Approximate energy correction for particle number symmetry breaking in constrained Hartree-Fock plus BCS calculations

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An approximate restoration of the particle number symmetry, in the manner of Lipkin-Nogami, is numerically investigated in the context of constrained Hartree-Fock plus BCS calculations. Its effect is assessed in a variety of physical situations like potential energy landscapes in transitional nuclei, shape isomerism at low spin, and fission barriers of actinide nuclei.

I. INTRODUCTION

Following the suggestion of Bohr, Mottelson, and Pines[1] and Belyaev,[2] it has become customary to use the BCS ansatz[3] to approximately account for pairing correlations in atomic nuclei. As is well known however, this approximation breaks the particle number (N) symmetry of the Hamiltonian. Whereas for large fermion number, the resulting fluctuations in N are negligible, this is not at all the case for the relatively small number of particles interacting in the nucleus. Bayman[4] has shown that the BCS wave function could be derived from a fixed particle-number solution as a saddle point approximation under conditions that are not met, in general, in actual nuclei. It is then clear that the description of any observable as expectation values in such BCS states may be impaired by this artificial symmetry breaking. To restore the symmetry, one has currently used either the projection formalism (projection after[5] or better before[6] variation) or a removal of number-dispersion spurious effects in a random-phase approximation (RPA) type of approach.[7] For the study of ground-state wave functions, the projection method has been the most widely used and many approximation schemes for it have been devised as (i) a renormalization of pairing matrix elements,[8] (ii) a discretization of the Fowler-Darwin-type integrals entering an expression of the projected energy[9] from which practical calculations have been performed,[10] (iii) the Gaussian overlap approximation,[11] (iv) a Taylor expansion of the BCS energy as a function of the number of particles around the BCS expectation value of the particle-number operator,[12] (v) the limit of weak symmetry violation,[13–14] (vi) a method initiated in a broader context by Lipkin[15] and specifically proposed[16] and further developed[17–20] by Nogami and collaborators for the BCS wave-function problem.

In this paper, we focus on the latter approximate formulation of the broken symmetry restoration, which is usually referred to and used[21] as the Lipkin-Nogami approach. Within this formalism, we assess the importance of correctly handling the particle-number symmetry for the microscopic evaluation of potential energy surfaces. In Sec. II, we review the general concepts and notation that are involved in this approach and generalize them to our constrained variational problem. The results of self-consistent calculations performed in different regions of nuclei are discussed in Sec. III, whereas our main conclusions are drawn in Sec. IV.

II. GENERAL OUTLINE OF THE METHOD

A. The original Lipkin-Nogami approach

Independent particle many-body descriptions meet with the general problem of correlations necessarily brought in by the conservation laws arising from dynamical symmetries. Lipkin has proposed in Ref. 15, to interpret uncorrelated wave functions as eigensolutions of a modified Hamiltonian $\overline{H}$ derived from the original one H by substracting the characteristic energy H_c associated with the conserved quantity. He took as examples of H_c the translational energy of a localized system of bound particles, the plasmon energy of a free electron gas, the rotational energy of a deformed quantal object, and finally the energy associated with a change in the number of particles for a BCS wave function. In the latter case, Lipkin defines $\overline{H}$ as

$$\overline{H}=H-f(N)\ , \tag{2.1}$$

where the characteristic energy H_c is here a function f of the particle number operator N. Assuming the latter to be a smoothly varying function of N, one can Taylor-expand it. At first order, one gets the Lagrange multiplier variational method in use in ordinary BCS treatments. Lipkin[15] questioned the validity of dropping the next terms in the expansion, and Nogami[16] further developed the approach by explicitly considering the second-order term.

For that, let us consider a normalized BCS wave function $|\psi_n\rangle$ for which the expectation value of N is denoted n (hence the subscript). We may project $|\psi_n\rangle$ on normalized eigenstates $|\phi_m\rangle$ of the operator N with the eigenvalue m:

$$|\psi_n\rangle = \sum_m c_{nm}|\phi_m\rangle \ . \tag{2.2}$$

Given an operator Q commuting with N, we define by $q(m)$ its expectation values on the $|\phi_m\rangle$ projected states. At this point, we make the assumption formulated by Lipkin, stating that $q(m)$ is an analytical function of m:

$$q(m)=\langle\phi_m|Q|\phi_m\rangle=q_0+q_1m+q_2m^2+\cdots \ , \tag{2.3}$$

where the q_p coefficients are real, given the hermiticity of Q and hereby defining a Hermitian operator $q(N)$ as

$$q(N)=q_0+q_1N+q_2N^2+\cdots \ . \tag{2.4}$$

It should be made clear now that $q(m)$ and $q(N)$ depend on the initial BCS wave function $|\psi_n\rangle$.

It follows from the definition (2.4) of $q(N)$ that the diagonal matrix elements of $Q-q(N)$ between $|\phi_m\rangle$ states are vanishing. Its nondiagonal matrix elements are equal to zero as well, if we define the ϕ's as common eigenvectors of the commuting Q and N operators. From the preceding, we trivially infer that

$$\langle\psi_n|(Q-q(N))N^\alpha|\psi_n\rangle=0 \tag{2.5}$$

for any non-negative integer α.

We now make a second assumption, which consists in truncating up to second order the expansions (2.3) and (2.4). It therefore results from Eq. (2.5) that

$$q_0=\langle\psi_n|Q-q_1N-q_2N^2|\psi_n\rangle \ . \tag{2.6}$$

In what follows we will denote as $\bar{Q}$ the *corrected* operator $Q-q_1N-q_2N^2$. As a consequence of Eq. (2.6), one is able to express, upon assuming a practical knowledge of q_1 and q_2, the expectation values of the *true* operator Q in projected states $|\phi_n\rangle$ in terms of expectation values of $\bar{Q}$ in the (unprojected) BCS wave function $|\psi_n\rangle$:

$$\langle\phi_n|Q|\phi_n\rangle=\langle\psi_n|\bar{Q}|\psi_n\rangle+q_1n+q_2n^2 \ . \tag{2.7}$$

To completely solve our problem, we need therefore to provide satisfactory requirements about the determination of q_1 and q_2. At this step, the inherent arbitrariness is manifested as a choice to be made among an infinity of relations that these coefficients should fulfill in an exact (not truncated) expansion of $q(m)$. The criterion for such a guess consists in a reproduction of exact results in some model case situations, as well as possible for all regimes of pairing correlations, singularly in the weak pairing strength *critical* case. In previous versions of the Lipkin-Nogami method[16–18] a prescription has been proposed that was later proven[19–20] to be advantageously replaced as defined in the following. Indeed, Goodfellow and Nogami[19] have determined q_1 and q_2 through

$$\langle\phi_m|\bar{Q}N|\phi_n\rangle=\langle\phi_n|\bar{Q}N^2|\phi_n\rangle=0 \ , \tag{2.8}$$

which is clearly fulfilled in the exact case [see Eq. (2.5)] and is merely postulated in the present case.

B. Variational ground state solutions

In what follows, we will restrict ourselves to the particular case where Q is the microscopic Hamiltonian H (including a kinetic energy T and a two-body interaction V) and only the component $|\phi_n\rangle$ of the BCS wave function $|\psi_n\rangle$ (i.e., only the $|\phi_m\rangle$ with $m=n$) is considered. The projected energy E_n is thus given in this case, through Eq. (2.7), as

$$E_n=\langle\phi_n|H|\phi_n\rangle=\langle\psi_n|\bar{H}|\psi_n\rangle+\lambda_1n+\lambda_2n^2 \ , \tag{2.9}$$

where the expansion coefficients of the expectation value of H between projected states are noted, as is customary, by λ_1 and λ_2.

Now, in the context of a projection before variation approach, one must minimize E_n with respect to all possible BCS wave functions $|\psi_n\rangle$, i.e. (assuming λ_1 and λ_2 to be known),

$$\delta(E_n)=\delta(\langle\psi_n|\bar{H}|\psi_n\rangle)=0 \ . \tag{2.10}$$

The present variational problem assumes therefore the form discussed by Lipkin,[15] where symmetry-breaking solutions are to be interpreted as eigensolutions of an *effective* (i.e., corrected) energy operator.

For a BCS wave function $|\psi_n\rangle$ built on the so-called canonical basis $\{i,j,\ldots\}$ (made of the eigenstates of the one-body reduced density matrix ρ with eigenvalues v_i^2), one has

$$\langle\psi_n|H|\psi_n\rangle=\sum_i v_i^2t_i+\tfrac{1}{2}\sum_{ij}v_i^2v_j^2V_{ij}+\tfrac{1}{4}\sum_{ij}u_iu_jv_iv_jG_{ij} \ , \tag{2.11}$$

where with the usual notation one defines

$$u_i^2=1-v_i^2, \quad t_i=\langle i|T|i\rangle \ ,$$

$$V_{ij}=\langle ij|V|\tilde{i}\tilde{j}\rangle, \quad G_{ij}=\langle i\tilde{i}|V|j\tilde{j}\rangle \ .$$

Upon varying

$$E_n=\langle\psi_n|H|\psi_n\rangle-\lambda_1\langle\psi_n|N|\psi_n\rangle-\lambda_2\langle\psi_n|N^2|\psi_n\rangle$$

with respect to the single particle states $|i\rangle$ and the occupation probabilities v_i^2, one gets Hartree-Fock-type equations and BCS-type equations, respectively. The latter is written as

$$e_i-\Delta_i\frac{u_i^2-v_i^2}{2u_iv_i}-\lambda_1-2\lambda_2(n+u_i^2-v_i^2)=0 \ , \tag{2.12}$$

where

$$e_i=t_i+\sum_j v_j^2V_{ij}, \quad \Delta_i=-\tfrac{1}{2}\sum_j G_{ij}u_jv_j, \quad n=\sum_i v_i^2 \ .$$

Equation (2.12) can be cast into the standard BCS formal framework by defining

$$\epsilon_i=e_i+4\lambda_2v_i^2 \ ,$$
$$\lambda=\lambda_1+2\lambda_2(n+1) \tag{2.13}$$

to yield the variational equations

$$\epsilon_i-\lambda-\Delta_i\frac{u_i^2-v_i^2}{2u_iv_i}=0\ , \tag{2.14}$$

whose solutions are

$$v_i^2=\frac{1}{2}\left[1-\frac{\epsilon_i-\lambda}{E_i}\right]^{1/2}\ ,$$
$$E_i=[(\epsilon_i-\lambda)^2+\Delta_i^2]^{1/2}\ . \tag{2.15}$$

From now on, we will make the standard seniority force ansatz

$$\forall i,j;\ \langle\bar{i}\bar{i}|V|\tilde{j}\tilde{j}\rangle=-G\ , \tag{2.16}$$

and consequently

$$\forall i;\ \Delta_i=-\frac{G}{2}\sum_j u_jv_j\ . \tag{2.17}$$

The next problem consists in determining λ_1 and λ_2 through Eqs. (2.8) for $\bar{H}$. The first one is equivalent to the variational equation (2.12), whereas the other leads after lengthy but straightforward calculations[19,22] to

$$\lambda_2=\frac{G}{4}\frac{\left[\sum'u_i^3v_i\right]\left[\sum'u_iv_i^3\right]-\sum'u_i^4v_i^4}{\left[\sum'u_i^2v_i^2\right]^2-\sum'u_i^4v_i^4}\ , \tag{2.18}$$

where, throughout this paper, the $\sum'$ over i runs only over half the single-particle states i. As in usual BCS calculations, the Lagrange multiplier λ (and therefore λ_1 since λ_2 is known) is fixed by the particle number conservation.

The energy difference between the approximate projected energy and the BCS (unprojected) energy is thus given as

$$\Delta E=\lambda_1 n+\lambda_2\langle\psi_n|N^2|\psi_n\rangle\ , \tag{2.19}$$

which leads to

$$\Delta E=-4\lambda_2\sum'u_i^2v_i^2\ . \tag{2.20}$$

C. The case of one-body operators

Even though the Lipkin-Nogami projection method is *a priori* designed for the correction of the energy expectation value in a variational approach, one may try to use the BCS wave function resulting from the approximate projection process to compute expectation values of operators other than the energy. The basic motivation for that is to yield in cases where ordinary BCS approaches yield zero gap trivial solutions an educated guess of the influence of pairing correlations that would emerge from a more sophisticated pairing treatment. There are cases where this would be clearly useless when for instance one considers the particle number variance. One expects, however, that for one-body operators, the Lipkin-Nogami BCS wave function might be of interest.

Let us therefore consider a one-body operator Q (thus commuting with N) assuming further its even character under time reversal. We may consider it as the Q operator of Sec. II A.

Defining $\bar{Q}$ as previously, q_1 and q_2 are given by the solution of two linear equations stemming from Eqs. (2.8):

$$\sum'u_i^2v_i^2(Q_i-q_1-2q_2w_i)=0 \tag{2.21}$$

$$\sum'u_i^2v_i^2w_i(Q_i-q_1-2q_2w_i)-4q_2\left[\left[\sum'u_i^2v_i^2\right]^2-\sum'u_i^4v_i^4\right]=0\ . \tag{2.22}$$

From Eqs. (2.21) and (2.22) one gets q_1 and q_2. For instance the latter is given by

$$q_2=\frac{1}{2}\frac{\left[\sum'Q_ik_i^2\right]\left[\sum'k_i^2w_i\right]-\left[\sum'k_i^2\right]\left[\sum'Q_ik_i^2w_i\right]}{\left[\sum'k_i^2w_i\right]^2-\left[\sum'k_i^2w_i^2\right]\left[\sum'k_i^2\right]-2\left[\sum'k_i^2\right]\left[\left[\sum'k_i^2\right]^2-\sum'k_i^4\right]}\ , \tag{2.23}$$

where

$$w_i=u_i^2-v_i^2+n\ ,$$
$$k_i^2=u_i^2v_i^2\ , \tag{2.24}$$
$$Q_i=\langle i|Q|i\rangle\ .$$

The effect of the projection onto good particle number states is given by

$$\Delta Q=-4q_2\sum'k_i^2\ . \tag{2.25}$$

This will be applied below to the case where Q is the axial quadrupole operator, in the context of constrained Hartree-Fock calculations. Indeed, in adiabatic time-dependent Hartree-Fock descriptions of large amplitude collective motion, one computes the deformation energy surface through constrained Hartree-Fock calculations, where the constraining field defines the collective variable by its expectation value.[23] For the matter under discussion here, one is thus led to replace in the variational approach H with $H-\mu Q$, or $\bar{H}$ with $\bar{H}-\mu\bar{Q}$. Consequently the BCS-type variational equations are formally unchanged upon replacing λ_1 with $\tilde{\lambda}_1=\lambda_1-\mu q_1$ and λ_2 with $\tilde{\lambda}_2=\lambda_2-\mu q_2$. As a result, one then obtains a deformation energy surface where *both* the energy and the collective variables are corrected for particle-number spurious fluctuations.

In another case of interest, one could focus on the

particle-number fluctuation corrections related with the expectation value of a one-body operator Q in a given single-particle state (as for instance the occupation of a particular Hartree-Fock single-particle state i_0). One readily reduces the previous equations for q_2 by noting that

$$Q_i=\delta_{i,i_0}Q_{i_0}\ ,$$

leading to

$$\Delta Q_{i_0}=\frac{-2Q_{i_0}k_{i_0}^2\left[\sum{}'k_i^2\right]\left[\sum{}'k_i^2w_i-w_{i_0}\sum{}'k_i^2\right]}{\left[\sum{}'k_i^2w_i\right]^2-\left[\sum{}'k_i^2w_i^2\right]\left[\sum{}'k_i^2\right]-2\left[\sum{}'k_i^2\right]\left[\left[\sum{}'k_i^2\right]^2-\sum{}'k_i^4\right]}\ . \tag{2.26}$$

The above result[22] has recently been used by the authors of Ref. 24 to study the depletion of the $3s_{1/2}$ proton state in nuclei near ^{208}Pb.

III. SOME CALCULATIONAL DETAILS

We have performed constrained Hartree-Fock plus BCS calculations using the Skyrme *SIII* effective interaction.[25] The constraining operator was the axial quadrupole moment. It is important to note that no inert core has been used. Pairing correlations have been approximately taken into account with a seniority force whose strength has been adjusted so as to reproduce the bulk variation of odd-even binding energy differences. Throughout this work axial symmetry has been assumed. The solution of the Hartree-Fock-type variational equations has been performed by projecting the single-particle states onto axially symmetrical harmonic oscillator states using a so-called deformed truncation scheme.[26] In Table I, some specific details about our calculations are reported: namely, the number N of oscillator major shells in the spherical case together with the pairing strength G_p and G_n (for proton and neutron, respectively) corresponding to a BCS variational space defined by a cutoff energy located at an energy e_c above the chemical potential.

The basis size is sufficient to ensure a good stability of the relative energies provided that the optimized two axial harmonic oscillator parameters have been chosen such as to yield a minimal total energy. In principle, one should optimize for the projected energy (i.e., Lipkin-Nogami corrected in our case). In practice, it turns out that optimizing for unprojected BCS solutions corresponds to a minimal energy also for the projected solution. This is exemplified on Fig. 1 for a deformed solution of the ^{196}Pt nucleus, with a basis size corresponding in the spherical case to 11 major shells.

The simultaneous solution of the Hartree-Fock-type and BCS-type variational equations is performed iteratively. After each Hartree-Fock iteration, a system of three equations is solved: (a) the gap equation (2.17), (b) the particle number conservation equation $n=\sum_i v_i^2$, and (c) the equation (2.18) yielding $\tilde{\lambda}_2$.

In order to achieve a convergence, in such an iterative process, one should first guess a $\tilde{\lambda}_2$ value and solve the nonlinear equations (a) and (b) to get Δ and $\tilde{\lambda}_1$, from which through equation (c) a new $\tilde{\lambda}_2$ value is determined and so forth. Knowing $\tilde{\lambda}_1$ and $\tilde{\lambda}_2$, one evaluates through the corresponding u_i's and v_i's, the q_1 and q_2 quantities according to Eqs. (2.21) and (2.22). From the latter one deduces—the Lagrange multiplier μ being known—λ_1 and λ_2 by proper substraction from $\tilde{\lambda}_1$ and $\tilde{\lambda}_2$. In practice it turns out that μq_1 and μq_2 are significantly smaller than $\tilde{\lambda}_1$ and $\tilde{\lambda}_2$, and therefore $\tilde{\lambda}_1\sim\lambda_1$ as well as $\tilde{\lambda}_2\sim\lambda_2$. Finally, one computes the corrected energy and the corrected quadrupole moment from Eqs. (2.20) and (2.25).

The matrix elements of Q_{20} involved in the computation of Q_1 and Q_2 have been calculated analytically in the

TABLE I. Numerical details of our CHF+BCS calculations: the number of major shells N, the e_c pairing cutoff constant (in MeV) and the $G_{n,p}$ constant pairing strengths (in MeV).

Nuclei	N	e_c	G_p	G_n
^{40}Ca	7	10	15.5	15.5
^{106}Cd	11	10	13.0	13.0
$^{92-102}$Zr	11	5	16.5	13.5
Os-Pt	11	10	12.5	12.5
^{240}Pu	13	10	12.9	12.9

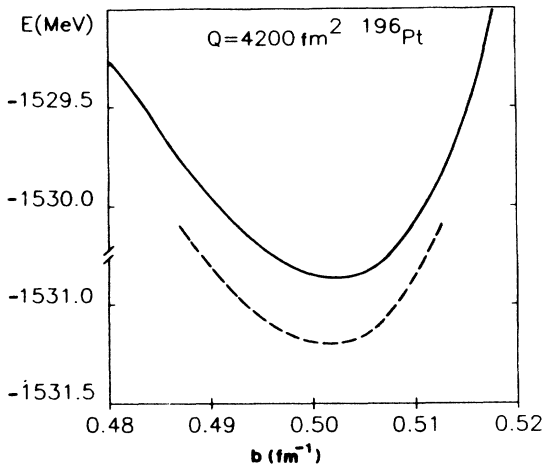

FIG. 1. Convergence of the total HF plus BCS energy E in MeV as a function of the usual monopole basis parameter b in fm^{-1}. The solid (dashed) line corresponds to unprojected (projected) calculations for a given value of the mass quadrupole moment Q (namely, $Q=42$ b).

deformed harmonic oscillator basis according to the method of Ref. 27. Incidentally the validity of the evaluation of expectation values of one-body operators in the BCS wave function by numerical integration over the density function through a Gauss-Hermite and Gauss-Legendre method (which is current practice in such Skyrme Hartree-Fock calculations on a deformed oscillator basis) has been checked. Indeed, comparing the result of such an approximate integration and the trace, in our basis, of the product of the density matrix by the Q_{20} operator yields equivalent results.

IV. RESULTS

A. An illustrative example: the ^{40}Ca nucleus

The doubly magical ^{40}Ca nucleus is well known to have a spherical equilibrium solution. It corresponds to a trivial BCS solution—i.e., with $\Delta_n = \Delta_p = 0$—upon using realistic G values.[26,28] Figure 2 shows the neutron and proton gaps obtained when taking into account the Lipkin-Nogami corrective terms. For the spherical equilibrium solution, the approximate projection has had the effect of switching on the pairing correlations. Indeed, we have then obtained for $Q=0$ nonzero neutron and proton gaps (dashed lines), whereas the usual BCS treatment (solid lines) leads to the trivial solution. Out of equilibrium, the change is not so important: the projected and unprojected gaps are of the same order of magnitude, except for large prolate shapes near $Q=4$ b, where they differ by a factor of 2. If now we consider the potential-energy curve $E(Q)$ with and without projection (see Fig. 3), we notice as expected that projected energies are lower than unprojected ones by 0.5–1.5 MeV. As a result the trend of both projected and unprojected potential-energy curves are found to be rather similar.[29]

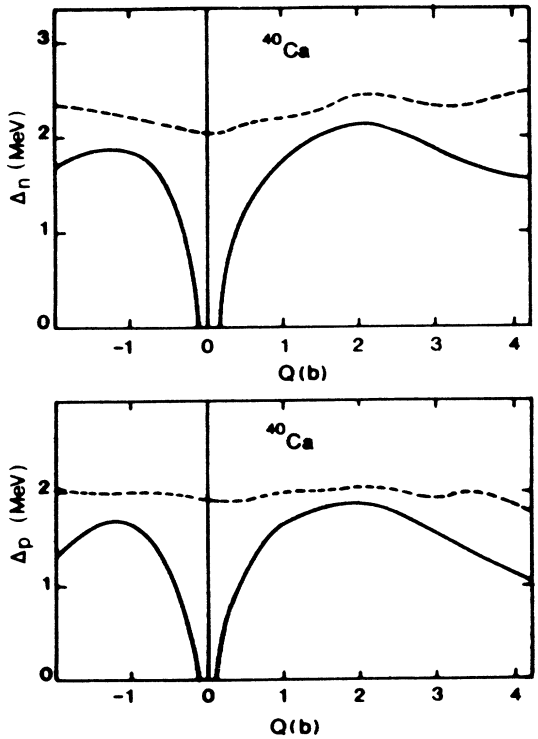

FIG. 2. Neutron Δ_n and proton Δ_p gap energies in MeV as a function of the mass quadrupole moment Q (in b) for the ^{40}Ca nucleus. Solid lines show the standard CHF plus BCS results while the dotted lines correspond to calculations including the Lipkin-Nogami corrections.

B. Transitional nuclei

Transitional nuclei are, by definition, very soft against β deformation. A correct treatment of pairing correlations appears quite mandatory. Nuclei in three different regions have been investigated: (i) a typically soft and weakly deformed nucleus, the ^{106}Cd isotope; (ii) the sharp transition from spherical to prolate shape in Zr isotopes; and (iii) the well-known Os-Pt-Hg transitional region with a particular study of the energy differences between oblate and prolate minima (the so-called V_{po} energies).

1. A typical transitional weakly deformed nucleus: the ^{106}Cd isotope

We have calculated the complete axial energy potential curve for the ^{106}Cd nucleus known as a weakly deformed nucleus close to the spherical ^{98,100,102}Cd isotopes.[30] Figure 4 shows the results without and with the Lipkin-Nogami (LN) correcting terms. Without LN corrections the equilibrium shape is prolate while an oblate secondary minimum exists. The V_{po} energy is equal to 0.77 MeV. The spherical barrier height H_S (the difference between the energies of the spherical solution and the absolute minimum) is found to be 1.3 MeV. Upon including LN corrections, the equilibrium solution remains prolate shaped (with $Q=419$ fm^2 instead of 435 fm^2), but the energy difference between the two local minima decreases by about 500 keV, now yielding $V_{po}=0.27$ MeV and $H_S=0.9$ MeV. The two local minima become therefore quasidegenerate and the ^{106}Cd nucleus appears globally more soft.

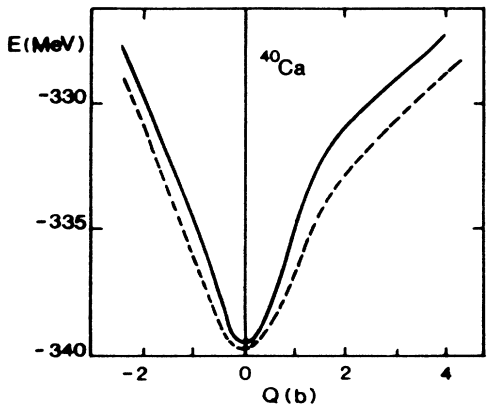

FIG. 3. Deformation potential energy curve in MeV as a function of the intrinsic quadrupole moment Q (in b) for the ^{40}Ca nucleus. The solid line shows the results for the standard CHF plus BCS calculations while the dotted line corresponds to calculations including the Lipkin-Nogami corrections.

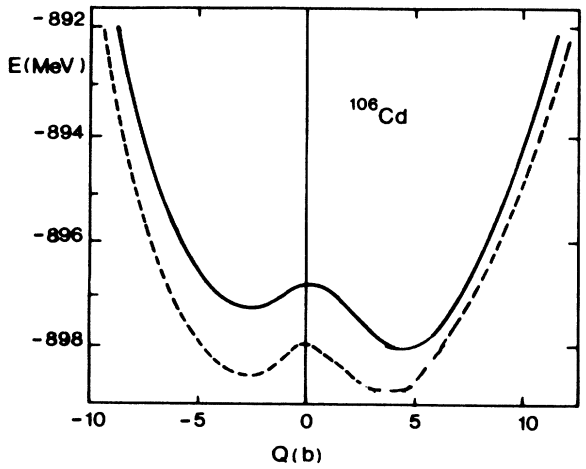

FIG. 4. Same as Fig. 3 for the ^{106}Cd nucleus.

2. *The shape phase transition in Zr isotopes*

In HF plus (ordinary) BCS calculations, the isotopes of Sr and Zr exhibit a sharp transition from spherical to prolate shape below $N=60$, while the isotopes of Mo, Ru, and Pd present rather a smooth transition.[31] Arima and Sugita[32] have suggested that the particle-number projection could be important to explain this difference in the behavior of such a *phase* transition (sharp versus smooth).

Figure 5 displays the equilibrium proton deformation obtained in projected and unprojected axial HF plus BCS calculations for the ^{102,100,98,96,94,92}Zr isotopes. As a result of our calculations (see Table II), the fluctuations due to the particle number are rather small. Indeed, on the usual β_2 quadrupole deformation parameter they never induce a change higher than 3%. We are therefore led to a conclusion at variance with what was suggested in Ref. 32.

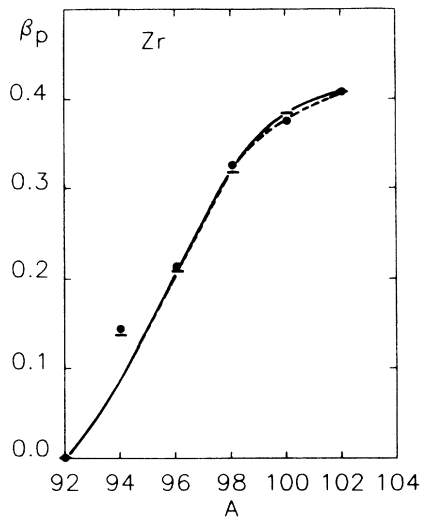

FIG. 5. Equilibrium proton quadrupole deformation parameter β_p as a function of the nucleon number A near the shape transition for Zr isotopes. Solid circles (horizontal marks) correspond to unprojected (projected) equilibrium solutions. The solid (dashed) lines are only drawn to give the trend of the shape transition in unprojected (projected) axial calculations. The parameters corresponding to the ^{94}Zr nucleus need not be included in this systematical representation, since it is known that its equilibrium solution breaks axial symmetry (as found in Ref. 31).

TABLE II. Effect of LN corrections on the proton axial quadrupole deformation parameter β_2 for the Zr isotopes under study. The last column gives the variation in percent. The ^{94}Zr isotope has a triaxial equilibrium shape in the calculations of Ref. 31 while the present approach deals only with axial shapes.

A	Without LN	With LN	Variation
100	0.375	0.381	1.6
98	0.323	0.319	1.3
96	0.209	0.208	0.4
94	0.142	0.139	2.9
92	0.0	0.0	0.0

3. *The Os-Pt-Hg transitional region*

This region has been extensively studied both experimentally and theoretically (see, e.g., Refs. 33–35). Axial calculations using the same force as here have been in particular performed by Sauvage *et al.*,[33] where some nuclei (such as the ^{186}Pt isotope) present locally trivial equilibrium solutions where one of the pairing gaps is vanishing. We have searched for the possible effects of the projection on V_{po} energy differences.

Including LN corrections, V_{po} values generally decrease. They do it for instance by 350 keV in the ^{186}Pt case, as shown in Fig. 6. These corrections, however,

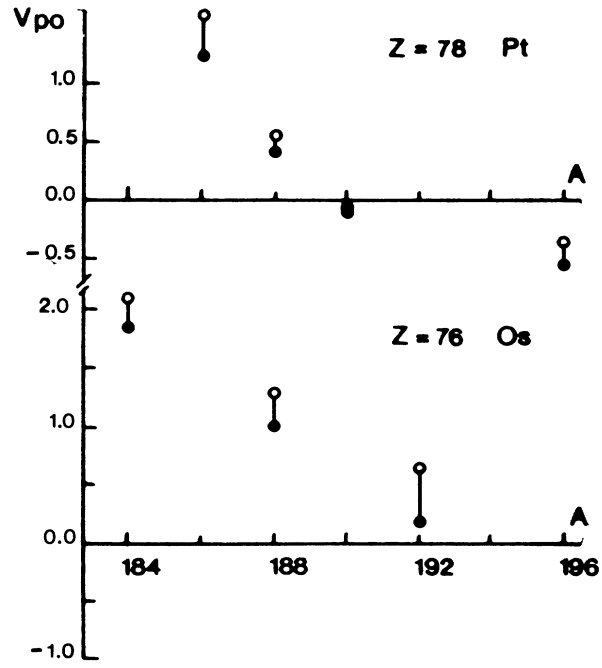

FIG. 6. Energy differences V_{po} in MeV between the prolate and oblate local minima versus the nucleon number A for Os and Pt isotopes. Open circles display the result of standard CHF plus BCS calculations whereas solid circles correspond to calculations including Lipkin-Nogami corrections.

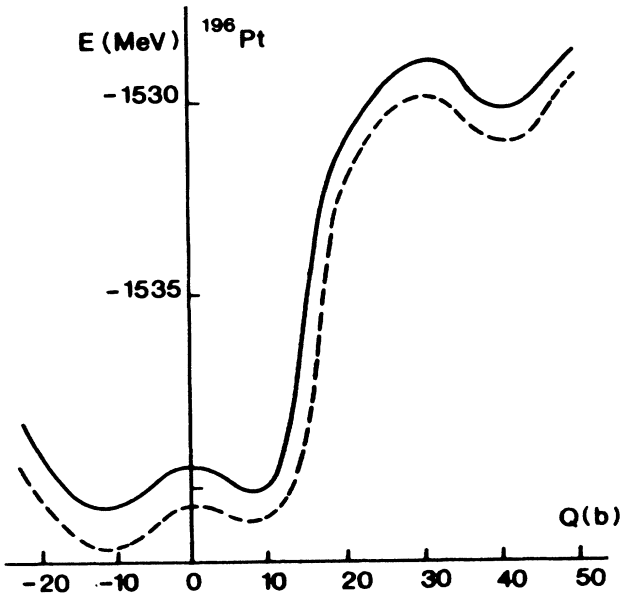

FIG. 7. Axial deformation potential energy E (in MeV) as a function of the intrinsic quadrupole moment Q (in b) for the ^{196}Pt nucleus. The dotted line shows the results of standard CHF plus BCS calculations while the solid line corresponds to calculations including Lipkin-Nogami corrections.

remain weak and do not exceed 500 keV. Nevertheless, in such soft nuclei, the two local axial minima are almost degenerate and such a projection on the particle number may appear quite necessary for an accurate static description.

C. Superdeformation at low spin

1. *Nonfissile nuclei*

Recent calculations have predicted superdeformed shapes in nonfissile nuclei at zero spin in the Os-Pt-Hg region.[35–38] Experimental evidence for a corresponding superdeformed rotational band in ^{191}Hg (Ref. 39) at low spin ($\frac{17}{2}\hbar$) has recently been brought up. It is therefore important to check the stability of this shape isomerism against the particle-number projection in CHF plus BCS calculations.

We have performed projected self-consistent calculations imposing axial symmetry to one nonfissile candidate for shape isomerism at zero spin,[35] i.e., the ^{196}Pt nucleus. Indeed, a large number of even-even Pt isotopes from ^{190}Pt to ^{210}Pt exhibit a secondary prolate minimum at $Q \sim 4.5$ b and lies at a few MeV above the absolute equilibrium minimum. The depth of this secondary minimum

TABLE III. Effect of the LN correction on the properties of the superdeformed isomeric state in the ^{196}Pt nucleus. All energies are expressed in MeV.

^{196}Pt isomer	Without LN	With LN
V_{po}	0.4	0.5
Excitation energy	11.3	11.0
Second well depth	1.4	1.2

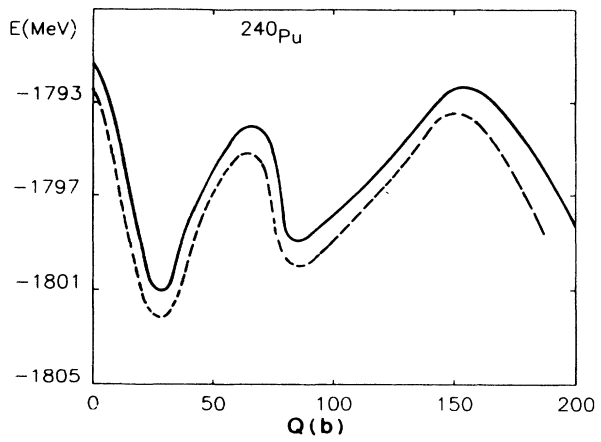

FIG. 8. Same as Fig. 7 for the fission barrier of the ^{240}Pu nucleus.

depends strongly on the isotopic mass. In the ^{196}Pt case, the second well is calculated rather deep (its depth is approximately 1.25 MeV). This is why this nucleus was chosen as an interesting test case to see whether or not the LN correction energies would be able to destroy such a secondary well. Numerical results of our calculations are summarized in Table III. As shown also in Fig. 7, the second well subsists at the same prolate deformation and with quite the same depth. We may therefore infer with some confidence that the shape isomerism in nonfissile nuclei at no spin found without LN corrections should survive when including a proper particle-number projection.

2. *The fission barrier of ^{240}Pu*

In many calculations,[40–42] the fission barrier of the ^{240}Pu nucleus has constituted a useful testing ground for HF plus BCS calculations using Skyrme forces. As is also well known, the Sk M^* force,[43] yields the best agreement with experimental fission barrier heights. We have therefore calculated the fission barrier of this nucleus with this force in order to provide at such extreme deformations, some results of our approximate projection method. As for the ^{196}Pt nonfissile nucleus, the second minimum takes place along the elongation axis at the same deformation (see Fig. 8) without or with LN corrections. The same conclusions hold for the whole fission barrier: projected and unprojected energy curves are found very similar indeed.

V. DISCUSSION AND CONCLUSION

The approximate Lipkin-Nogami projection method developed in this paper for the microscopic total energy in self-consistent HF plus BCS calculations has proven very easy to handle. As shown here a rather arbitrary extension of its physical foundation can be made to yield projection effects on expectation values of one-body operators. As a result, however, these effects (evaluated in this tentative fashion) are very small indeed for *collective* one-body operators as the quadrupole operator and could be as well neglected. It would be desirable to com-

pare the results of our approach with exact projection approaches. It should be stressed that it is of course an essential fact that such projections should be made before variation. If not there would be of course no way through which a trivial solution would be corrected into a more physical one. This remark applies *a fortiori* to the approximate projection after variation approaches as performed in Ref. 11, for instance.

The physical problem under study can be summarized as follows. When evaluating, through HF plus BCS calculations, an adiabatic path for a large amplitude collective motion, there are intervals for the collective parameter where no other solutions than zero gap ones are found. Therefore one is entitled to seek how a more physical treatment of pairing correlations would affect the conclusion drawn from such *static* calculations.

It is well known that the Lipkin-Nogami prescription reproduces very well, even in the low-level density regime, exact pairing calculations in restricted model cases.[20] Even though the relevance of the latter for realistic nuclear systems is of course questionable *a priori*, such a result provides, however, a reasonable theoretical justification for the present investigation.

Practical calculations have been performed here pertaining to three interesting phenomena: shape transition, shape coexistence, and shape isomerism. In all three cases, we have found that the location of extrema in the potential-energy curves was almost not affected by the inclusion of projection effects. It is undoubtedly due to the fact, which is the second finding of our calculations, that relative energies are not affected much by these effects. Yet, in some cases (as when studying shape coexistence) a near degeneracy appears. There, tiny energy differences might entail sizeable consequences for the (collective) properties of the nucleus (e.g., for the sign of the intrinsic quadrupole moment of its ground state).

A correct description of nuclear collective motion should contain, of necessity, a consistent dynamical part. The next step of this study should therefore be an assessment of the effect of such an improved treatment of pairing correlations on the solutions of the time-odd adiabatic TDHFB equations of motion which are known[42] to be the dynamical counterparts of the CHF plus BCS description of low-energy collective excitations. Indeed, it is known (see, e.g., Ref. 42) that pairing correlations play a very important role to determine the adiabatic masses. One might therefore expect that the consequence of such projection on these masses should be quite sizeable near spurious normal superfluid *phase transition*.

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