nu}^{\dagger} a_{\nu} + a_{\nu}^{\dagger} a_{\nu} \right) , \qquad (3)
$$

as only the mean value of this operator is supposed to be constant and equal to the real number of particles. The quasiparticle states describe rather a superposition of states of nuclei of neighboring masses. These differ by an even number of nucleons and correspond to the same value of the chemical potential λ , as well as the same half-width of the gap Δ .

Equation (2) shows clearly that the quasiparticles describe a superposition of states with $0, 2, 4, \ldots, 2\Omega$ particles, where Ω is the total degeneracy of the system.

It has been shown²⁴ that the sequence of states corresponding to P pairs of paired particles,

$$
|\psi_n\rangle = C_n \left[\sum_{k=0}^{n+1} \xi_k z_k^{-P} \prod_{\nu > 0} (u_{\nu} + z_k v_{\nu} a_{\bar{\nu}}^{\dagger} a_{\bar{\nu}})|0\rangle + \text{c.c.} \right],
$$
\n(4)

where C_n is a normalization factor and

$$
z_k = \exp[i k \pi/(n+1)] ,
$$

\n
$$
\xi_k = \begin{cases} 1 & \text{if } 0 < k < n+1, \\ \frac{1}{2} & \text{if } k = 0 \text{ or } k = n+1 \end{cases}
$$

converges toward the projected BCS (PBCS) state²⁵ or toward the fixed BCS (FBCS) state.²⁶ This convergence depends on whether the variational parameters u_v and v_v are evaluated before or after the projection. The relatively high speed at which this convergence occurs, as shown in Sec. IV, is explained by the fact that the state (4) has only components which correspond to $2P \pm 2l(n + 1)$ pairs, where l is any integer. In all that follows, we denote our discrete method of projection from the usual ones by SBCS.

In the same manner, the fluctuations of the number of nucleons can be easily dropped out of the states with any number of quasiparticles. As the moment of inertia is written in terms of matrix elements of the angular momentum operator, the only projected states having a nonzero contribution are

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$$
|(\nu\mu)_n\rangle = C_n^{\nu\mu} \left(\sum_{k=0}^{n+1} \xi_k z_k^{-(P-1)} a_{\nu}^{\dagger} a_{\mu}^{\dagger} \prod_{j \neq (\nu,\mu)} (u_j + z_k v_j a_j^{\dagger} a_j^{\dagger}) |0\rangle + \text{c.c.} \right),
$$
 (5a)

$$
|(\nu\nu\mu\eta)_n\rangle = C_n^{\nu\mu\eta} \left[\sum_{k=0}^{n+1} \xi_k z_k^{-(P-1)}(-v_\nu + z_k u_\nu a_\nu^\dagger a_\nu^\dagger) a_\mu^\dagger a_\eta^\dagger \prod_{j \neq (\nu,\mu,\eta)} (u_j + z_k v_j a_j^\dagger a_j^\dagger) |0\rangle + \text{c.c.} \right],
$$
 (5b)

and in general all states with an even number of paired quasiparticles in the states $(|v_1\rangle, |\tilde{v}_1\rangle), \ldots, (|v_k\rangle, |\tilde{v}_k\rangle)$ except in the states $(|\mu \rangle, |\tilde{\eta} \rangle)$:

$$
|(\nu_1\nu_1,\ldots,\nu_s\nu_s,\mu\eta)_n\rangle = C_n^{\nu_1\cdots\nu_s\mu\eta} \left[\sum_{k=0}^{n+1} \xi_k z_k^{-(P-1)} \prod_{l=1}^s (-\nu_l + z_k u_l a_l^\dagger a_l^\dagger) \prod_{j \neq \nu_1,\ldots,\nu_s} (u_j + z_k v_j a_j^\dagger a_j^\dagger)|0\rangle + \text{c.c.} \right], \quad (5c)
$$

where the coefficients $C_n^{\nu\mu},C_n^{\nu\mu\eta},C_n^{\nu_1\cdots\nu_s\mu\eta}$ are normalization factors.

B. Energies of the projected states

It may appear at first glance that it is difficult to evaluate the matrix elements of physical operators with the help of Eqs. (4) and (5). However, in general these observables commute with the number of particles operator, and furthermore their matrix elements exist only between those components with the same number of particles.

As such, the calculations in the quasiparticle representation are simplified. It is well known that any ket $|\phi\rangle$ of the Hilbert space of the states of a physical system described within the BCS method allows the following:

$$
|\phi\rangle = |\psi\rangle \langle \psi|\phi\rangle + \sum_{\nu} \alpha^{\dagger}_{\nu} |\psi\rangle \langle \psi|\alpha_{\nu}|\phi\rangle + \frac{1}{2} \sum_{\nu,\mu} \alpha^{\dagger}_{\nu} \alpha^{\dagger}_{\mu} |\psi\rangle \langle \psi|\alpha_{\mu} \alpha_{\nu}|\phi\rangle + \cdots
$$

It appears clearly that for zero and two paired quasiparticles, respectively, we have

$$
|\psi_n\rangle = C_n \left[\sum_{k=0}^{n+1} \xi_k z_k^{-P} \prod_v (u_v^2 + z_k v_v^2) \left[1 + (z_k - 1) \sum_v \frac{u_v v_v}{(u_v^2 + z_k v_v^2)} A_v^{\dagger} + \cdots \right] + \text{c.c.} \right] |\psi\rangle \tag{6a}
$$

$$
|(\nu\mu)_n\rangle = C_n^{\nu\mu} \left[\sum_{k=0}^{n+1} \xi_k z_k^{-(P-1)} \prod_{j \neq (\nu,\mu)} (u_j^2 + z_k v_j^2) \left[1 + (z_k - 1) \sum_{j \neq (\nu,\mu)} \frac{u_j v_j}{u_j^2 + z_k v_j^2} A_j^+ + \cdots \right] + \text{c.c.} \right] \alpha_v^{\dagger} \alpha_{\mu}^{\dagger} |\psi\rangle \;, \tag{6b}
$$

expressions in which $A_v^{\dagger} = \alpha_v^{\dagger} \alpha_v^{\dagger}$ is the pair creation operator for paired quasiparticles invariant under time reversal. It is shown below that it is unnecessary to write explicitly the development of the states (5b) and, in general, the states (5c) or their energies because they do not contribute to the moment of inertia.

The Hamiltonian H and its canonical transform in the quasiparticle representation connects only those components with the same number of pairs and keeps the number of nucleons invariant. As a result,

$$
E_n^0 = \langle \psi_n | H | \psi_n \rangle = 2(n+1)C_n \langle \psi_n | H | \psi \rangle \tag{7a}
$$

$$
E_n^{\nu\mu} = \langle (\nu\mu)_n | H | (\nu\mu)_n \rangle = 2(n+1) C_n^{\nu\mu} \langle (\nu\mu)_n | H \alpha_\nu^\dagger \alpha_\mu^\dagger | \psi \rangle \tag{7b}
$$

Using (6a) and (6b) allows (7) to become

$$
E_n^0 = E_0 + G \sum_{\gamma,\eta} u_{\gamma}^3 u_{\eta} v_{\eta}^3 v_{\gamma} \left[2(n+1)C_n^2 \left(\sum_{k=0}^{n+1} \xi_k z_k^{-P} (z_k - 1)^2 \prod_{j \neq (\gamma,\eta)} (u_j^2 + z_k v_j^2) + \text{c.c.} \right) \right],
$$

\n
$$
E_n^{\gamma\mu} = E_0 + E_{\gamma} + E_{\mu} + G \sum_{\gamma,\eta \neq (\gamma,\mu)} u_{\gamma}^3 u_{\eta} v_{\eta}^3 v_{\gamma} \left[2(n+1) (C_n^{\gamma\mu})^2 \left(\sum_{k=0}^{n+1} \xi_k z_k^{-(P-1)} (z_k - 1)^2 \prod_{j \neq (\gamma,\mu)} (u_j^2 + z_k v_j^2) + \text{c.c.} \right) \right],
$$

and the real part of (7) gives

$$
E_n^0 = E_0 - 4G \sum_{\gamma, \eta} u_{\gamma}^3 u_{\eta} v_{\eta}^3 v_{\gamma} \left[4(n+1) C_n^2 \sum_{k=0}^{n+1} \xi_k \sin^2 x_k R_k^{\gamma} \cos \psi_k^{\gamma} \eta \right],
$$
\n(8a)

$$
E_{n}^{\nu\mu} = E_{0} + E_{\nu} + E_{\mu} - 4G \sum_{\gamma, \eta \neq (\nu, \mu)} u_{\gamma}^{3} u_{\eta} v_{\eta}^{3} v_{\gamma} \left[4(n+1)(C_{n}^{\nu\mu})^{2} \sum_{k=0}^{n+1} \xi_{k} \sin^{2}(x_{k} R_{k}^{\nu\mu\gamma\eta}) \cos(\psi_{k}^{\nu\mu\gamma\eta} + 2x_{k}) \right],
$$
 (8b)

where E_0 and E_v are the BCS and quasiparticle energies, respectively, given by

$$
E_0 = 2 \sum_{v>0} (\varepsilon_v - \lambda - Gv_v^2) v_v^2 - \Delta^2 / G,
$$

\n
$$
E_v = [(\varepsilon_v - \lambda - Gv_v^2)^2 + \Delta^2]^{1/2}, \quad \Delta = G \sum_{v>0} u_v v_v.
$$

The normalization factors C_n and $C_n^{\nu\mu}$ are given by

$$
4(n+1)C_n^2 \sum_{k=0}^{n+1} \xi_k R_k \cos \psi_k = 1,
$$
\n
$$
4(n+1)(C_n^{\gamma \mu})^2 \sum_{k=0}^{n+1} \xi_k R_k^{\gamma \mu} \cos(\psi_k^{\gamma \mu} + 2x_k) = 1.
$$
\n(9b)

In Eqs. (8) and (9) we have chosen

$$
\gamma_{v} = 2u_{v}v_{v}, \quad \delta_{v} = u_{v}^{2} - v_{v}^{2},
$$
\n
$$
x_{k} = k\pi/[2(n+1)], \quad R_{k} = \prod_{v} \rho_{vk},
$$
\n
$$
\psi_{k} = \sum_{k} \phi_{vk} + (\Omega - 2P)x_{k}, \quad \rho_{vk} = (1 - \gamma_{v} \sin^{2} x_{k})^{1/2},
$$
\n
$$
\tan \phi_{vk} = -\delta_{v} \tan x_{k}, \quad |\phi_{vk}| \le \pi/2,
$$
\n
$$
R_{k}^{\nu_{1} \cdots \nu_{l}} = \prod_{v \ne \nu_{1}, \ldots, \nu_{l}} \rho_{vk},
$$
\n
$$
\psi_{k}^{\nu_{1} \cdots \nu_{l}} = \sum_{v \ne \nu_{1}, \ldots, \nu_{l}} \phi_{vk} + (\Omega - 2P + 2I)x_{k}.
$$

Although they are complicated forms, expressions (8) and (9) can be evaluated quite easily numerically.

III. MOMENT OF INERTIA

A. Orthonormalization of the projected BCS states

States (4) and (5), although they are normalized to unity, cannot be used to calculate the moment of inertia for they are not orthogonal and therefore cannot describe the excited states of the system. A basis of orthogonal states which keeps the number of particles strictly invariant can be obtained following the Schmidt procedure. The first two states of such a basis are the orthogonal states (4) and (5a). The projected state which is orthogonal to both (4) and (5a) and built from (5b) can be written as

$$
|(\nu\nu\mu\eta)_n\rangle_p = N_n(\nu\mu\eta) \left[|(\nu\nu\mu\eta)_n\rangle - |\psi_n\rangle \langle \psi_n |(\nu\nu\mu\eta)_n\rangle - \sum_{kl} |(kl)_n\rangle \langle (kl)_n |(\nu\nu\mu\eta)_n\rangle \right],
$$
\n(10a)

where $N_n(v, \mu, \eta)$ is a normalization factor.

In general, the orthonormal state having $(2s+2)$ quasiparticles of which 2s are paired is obtained from the recurrence relation

$$
\begin{split}\n&|\langle v_1v_1,\ldots,v_sv_s\mu\eta\rangle_n\rangle_P \\
&=N_n(v_1,\ldots,v_s\mu\eta)\left|\left|\langle v_1v_1,\ldots,v_sv_s\mu\eta\rangle_n\rangle-\left|\psi_n\right\rangle\langle\psi_n|\left(v_1v_1,\ldots,v_sv_s\mu\eta\rangle_n\rangle\right.\right.\\
&\left.-\sum_{kl}|\langle kl\rangle_n\rangle\langle\langle kl\rangle_n|\langle v_1v_1,\ldots,v_sv_s\mu\eta\rangle_n\rangle\right.\\
&\left.-\sum_{r=1}^{s-1}\sum_{t_1\cdots t_rkl}|\langle t_1t_1,\ldots,t_rt_rkl\rangle_n\rangle_P\langle\langle t_1t_1,\ldots,t_rt_rkl\rangle_n|\langle v_1v_1,\ldots,v_sv_s\mu\eta\rangle_n\rangle\right],\n\end{split} \tag{10b}
$$

for $s = 1, 2, \ldots$.

In fact, it is not necessary to write explicitly the states of this new basis because the only ones that have a nonzero contribution to the moment of inertia are the projected states with two quasiparticles. Indeed, as

$$
J_i|\psi_n\rangle = \sum_{kl} \frac{C_n}{C_n^{kl}} \langle k|J_i|1\rangle u_k v_l |(kl)_n\rangle, \quad i = x \text{ or } z \text{ ,}
$$
 (11)

where J_i is the *i* component of the angular momentum operator, and as the angular momentum keeps the number of particles invariant, we have

$$
\langle \psi_n | J_i | (\psi \mu)_n \rangle = (C_n / C_n^{\psi \mu}) \langle \nu | J_i | \mu \rangle (u_\nu v_\mu - u_\mu v_\nu) . \tag{12}
$$

Those relations show that the projection in the occupation number space changes the matrix elements of J_i in the quasiparticle representation by the multiplying factor $C_n/C_n^{\nu\mu}$. As for the other projected states, their contribution to the moment of inertia is zero. For example, for the state with four quasiparticles, we have

$$
\langle \psi_n | J_i | (\nu \nu \mu \eta)_n \rangle_p = N_n(\nu \mu \eta) \left[\langle \psi_n | J_i | (\nu \nu \mu \eta)_n \rangle - \sum_{kl} \langle \psi_n | J_i | (kl)_n \rangle \langle (kl)_n | (\nu \nu \mu \eta)_n \rangle \right]
$$

= 2(n+1)C_n^{\nu \mu \eta} N_n(\nu \mu \eta) \left[\langle \psi | J_i | (\nu \nu \mu \eta)_n \rangle - \sum_{kl} \langle \psi | J_i | kl \rangle \langle kl | (\nu \nu \mu \eta)_n \rangle \right],

and using the closure relation, it can easily be verified that

$$
\langle \psi | J_i | (\nu \nu \mu \eta)_n \rangle = \sum_{kl} \langle \psi | J_i | kl \rangle \langle kl | (\nu \nu \mu \eta)_n \rangle ,
$$

and so

 $\langle \psi_n | J_i | (\nu \nu \mu \eta)_n \rangle = 0$.

In general, for an even number of quasiparticle states, we still have

$$
\langle \psi_n | J_i | (\nu_1 \nu_1 \cdots \nu_s \nu_s \mu \eta)_n \rangle_P
$$

= $N_n(\nu_1, \ldots, \nu_s \mu \eta) \left[\langle \psi_n | J_i | (\nu_1 \nu_1 \cdots \nu_s \nu_s \mu \eta)_n \rangle - \sum_{kl} \langle \psi_n | J_i | (kl)_n \rangle \langle (kl)_n | (\nu_1 \nu_1 \cdots \nu_s \nu_s \mu \eta)_n \rangle \right] = 0.$

The cranking method allows the formulation of the moment of inertia without the fluctuation of the number of particles using the orthonormalized states previously developed. Let Oz be the symmetry axis for the nucleus supposed to be adiabatically cranked around the 0x axis. The moment of inertia is given by

$$
\mathcal{J} = \frac{\hbar^2}{2} \sum_{\nu\mu} \frac{|\langle \psi_n | J_x | (\nu\mu)_n \rangle|^2}{E_n^{\nu\mu} - E_n^0}, \qquad (13a)
$$

and with the help of (12), we get

$$
\mathcal{J} = \frac{\hbar^2}{2} \sum_{\nu\mu} \left[\frac{C_n}{C_n^{\nu\mu}} \right]^2 \frac{|\langle \nu | J_x | \mu \rangle|^2}{E_n^{\nu\mu} - E_n^0} (u_\nu v_\mu - u_\mu v_\nu)^2 , \quad (13b)
$$

where the $\langle v|J_x|\mu\rangle$ are the matrix elements in the particle-state representation of the operator J_{κ} .

The energies of the states of the system in the BCS method are modified because of the strict conservation of the number of particles. In addition to the usual reduction factor $(u_v v_\mu - u_\mu v_v)$ that is introduced in the matrix element $\langle v|J_x|\mu\rangle$ by the BCS method, the cancellation of the false components can be seen by the introduction of a supplementary factor $(C_n/C_n^{\nu\mu})$. This factor is the ratio of the overlap integral calculated between the wave functions written with the BCS and SBCS methods for two quasiparticles over that of the same for zero quasiparticles. Regarding the energies, as can be noted from (8), the fluctuation of the number of particles implies a second-order approximation which can be neglected in a first approximation. However, this fluctuation can modify considerably the matrix elements of J_x and hence the values of the moment of inertia.

B. Theoretical relation of the moment of inertia IV. NUMERICAL RESULTS: DISCUSSION

In order to show the numerical importance of the nonphysical effects contained in the BCS wave functions, the discrete projection method developed previously (see Secs. II and III) is applied to the rare-earth and actinide nuclei in their ground and fission isometric states. The energies and single-particle states of the Woods-Saxon mean field explicitly dependent on the nuclear shape have been chosen for this work. The elongation and neck pa-

FIG. 1. Variation of the overlap integral of the BCS and projected wave functions versus the elongation parameter c for the fundamental state of the (a) proton and (b) neutron systems of 230 Th.

TABLE I. Evolution of the energy difference of the zero quasiparticle projected states and BCS as well as the moment of inertia of neutrons, protons, and nucleus systems versus the extraction degree n of the false components for ^{236}U and ^{240}Pu in their fundamental and isomeric states.

236 U		Fundamental state					Isomeric state					
\boldsymbol{n}	BCS	$\mathbf 0$		2	3	4	BCS	0		2	3	$\overline{4}$
$E_n^0 - E_0$	$\mathbf{0}$	-0.59	-1.23	-1.24			$\mathbf{0}$	-0.85	-1.91	-2.11		
$(\mathcal{J})_{\text{neut}}$	81.38	92.90	95.01	95.03			169.31	214.17	218.95	218.95		
$(\mathcal{J})_{\text{prot}}$	37.79	39.23	40.26	40.26			74.32	70.09	69.14			
F	119.18	132.13	135.27	135.29			243.63	284.26	288.10			
240 Pu												
$E_n^0 - E_0$	$\mathbf{0}$	-0.05	-2.06	-2.61	-2.63		$\mathbf{0}$	-0.17	-0.36	-0.67		
$(\mathcal{J})_{\text{neut}}$	73.99	90.33	91.97	92.46	92.47		171.52	201.60	210.84	210.87		
$(\mathcal{J})_{\text{prot}}$	42.60	42.54	43.84	44.06			80.88	84.71	88.63	88.64		
F	116.54	132.87	135.81	136.52	136.53		252.40	286.31	299.47	299.52		

rameters of the nucleus c and h , respectively, are those obtained in minimizing the total deformation energy following the Strutinsky prescription.²⁷ For the rare-earth nuclei, those parameters have been calculated using the deformation parameters ε_2 and ε_4 (see Nilsson²⁸). The relation between c and h, and ε_2 and ε_4 , is obtained from the conservation of the nuclear volume. As for the actinides, c and h are taken directly from Ref. 13.

The pairing strength is chosen to be different for neutrons and protons and linearly dependent on the nuclear isospin 28 (see Fig. 1).

A. Numerical estimation of the fluctuation

The importance of the fluctuation of the number of particles and the efficiency of the method developed to calculate such fluctuations can be seen by numerical study of the convergence of the series of some observables. These observables are the moments of inertia (J)_{neut} and (J)_{prot} of the neutron and proton systems, the energy difference $(E_n^0 - E_0)$ of the zero quasiparticle projected states and BCS, and the overlap integral. The variation of these observables evaluated for 236 U and 240 Pu in their ground and isomeric states for an extraction degree

of false components n between 0 and 4 are given in Table I. A very rapid convergence is observed for each of these observables. The corresponding critical value is practically obtained for n close to 3 or 4 for all the sets. In addition to the appreciable difference between the values obtained by the BCS and projection methods, the cancellation of the fluctuation is reflected, as was expected, by an increase of the moment of inertia. Table II gives the behavior of the overlap integrals of the zero quasiparticle BCS and projected states as a function of n . It can be seen in Table II that for the case, chosen as an example, of wave functions of the neutrons of 254 Fm, the value of the overlap integral can be small compared with unity (up to 37%). This shows the importance of the false components in the BCS states and the need for their cancellation. Also, it can be seen that the nonphysical effects are mainly due to the components corresponding to $n = 1$ and 2, i.e., those components with a number of pairs equal to $P\pm 1$, $P\pm 3$, $P\pm 5$, ... and $P\pm 2$, $P\pm 6$, $P\pm 1Q, \ldots$.

Therefore, the main reason for the errors in the calculation of the moment of inertia is the consideration, in the BCS states, of the components of the nuclei with a mass close to that of the studied nucleus.

TABLE II. Convergence of the overlap integral of the zero quasiparticle BCS and projected wave functions versus the extraction degree n of the nonphysical components for the fundamental state of neutrons (up) and protons (down) systems.

$n_{\rm cut}$ and									
n	0		2	3	4				
156 Gd	0.7205	0.6565	0.6561						
	0.7163	0.6393	0.6386						
164 Dy	0.7071	0.5497	0.5400	0.5398					
	0.8239	0.8075							
176 Hf	0.7071	0.5176	0.4896	0.4883					
	0.7049	0.5892	0.5866						
236 U	0.7479	0.6973	0.6970						
	0.7483	0.7084	0.7083						
	0.7073	0.548	0.5330	0.5328					
^{240}Pu	0.7065	0.5699	0.5645						
	0.7071	0.5000	0.4126	0.3801	0.3730				
254 Fm	0.7071	0.5057	0.4585	0.4543	0.4541				

B. Results of the moment of inertia

The theoretical values for the moment of inertia of a large number of deformed even-even nuclei are calculated using (13b). These values are compared to both those obtained by other methods and experimental data. The moment of inertia of the ground state of rare-earth and actinide nuclei are given in Tables III and IV, respectively. The availability of the experimental results allows the representation of the ratio $\mathcal{I}_{\text{theor}} \mathcal{I}_{\text{expt}}$ of the theoretical moment, calculated by both the BCS and projection methods, over the experimental one (see Figs. 2 and 3). For the sake of comparison, in Fig. 2, the ratios, obtained by Ma and Tsang¹⁵ using the BCS method and by Mishra and Mantri¹¹ using the IBM model⁹ are plotted for the rare earths. In Fig. 3 the ratios corresponding to the results of Brack, Ledergerber, and Pauli,¹³ and the IBM model 11 are added for the actinides. Our BCS values for the rare earths are of the same order of slightly greater than those of Ma and Tsang. Both of these results lead to a ratio of $75-95\%$. For the actinides our BCS predictions are systematically lower by 25% than those of Brack, Ledergerber, and Pauli, except in the case of the californium isotopes, for which the present BCS calculations are closer to the experimental data. This discrepancy is probably due to the different choice of the pairing strength. The linear dependence of the nuclear isospin seems to lead to a better estimation of the moment of inertia than a dependence on the level density in the vicinity of the Fermi sea. Indeed, our results are in good agreement with those obtained by Sobiczewski and Bjornholm¹⁴ using a Nilsson mean field and a pairing strength dependent on the isospin as it is in our present work with a Woods-Saxon potential. Apart from the 236 U and 240 Pu nuclei, for which the IBM model gives a perfect agreement, it can be seen clearly from Figs. 2 and 3 that the results obtained by the projection method are closer to the experimental data than those of any other method. The good results obtained with the IBM model are due to the great number of phenomenologica1 parameters of the model. 9 The quality of the estimation obtained with the projection method proves the usefulness

TABLE III. Moments of inertia $(2J/\hbar^2)$ (MeV⁻¹) of rare-earth nuclei in their fundamental states evaluated by the BCS and SBCS calculations of the present work (the first two columns), the BCS model of Ref. 15 (third column), and the IBM cranking method of Ref. 11 (fourth column). The experimental values are in the fifth column.

	BCS	SBCS	BCS	IBM	
Nucleus	(present work)	(present work)	(Ref. 15)	cranking	Expt.
152 Sm	41.13	49.86	40.38		49.26
$^{154}\mathrm{Sm}$	66.06	77.39	54.97		73.17
$\rm ^{154}Gd$	36.59	45.89	38.22	60.6	46.6
$^{156}\mathrm{Gd}$	61.15	71.59	50.75	73.2	67.42
158 Gd	67.27	77.97	53.26	80.6	75.41
160 Gd	68.48	77.16	56.28	84	79.68
156 Dy	36.96	47.47	38.3	40.2	46.6
$^{158}\mathrm{Dy}$	47.90	58.90	45.6	59.6	57.4
$^{160}\mathrm{Dy}$	56.44	70.80	49.53	64.2	69.2
$\rm ^{162}Dy$	63.37	76.07	53.48	69.2	74.35
164 Dy	71.67	85.34	56.88		81.74
162 _{Er}	46.66	57.24	45.21	58.6	58.6
164 _{Er}	53.29	65.38	50.17	64.4	65.72
166 _{Er}	58.48	70.35	53.98	69.2	74.44
$^{168}\mathrm{Er}$	67.14	81.16	56.54		75.19
$^{170}\mathrm{Er}$	56.86	70.06	59.19		75.67
$\rm ^{166}Yb$	45.35	58.68	45.94	58.6	58.94
168 Yb	57.58	71.25	50.20	64.2	68.26
170Yb	60.77	73.55	53.51	69.2	71.26
172Yb	60.55	73.17	57.45	73.8	76.24
174Yb	64.35	75.55	59.44	78.4	78.43
$^{174}\mathrm{Hf}$	56.14	66.95	51.77		65.93
176 Hf	59.98	69.94	56.25		67.87
178 Hf	56.51	67.67	54.77		64.38
180 Hf	48.25	60.51	57.96		64.31
180W	43.82	56.80	49.98		57.91
182W	46.33	58.05	53.28		60.00
184W	45.48	56.67	46.07		53.96
186W	39.86	49.04	39.18		48.98
184 Os	40.71	51.57	48.58		50.08
186 Os	36.53	46.96	43.20		43.73
$^{188}\mathrm{Os}$	31.46	40.99	37.72		37.4

TABLE IV. Moments of inertia $(2J/\hbar^2)$ (MeV⁻¹) of the actinide nuclei in their fundamental states evaluated by the BCS and SBCS calculations of the present work (the first two columns), the BCS model of Refs. 13 and 14 (the following two columns), and the IBM cranking method of Ref. 11 (fifth column). The experimental values are in the sixth column.

					IBM	
	BCS	SBCS	BCS	BCS	cranking	
Nucleus	(present work)	(present work)	(Ref. 14)	(Ref. 13)	(Ref. 15)	Expt.
$\rm ^{224}Ra$	53.9	68.3		102		68
226 Ra	68.7	84.3	64	118		88
228 Ra	89.7	99.3		114		100
224 Th	47.1	60.5		102		62
226Th	60.7	76.1		140	103.8	82
$\rm ^{228}Th$	88.2	98.8		132	112.2	104
$\rm ^{230}Th$	98.7	108.2	88	128	120.4	113
$\rm ^{232}Th$	114.6	127.3	104	146	128.6	120
234 Th	119	132		132		126
230 [J	84.9	102.0		148	116.6	116
232 U	97.7	110.3		144	122.8	126
234 U	113.4	127.9	114	160	129	138
236 U	119.2	135.3	104	150	135.4	132
238 U	116.0	131.0	94	128		134
$^{236}\mathrm{Pu}$	114.1	132.2	111	156	130.2	135
^{238}Pu	124.4	140.3	103	140	135.2	136
240 Pu	116.6	136.5	102	130	140.4	140
242 Pu	114.7	129.0	108	126	145.8	135
244 Pu	120.2	138.6	114	138		133
$\mathrm{^{242}Cm}$	121.6	138.6	107	140		142
$\mathrm{^{244}Cm}$	120.2	138.1	108	136		140
$\rm ^{246}Cm$	128.1	146.8	109	150		140
$\mathrm{^{248}Cm}$	127	142.6	101	136		138
248 Cf	136.1	155.4		144		142
250Cf	133.7	150.9		126		142
252Cf	131.3	147.6		118		136
$^{254}\mathrm{Fm}$	105.3	131.8		118		136

of canceling the nonphysical components due to the Auctuations of the number of particles. The modifications of the moment of inertia due to this projection are approximately the same for all the nuclei within the same region. Indeed, the gap $|\mathcal{J}_n - \mathcal{J}_{BCS}|/\mathcal{J}_{expt}$ is practically constant and is of the order of 0.13 for the actinides and 0.18 for the rare earths. Moreover, a surprising agreement between the projected and experimental moments for the translational nuclei as the Ra and the light Th isotopes is clearly observed. Contrary to this observation, the disagreement for the other methods, previously attributed to a possible nonapplicability of the rotational model for these nuclei, is in fact mainly due to the important

fluctuations of the number of particles. The cancellation of the false components in these nuclei leads to an important increase of the pairing factors in comparison with other actinide nuclei. For example, in Table V some of the ratios $(C_n/C_n^{\gamma\mu})$ are given for levels of the ²³⁰Th in the vicinity of the Fermi level. This shows that the ratio is generally higher than unity. Table VI gives the values of the moment of inertia for the isomeric states of the actinides, calculated by the different methods mentioned in this paper. The intrinsic quality of the results obtained using the different methods cannot be appreciated because of the lack of experimental data. However, for the three nuclei ²³⁶U, ²³⁸U, and ²⁴⁰Pu, the projection method

TABLE V. Values of the $(C_n/C_n^{\gamma\mu})$ ratio for the closest levels to the Fermi level for the proton and neutron systems of ²³²Th.

		Protons					Neutrons		
	43	44	45	-46		69	70		
44	1.060				70	1.076			
45	1.134	1.152			71	1.089	1.096		
46	1.232	1.265	1.418		72	1.215	1.228	1.252	
47	1.043	1.062	1.141	.216	73	1.076	1.084	1.099	1.189

FIG. 2. Comparison between experimental and theoretical values of moments of inertia for rare-earth nuclei in their fundamental state. Points $(+ - - +)$ are our BCS results, $(\bullet \rightarrow \bullet)$ our SBCS results, $(\bullet \rightarrow \bullet)$ show the calculations of Ref. 15 with the BCS model, and $(X - - \times)$ those of Ref. 11 with the IBM model.

FIG. 3. Same as Fig. 2 for actinide nuclei. Points $+$ - $-$ + $+$) are our BCS results, (\bullet - \bullet) our SBCS results,
 \blacktriangle - \blacktriangle) show the calculations of Ref. 13 with the BCS model, and $(X - - \times)$ those of Ref. 11 with the IBM model.

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leads to results in excellent agreement with the experimental values. Furthermore, it can be seen that the BCS estimation of the present work is systematically lower by about 15% than that of the projection method. It should be noted that the SBCS results are closer to those of Brack, Ledergerber, and Pauli than those of Sobiczewski and Bjornholm, while for the fundamental states we have better agreement with the results of Sobiczewski and Bjornholm than those of Brack, Ledergerber, and Pauli.

V. CONCLUSION

We have studied the effects of the fluctuations of the number of particles inherent to the usual BCS method on the moment of inertia of many even-even rare-earth and actinides nuclei. The nonphysical effects due to these fluctuations have been canceled by a discrete projection method on the eigenstates of the particle-number operator. After having built new states which strictly conserve the number of particles and the corresponding energies, a

new expression for the moment of inertia was deduced using the usual cranking method.

The cancellation of the nonphysical effects is reflected by the variation of the usual pairing reduction factor of the matrix elements of the angular momentum. This projection method is found to be easy, powerful, and well adapted to the numerical calculation. The theoretical predictions of the moment of inertia are in good agreement with the corresponding experimental values both for the rare-earth and actinide nuclei. Some improvements to these calculations could be obtained by relaxing some restrictive hypothesis such as the taking into account of the rotation-pairing interaction term or the nonaxiality of the mean potential, which can modify the values of the moment of inertia of some nuclei as the light actinides.

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- ¹S. T. Belyaev, Mat. Fys. Medd. Dan. Vid. Selsk. 31, 11 (1959).
- D. R. Bes, Mat. Fys. Medd. Dan. Vid. Selsk. 33, 11 (1961).
- 3D. R. Inglis, Phys. Rev. 96, 1059 (1954); 97, 701 (1955).
- 4A. B. Migdal, Nucl. Phys. 13, 655 (1959).
- 5S. T. Belyaev, Nucl. Phys. 64, 16 (1965).
- ⁶M. Brack, J. Damgaard, A. S. Jensen, H. C. Pauli, V. M. Strutinski, and C. Y. Wong, Rev. Mod. Phys. 44, 320 (1972).
- 7D. J. Thouless and J. G. Valatin, Nucl. Phys. 31, 211 (1962).
- ⁸J. Kunz and J. R. Nix, Nucl. Phys. A426, 353 (1984).
- $9H$. Schaaser and D. M. Brink, Nucl. Phys. A452, 1 (1986).
- ¹⁰A. Bohr and B. R. Mottelson, Nuclear Structure (Benjamin, Reading, MA, 1975), Vol. II.
- ¹¹A. Mishra and A. N. Mantri, Z. Phys. A 328, 171 (1987).
- ¹²S. G. Nilsson and O. Prior, Mat. Fys. Medd. Dan. Vid. Selsk. 32, 2 (1960); J. J. Griffin and M. Rich, Phys. Rev. 118, 850 (1960); G. Gustafsson, I. L. Lamm, B. Nilsson, and S. G. Nilsson, Ark. Fys. 36, 613 (1967); J. Krumlinde, Nucl. Phys. 160, 471 (1971)[~]
- ¹³M. Brack, T. Ledergerber, and H. C. Pauli, Nucl. Phys. A234, 185 (1974).
- ¹⁴A. Sobiczewski and S. Bjornholm, Nucl. Phys. A202, 274 (1973).
- ¹⁵C. W. Ma and C. F. Tsang, Phys. Rev. C 11, 213 (1975).
- ¹⁶M. Rho and J. O. Rasmussen, Phys. Rev. 135, B1295 (1964); H. J. Mang, J. O. Rasmussen, and M. Rho, Phys. Rev. 141, 941 (1966); H. C. Pradhan, Y. Nogami, and J. Law, Nucl. Phys. A201, 357 (1973).
- $17K.$ Goeke, J. Garcia, and A. Faessler, Nucl. Phys. A208, 477 (1973).
- M. Fellah, T. F. Hammann, and D. E. Medjadi, Phys. Rev. C 8, 1585 (1973).
- $19M$. Fellah and T. F. Hammann, Phys. Rev. C 10, 284 (1974); J. Phys. (Paris) 36, 461 (1975).
- 20 M. Fellah and T. F. Hammann, Nuovo Cimento A 30, 239 (1975).
- 21 B. F. Bayman, Nucl. Phys. 15, 33 (1960).
- $22M$. Rich, Nucl. Phys. A90, 407 (1967).
- ²³S. Frauendorf, Nucl. Phys. **A263**, 150 (1976).
- 24 M. Fellah and T. F. Hammann, Phys. Rev. C 20, 1560 (1979).
- ²⁵A. K. Kerman, R. D. Lawson, and M. H. Macfarlane, Phys. Rev. 124, 162 (1961).
- ²⁶K. Dietrich, H. J. Mang, and J. H. Pradal, Phys. Rev. 135, B22 (1964).
- ²⁷H. C. Pauli, Phys. Rep. C 7, 35 (1973).
- 28 G. Nilsson et al., Nucl. Phys. A131, 1 (1969).