Pairing-correlations and particle-number projection methods

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Abstract

A systematic study of the pairing-correlations derived from various particle-number projection methods is performed in an exactly soluble cranked-deformed shell model Hamiltonian. It is shown that most of the approximate particle-number projection methods including the method of Lipkin-Nogami, which is used quite extensively in nuclear structure studies, breakdown in the weak pairing limit. The results obtained from the recently formulated number-projected Hartree-Fock-Bogoliubov (PHFB) equations, on the other hand, are in complete agreement with the exact solutions of the model Hamiltonian. The pairing-energy calculated from PHFB method is shown to be finite in all the studied limits. More importantly, the numerical work involved in the solution of the PHFB equations appears to be comparable to the solution of the bare HFB equations.

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I. INTRODUCTION

Pairing-correlations play a central role in describing the properties of atomic nuclei \cite{1,2}. The bulk of the nuclear phenomena, for instance, the odd-even mass differences and moments of inertia of deformed nuclei can be described by considering nucleons to be in a superfluid paired phase. The recent discovery of halo nuclei have also elucidated the importance of pairing-correlations in the formation of such structures \cite{3,4,5}. In the traditional nuclear structure models, the pairing-correlations are treated in Bardeen-Cooper-Schrieffer (BCS) or Hartree-Fock-Bogoliubov (HFB) approximations \cite{2}. These approaches use a simple ansatz of a product-state of quasiparticles for the ground-state wave function. The product ansatz leads to a set of non-linear equations in the BCS theory or to the diagonalization of a matrix in the case of HFB approach. There exist now very fast numerical methods to find accurate solutions of these problems. The major advantage in the mean-field models is that the number of non-linear equations or the dimensionality of the matrix to be diagonalised is quite small as compared to the exact analysis, which is impossible to apply in a realistic configuration space of medium and heavy mass nuclei.

Nevertheless, the product ansatz of the mean-field approach breaks the symmetries which the orginal many-body Hamiltonian obeys. For instance, in the case of BCS theory, the product-state violates the gauge-symmetry associated with the particle-number. The BCS product-state of quasiparticles does not have a well defined particle-number. The most undesirable feature associated with the broken symmetry is that it leads to sharp phase transitions. These phase transitions may be reasonable for a system with a very large number of particles, for example, a metallic superconductor. But for a finite mesoscopic system these phase transitions are washed out by fluctuations and are not observed in the experimental data or in the exact study of toy models. The sharp transition is an artifact of the simple ansatz of the product-state, which does not contain fluctuations.

The symmetry restoration in the mean-field studies is a major challenge to the nuclear structure models. Although, the projection methods which restore the broken symmetries have been known for more than thirty years, but have been studied only in simple model cases due to the numerical difficulties. In most of the realistic studies, approximate projection methods have been employed \cite{6}. Only recently, the gradient method in the projected-energy surface has been employed in realistic calculations with Gogny forces \cite{7}. There has been an unsolved problem whether a simple HFB like equations can be obtained with the projected-energy functional. This would allow the usage of fast numerical algorithms for diagonalisation of matrices as is done in the ordinary HFB theory. This problem has been recently addressed and it has been shown that the variation of an arbitrary energy-functional, which is completely expressed in terms of the HFB density matrix $\rho$ and the pairing tensor $\kappa$, results in the HFB like equation \cite{8}. It is noted that the projected-energy functional can also be expressed in terms of the HFB density matrices $\rho$ and $\kappa$ and, therefore, one obtains HFB like equations with modified expressions for the pairing-potential and the Hartree-Fock field.

In the present work, we shall limit ourselves to the restoration of the gauge symmetry associated with the particle-number projection, which is important in the discussion of the pairing-correlations. Several approximate particle-number projection methods have been developed and the most popular of these is the method of Lipkin and Nogami \cite{9}. The
The purpose of the present work is to perform a systematic study of these various approximate projection methods and to compare them with the recently developed number-projected HFB (PHFB) approach. It is shown that most of the approximate methods including the Lipkin-Nogami method breakdown in the weak pairing limit. The PHFB method, on the other hand, gives finite pair-correlations in all the cases studied. The paper is organised as follows: a brief survey of the particle-number projection methods is given in the next section and in the appendix. The model Hamiltonian used in the present work is expressed in section III, the numerical results are discussed in section IV and finally the present work is summarised in section V.

II. PROJECTION METHODS

In this section, we shall briefly describe the approximate particle-number projection methods used in the literature and the exact number-projected HFB method proposed recently [8]. Although, the approximate methods are quite standard and the details can be found, for example, in the textbook [2]. But for completeness, the essential elements of these methods are discussed in the following subsections.

A. HFB method

The many-body Hamiltonian of a system of fermions is usually expressed in terms of a set of annihilation and creation operators \((c, c^{\dagger}) = (c_1, \ldots, c_M; c_1^{\dagger}, \ldots, c_M^{\dagger})\):

\[
H = \sum_{n_1n_2} e_{n_1n_2} c_{n_1}^{\dagger} c_{n_2} + \frac{1}{4} \sum_{n_1n_2n_3n_4} \tau_{n_1n_2n_3n_4} c_{n_1}^{\dagger} c_{n_2}^{\dagger} c_{n_4} c_{n_3},
\]

where the anti-symmetrized two-body matrix-element is defined by

\[
\tau_{n_1n_2n_3n_4} = \langle n_1n_2 | V | n_3n_4 - n_4n_3 \rangle.
\]

The operators annihilate the bare fermion vacuum

\[
c_n | - \rangle = 0,
\]

for all \(n\) and provide a basis in the present analysis.

The most basic of the mean-field approaches to describe the pairing-correlations is the HFB method. In this method, the ground-state wavefunction is a product-state of quasiparticle operators \((\alpha, \alpha^{\dagger}) = (\alpha_1, \ldots, \alpha_M; \alpha_1^{\dagger}, \ldots, \alpha_M^{\dagger})\). These quasiparticle operators are connected to the original particle operators by a linear transformation

\[
\alpha_k = \sum_n \left( U_{nk}^{*} c_n + V_{nk}^{*} c_n^{\dagger} \right),
\]

\[
\alpha_k^{\dagger} = \sum_n \left( V_{nk} c_n + U_{nk} c_n^{\dagger} \right).
\]

This transformation can be rewritten in the matrix form as
\[
\begin{pmatrix}
\alpha \\
\alpha^\dagger
\end{pmatrix} = \begin{pmatrix}
U^\dagger & V^\dagger \\
V^T & U^T
\end{pmatrix} \begin{pmatrix}
c \\
c^\dagger
\end{pmatrix} = \mathcal{W} \begin{pmatrix}
c \\
c^\dagger
\end{pmatrix}.
\] (6)

The quasiparticle operators need to satisfy the same fermion commutation relations as the original operators in order to preserve the Fermi-Dirac statistics and, therefore, the transformation matrix is required to be unitary
\[
\mathcal{W}^\dagger \mathcal{W} = \mathcal{W} \mathcal{W}^\dagger = I,
\] (7)

which leads to following relations among the coefficients \(U_{nk}\) and \(V_{nk}\),
\[
U^\dagger U + V^\dagger V = I, \quad UU^\dagger + V^* V^T = I, \quad (8)
\]
\[
U^T V + V^T U = 0, \quad UV^\dagger + V^* U^T = 0. \quad (9)
\]

The quasiparticle operators annihilate the quasiparticle vacuum \(|\Phi\rangle\), defined by
\[
\alpha_k |\Phi\rangle = 0,
\] (10)

for all \(k\). In mean-field theory, it represents an approximation to the ground-state of a system and turns out to be a generalized Slater-determinant \([2]\). Since the quasiparticle transformation mixes creation and annihilation operators, \(|\Phi\rangle\) does not correspond to a wavefunction with good particle-number. In HFB theory, we have two kinds of densities, the normal density \(\rho\), and the pairing-tensor \(\kappa\), defined as
\[
\rho_{nn'} = \langle \Phi | c_{n'}^\dagger c_n | \Phi \rangle, \quad \kappa_{nn'} = \langle \Phi | c_{n'} c_n | \Phi \rangle. \quad (11)
\]

These can be expressed in terms of the HFB coefficients as
\[
\rho = V^* V^T, \quad \kappa = V^* U^T = -UV^\dagger. \quad (12)
\]

The HFB energy is given by
\[
E_{HFB}[\rho, \kappa] = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \text{Tr} \left\{ (e + \frac{1}{2} \Gamma) \rho \right\} - \frac{1}{2} \text{Tr} (\Delta \kappa^*), \quad (13)
\]

where the HFB fields are defined as
\[
\Gamma_{n_1n_3} = \sum_{n_2n_4} \sum_{n_2n_4} \gamma_{n_1n_2n_3n_4} \rho_{n_4n_2}, \quad (14)
\]
\[
\Delta_{n_1n_2} = \frac{1}{2} \sum_{n_3n_4} \sum_{n_3n_4} \delta_{n_1n_2n_3n_4} \kappa_{n_3n_4}. \quad (15)
\]

The variation of the HFB energy-functional \([13]\) results in the standard HFB equations :
\[
\mathcal{H} \begin{pmatrix}
U \\
V
\end{pmatrix} = E_i \begin{pmatrix}
U \\
V
\end{pmatrix}, \quad (16)
\]

where
\[
\mathcal{H} = \begin{pmatrix}
e + \Gamma - \lambda & \Delta \\
-\Delta^* & -(e + \Gamma)^* + \lambda
\end{pmatrix}. \quad (17)
\]

As already mentioned, the HFB wavefunction does not have a well defined particle-number and the Lagrangian parameter \((\lambda)\) is introduced to have the correct particle-number on the average. The diagonalisation of the HFB matrix \([17]\) gives rise to the quasiparticle energies \((E_i)\) and the excitation spectrum of the many-body system is constructed from these quasiparticle energies.
B. Variation after projection - Number-projected (PHFB) equations

It has been shown recently [8] that the variation after projection leads to the HFB like equations with modified expressions for the pairing-field and the Hartree-Fock potential. We have also obtained these equations using the method of statistical averages and the derivation is given in the appendix. In this section, we shall present the relevant expressions of the projected-fields which are used in the numerical study. The projected-energy functional is given by [2]

$$E^N[\rho, \kappa] = \frac{\langle \Phi | H P^N | \Phi \rangle}{\langle \Phi | P^N | \Phi \rangle} = \frac{\int d\phi \langle \Phi | H e^{i\phi(N-N)} | \Phi \rangle}{\int d\phi \langle \Phi | e^{i\phi(N-N)} | \Phi \rangle}, \quad (18)$$

where $\rho$ and $\kappa$ are the unprojected densities given in Eq. 12 and the particle-number projection operator is defined as

$$P^N = \frac{1}{2\pi} \int d\phi \ e^{i\phi(N-N)}. \quad (19)$$

It has been demonstrated in ref. [8] that the variation of the projected-energy results in the HFB equations of the same structure as in (17) except that the expressions for the fields are different. The projected HFB equation is given by

$$\mathcal{H}^N \begin{pmatrix} U \\ V \end{pmatrix} = \mathcal{E}_i \begin{pmatrix} U \\ V \end{pmatrix}, \quad (20)$$

where

$$\mathcal{H}^N = \begin{pmatrix} \varepsilon^N + \Gamma^N + \Lambda^N \\ -(\Delta^N)^* \\ -\varepsilon^N + (\Gamma^N)^* + (\Lambda^N)^* \end{pmatrix}. \quad (21)$$

The number-projected expressions for the fields are now given by

$$\varepsilon^N = \frac{1}{2} \int d\phi \ y(\phi) \left\{ Y(\phi) \text{Tr}[\rho(\phi)] + [1 - 2ie^{-i\phi} \sin \phi \rho(\phi)] e\mathcal{C}(\phi) \right\} + h.c. \quad (22)$$

$$\Gamma^N = \frac{1}{2} \int d\phi \ y(\phi) \left\{ Y(\phi) \frac{1}{2} \text{Tr}[\Gamma(\phi)\rho(\phi)] + \frac{1}{2} [1 - 2ie^{-i\phi} \sin \phi \rho(\phi)] \Gamma(\phi) \mathcal{C}(\phi) \right\} + h.c. \quad (23)$$

$$\Lambda^N = -\frac{1}{2} \int d\phi \ y(\phi) \left\{ Y(\phi) \frac{1}{2} \text{Tr}[\Delta(\phi)\kappa^*] - 2ie^{-i\phi} \sin \phi \ C(\phi) \Delta(\phi)\kappa^* \right\} + h.c. \quad (24)$$

$$\Delta^N = \frac{1}{2} \int d\phi \ y(\phi) e^{-2i\phi} \mathcal{C}(\phi) \mathcal{D}(\phi) - (..)^T, \quad (25)$$

with
\[ \Gamma_{n_1 n_3}(\phi) = \sum_{n_2 n_4} \tau_{n_1 n_2 n_3 n_4} p_{n_1 n_2}(\phi), \quad (26) \]
\[ \Delta_{n_1 n_2}(\phi) = \frac{1}{2} \sum_{n_3 n_4} \tau_{n_1 n_2 n_3 n_4} \kappa_{n_3 n_4}(\phi), \quad (27) \]
\[ \Delta_{n_3 n_4}(\phi) = \frac{1}{2} \sum_{n_1 n_2} \tau_{n_1 n_2}(\phi) \tau_{n_1 n_2 n_3 n_4}, \quad (28) \]
\[ \rho(\phi) = C(\phi) \rho, \quad (29) \]
\[ \kappa(\phi) = C(\phi) \kappa = \kappa C^T(\phi), \quad (30) \]
\[ \pi(\phi) = e^{2i\phi} \kappa C^*(\phi) = e^{2i\phi} C^*(\phi) \kappa, \quad (31) \]
\[ C(\phi) = e^{2i\phi} \left( 1 + \rho(e^{2i\phi} - 1) \right)^{-1}, \quad (32) \]
\[ x(\phi) = \frac{1}{2\pi} \frac{e^{i\phi(N)} \det(e^{i\phi})}{\sqrt{\det C(\phi)}}, \quad (33) \]
\[ y(\phi) = \frac{x(\phi)}{\int dg \ x(\phi)}, \quad \int dg \ y(\phi) = 1, \quad (34) \]

and

\[ Y(\phi) = i e^{-i\phi} \sin \phi \ C(\phi) - i \int d\phi' y(\phi') e^{-i\phi'} \sin \phi' \ C(\phi'). \quad (35) \]

The term designated by \( \Lambda^N \) in Eq. (24) does not appear in the normal HFB formalism and it can be immediately shown that it vanishes for the gauge-angle, \( \phi = 0 \). This term originates from the variation of the pairing-energy with respect to the density-matrix. In normal HFB theory, the pairing-energy depends only on the pairing-tensor, but the projected HFB pairing-energy also depends on the density-matrix through the norm-overlap. As a matter of fact, in a general case, the norm-overlap depends on both the density-matrix and the pairing-tensor (see appendix). But for the special case of number-projection, the term in the overlap-matrix, depending on the pairing-tensor, can be rewritten in terms of the density-matrix by using the HFB relation \( \rho - \rho^2 = \kappa \kappa^\dagger \). Due to this transformation, the expression for \( \Delta^N \) in (25) has a very simple appearance and reduces to the familiar form in the canonical representation [8,10].

It should be noted that as compared to the HFB case, the projected quasiparticle energies obtained from the diagonalisation of the projected HFB matrix Eq. (21) have no meaning. The only meaningful quantity is the total projected-energy, which is given by

\[ E_{\text{tot}} = \int d\phi y(\phi) H(\phi), \quad (36) \]
\[ = \int d\phi y(\phi) \left\{ H_{sp}(\phi) + H_{ph}(\phi) + H_{pp}(\phi) \right\}, \quad (37) \]

where,

\[ H_{sp}(\phi) = \text{Tr} (\epsilon \rho(\phi)), \quad (38) \]
\[ H_{ph}(\phi) = \frac{1}{2} \text{Tr} \left( \Gamma(\phi) \rho(\phi) \right), \quad (39) \]
\[ H_{pp}(\phi) = -\frac{1}{2} \text{Tr} \left( \Delta(\phi) \kappa^\dagger(\phi) \right). \quad (40) \]
In the present work, we shall discuss the pairing-energy \( E_{\text{pair}} \) and the aligned angular-momentum \( \langle J_x \rangle \) quite extensively, since these give a measure of the pairing-correlations. The expressions for these quantities are given by

\[
E_{\text{pair}} = \int d\phi H_{pp}(\phi), \quad (41)
\]

\[
\langle J_x \rangle = \int d\phi \text{Tr} (J_x \rho(\phi)). \quad (42)
\]

As is clear from Eq. (21), the projected equations have exactly the same structure as that of normal HFB. Therefore, one can employ the existing HFB computer codes and only the expressions for the projected-fields need to be evaluated. The projected-fields now involve the integration over the gauge-angle, \( \phi \). This integration has been performed using the Gauss-Chebyshev quadrature method \[11\]. In this method, the integration over the gauge-angle is replaced by a summation. It can be shown \[11\] that the optimal number of mesh-points in the summation which eliminates all the components having undesired particle numbers is given by

\[
M = \max \left( \frac{1}{2} N, \Omega - \frac{1}{2} \right) + 1, \quad (43)
\]

where \( N \) is the number of particles and \( \Omega \) is the degeneracy of the model space.

C. Projection after variation (PAV)

In this projection method, the HFB mean-field solution is used to calculate the projected quantities. The normal variational calculations are carried out in the HFB formalism and the solution obtained is then used to calculate the projected quantities as given by Eqs. (37,41,42). Therefore, this method is closely based on the HFB method and in the event that HFB solution depicts a transitional behaviour, it would also be reflected in the PAV results.

D. Lipkin-Nogami (LN) method

The Lipkin-Nogami (LN) method has been used quite extensively as an approximation to the particle-number projection approach. In this method, the HFB energy-function is modified to include the quadratic term in the Kamalh expansion of the projected-energy \[2\]. The HFB energy is replaced by

\[
E_{\text{HFB}} \rightarrow E_{\text{HFB}} - \lambda_2 \langle \Delta \hat{N}^2 \rangle, \quad (44)
\]

where \( \Delta \hat{N}^2 = (\hat{N} - \langle \hat{N} \rangle)^2 \) and the Lagrangian parameter \( \lambda_2 \) is given by \[3\]

\[
\lambda_2 = \frac{\langle \hat{H}(\Delta \hat{N}^2 - \langle \Delta \hat{N}^2 \rangle) \rangle - \langle \hat{H} \Delta \hat{N} \rangle \langle \Delta \hat{N}^3 \rangle / \langle \Delta \hat{N}^2 \rangle}{\langle \Delta \hat{N}^4 \rangle - \langle \Delta \hat{N}^2 \rangle^2 - \langle \Delta \hat{N}^3 \rangle^2 / \langle \Delta \hat{N}^2 \rangle}. \quad (45)
\]

In the above equations, the expectation value of an operator is calculated with respect to the HFB vacuum, i.e., \( \langle \hat{O} \rangle = \langle \Phi | \hat{O} | \Phi \rangle \) and can be calculated by differentiating the norm and the Hamiltonian overlaps as a function of the gauge-angle, i.e.,
\[ \langle \Delta \hat{N}^p \rangle = 2\pi \frac{1}{v^p} \frac{\partial^p x(\phi)}{\partial \phi^p} \bigg|_{\phi=0}, \]  
(46)

\[ \langle H \Delta \hat{N}^p \rangle = \frac{1}{v^p} \frac{\partial^p H(\phi)}{\partial \phi^p} \bigg|_{\phi=0}, \]  
(47)

where \( x(\phi) \) and \( H(\phi) \) are defined in Eqs. (33) and (36), respectively. The expressions for the expectation values required in Eq. (45) are given, for example in ref. [6]. We have rederived these expectation values using the expressions (33) and (36), which essentially involve differentiation of determinants and the matrix functions. The expectation values are given by

\[ \langle \Delta \hat{N}^2 \rangle = 2 \text{Tr}(\chi), \]  
(48)

\[ \langle \Delta \hat{N}^3 \rangle = 4 \text{Tr}(\gamma \chi), \]  
(49)

\[ \langle \Delta \hat{N}^4 \rangle = 3(\Delta \hat{N}^2)^2 + 8 \text{Tr}\{\chi(1 - 6\chi)\}, \]  
(50)

\[ \langle H \Delta \hat{N} \rangle = 2 \text{Tr}(h \chi) - \mathcal{R} \text{Tr}(\Delta \kappa^* \gamma), \]  
(51)

\[ \langle H(\Delta \hat{N}^2 - \langle \Delta \hat{N}^2 \rangle) \rangle = 4 \text{Tr}[(h \gamma + V_{HF}\{\chi\})\chi], \]  

\[ - \mathcal{R} \text{Tr}[\Delta \kappa^*(1 - 8\chi)] - \text{Tr}[V_P\{\gamma \kappa\}(\gamma \kappa)^*], \]  
(52)

where,

\[ \chi = \rho(1 - \rho), \]  
(53)

\[ \gamma = 1 - 2\rho, \]  
(54)

\[ h = e + \Gamma, \]  
(55)

\[ V_{HF}\{\chi\}_{ij} = \sum_{kl} \nu_{ijkl} \chi_{ij}, \]  
(56)

\[ V_P\{\gamma \kappa\}_{ij} = \frac{1}{2} \sum_{kl} \nu_{ijkl} (\gamma \kappa)_{kl}. \]  
(57)

\( \mathcal{R} \) in Eq. (52) denotes the real part of the expression. In the LN method, the calculations proceed exactly as in HFB case except for the extra \( \lambda_2 \) term. At each HFB iteration, the \( \lambda_2 \) is calculated using the expression (45) and this is then used in the solution of the HFB equations in the next iteration.

### III. MODEL HAMILTONIAN

In the present work, we have carried out extensive numerical calculations using the model Hamiltonian consisting of a cranked deformed one-body term, \( h' \) and a scalar two-body delta-interaction, \( V_2 \) [12]. The deformed shell model Hamiltonian employed is given by

\[ H = h'_{\text{def}} + V_2, \]  
(58)

\[ = h'_{\text{def}} - \omega J^2_x + V_2, \]  
(59)

where,
\[ h_{\text{def}} = -4\kappa \sqrt{\frac{4\pi}{5}} \sum_m <jm|Y_{20}|jm > c_{jm}^\dagger c_{jm}, \] (60)

and

\[ V_2 = \frac{1}{2} \sum_{LM} E_L A_{LM}^\dagger A_{LM}, \] (61)

with \( A_{LM}^\dagger = (c_{jL}^\dagger)^{LM} \) and \( A_{LM} = (A_{LM}^\dagger)^\dagger \). For the antisymmetric-normalized two-body matrix-element \( (E_J) \), we use the delta-interaction which for a single j-shell is given by [13]

\[ E_L = -G \left( \frac{2j+1}{2(2L+1)} \right)^2 \left[ \begin{array}{ccc} j & j & L \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{array} \right]^2, \] (62)

where the symbol \( [ \ ] \) denotes the Clebsch-Gordon coefficient. We use \( G = g \int R_{nl}^4 r^2 dr \) as our energy unit and the deformation energy \( \kappa \) is related to the deformation parameter \( \beta \). For the case of \( h_{11/2} \) shell, \( \kappa = 2.4 \) approximately corresponds to \( \beta = 0.23 \) [14].

Although, the present model Hamiltonian is not very realistic and the results obtained cannot be compared with the experimental data. Nevertheless, it contains most of the essential components of a realistic Hamiltonian. The advantage in this model is that it can be solved exactly and it is possible to test the quality of an approximate scheme. We consider that it is quite appropriate to test the number-projection methods in a cranking model, since with increasing rotational frequency the pairing-correlations drop and the results become quite sensitive to the projection method.

**IV. RESULTS AND DISCUSSIONS**

The detailed numerical calculations have been carried out for six-particles in \( j = 11/2 \) shell in order to investigate the validity of the particle-number projection methods presented in section II. The calculations have been done with three different pairing-interactions, monopole \([L=0 \text{ in Eq. (62)}]\), monopole plus quadupole \([L=0 \text{ and } 2 \text{ in Eq. (62)}]\) and with full delta-interaction to check the sensitivity of the projection method on the underlying pairing-interaction.

First, we would like to mention that the projected-HFB calculations almost completely agree with the exact solutions for all the cases studied and it is not possible to distinguish them in the figures. In all the figures, we present only the PHFB results and it should be kept in mind that these results coincide with the exact solution. In Fig. 1, the results of the total-energy \( (E_{\text{tot}}) \) and the pairing-energy \( (E_{\text{pair}}) \) are presented as a function of the strength of the pairing-interaction. For this set of calculations, we have employed the full delta-interaction. The HFB total-energy deviates from PHFB with increasing strength of the pairing-interaction. The results of total-energy with projection after variation appear to be in good agreement with the results of PHFB. The calculated total-energy in LN method interpolate between the PHFB and the HFB results. In general, it is noted from Fig. 1 that the total-energy is fairly reproduced by all the approximate projection methods.

The critical test of a projection method is how well it reproduces the pairing-energy. In the lower panel of Fig. 1, the pairing-energy obtained from different projection methods is
presented. The major problem associated with the HFB theory is that the pairing-energy shows a phase transition from finite pairing to zero pairing as is clearly evident from Fig. 1. The HFB pairing-energy is finite for pairing-strength, $G$ greater than 0.4, but collapses for $G$ less than or equal to 0.4. The PAV projected-energy has a similar behaviour as that of HFB energy and is expected since it uses the HFB mean-field solution. It should be noted that the PAV pairing-energy for certain values of the strength has a higher value than the HFB pairing-energy.

The LN pairing-energy is somewhat between HFB and PHFB pairing-energy and has a non-zero value for $G = 0.4$. But for the lower values of the pairing-strength, the LN pairing-energy also collapses. Therefore, the LN method which is used so extensively in the nuclear structure studies appears to be marginally better than the HFB approach and deviates substantially from the PHFB results. As is evident from Fig. 1, the PHFB pairing-energy is non-zero for all the values of the pairing-strength. In the following, we shall now turn to the rotational aspects of the pairing-energy.

The results of the cranking calculations with monopole-, (monopole plus quadrupole)- and delta-interactions are presented in Figs. 2, 3 and 4, respectively. In the upper panel of Fig. 2, a marked difference between the PHFB and HFB results are obtained for the monopole-interaction at lower rotational frequencies. The PAV on the other hand gives a good description for the total-energy and coincides with the PHFB total-energy at lower rotational frequencies. However, at higher rotational frequencies it shows a transitional behaviour and goes over to the HFB total-energy. The reason for this transition is that at higher rotational frequencies, the HFB pairing-energy vanishes and the results of PAV become identical to HFB. It should be noted that the mean-field potential, apart from the contribution of the pairing-interaction ($\Gamma$-term), is fixed in the present model study and as the pairing-energy vanishes the results of projected-energy are same as that of unprojected HFB in the PAV method. The LN total-energy is slightly lower than HFB, but is still far from the PHFB total-energy. At higher rotational frequencies all the approximate projection methods coincide with the PHFB, since the pairing-energy becomes quite weak.

The HFB pairing-energy, shown in the middle panel of Fig. 2, depicts a transitional behaviour as expected. For $\hbar\omega \leq 0.45G$, the pairing-energy is finite, but for higher rotational frequencies it vanishes. This is a major problem with the HFB theory and is related to the fact that it does not consider the particle-number fluctuations which become quite important for a mesoscopic system like an atomic nucleus. The PHFB pairing-energy, on the other hand, is clearly non-zero for all the rotational frequencies. It does drop at around $\hbar\omega = 0.55G$ and continues to drop with increasing rotational frequency, but decreases very smoothly. This smooth drop is due to the fluctuations which are inherent in the projection formalism. The PAV pairing-energy is somewhat better at low rotational frequencies, but after the HFB phase transition is same as that of HFB. The Lipkin-Nogami pairing-energy shows a slightly smoother drop at the transitional frequency, but then goes to zero at a slightly higher frequency as compared to HFB.

The observable quantity which is directly related to the pairing-energy is the aligned angular-momentum along the rotational axes ($< J_x >$). The nuclei in the ground-state are in a paired phase with maximal pairing-correlations. However, with increasing rotational frequency the particles are unpaired and are aligned towards the rotational axes. The aligned angular-momentum, therefore, is a measure of the unpaired particles or inversely of
pairing-correlations. It is evident from the bottom panel of Fig. 2 that the HFB aligned angular-momentum shows a transition from $< J_x > \approx 0$ to $\approx 10$. This jump is related to the transitional behaviour of the pairing-energy. The results of PAV closely follow the HFB results. The LN aligned angular-momentum has a smoother behaviour, but deviates from PHFB. The crossing frequency, which is given by the point of inflexion in the slope of the $< J_x >$ curve, is same for HFB and PAV. The crossing for LN is slightly higher than HFB, but is lower than PHFB by $\hbar \omega = 0.1G$.

The results of the projection methods with (monopole plus quadrupole)-interaction are presented in Fig. 3. The overall agreement between the approximate projection methods (HFB, PAV and LN) and the PHFB results is improved as compared to the results with a pure monopole-interaction. The results of the total-energy for PAV agree very well with PHFB at lower rotational frequencies as in the case of monopole interaction. The LN total-energy is slightly improved as compared to HFB, but deviates considerably from the PHFB total-energy. The results of the pairing-energy, shown in the middle panel of Fig. 3, are similar to the results with monopole pairing. The LN pairing-energy is smoother at the bandcrossing, but vanishes at higher rotational frequencies. The behaviour of the LN aligned angular-momentum, shown in the bottom panel of Fig. 3, is now quite similar to $< J_x >$ of PHFB. In particular, the slope of the curve, which is a measure of the interaction between the ground-state band and the s-band, is quite similar to that of HFB, although the bandcrossing is slightly lower than that of PHFB.

The results of the calculations with the full delta-interaction are shown in Fig. 4. The total-energy obtained from different approximate particle number-projection methods is considerably improved as compared to the previous two cases of monopole- and (monopole plus quadrupole)-interactions. However, the HFB pairing-energy shows the phase transition from finite pairing to zero pairing as in the other two cases. The LN pairing-energy on the other hand is quite smooth and is non-zero up to a very high rotational frequency. Due to this smooth behaviour, the aligned angular-momentum also shows a smooth behaviour and has a similar slope as that of PHFB.

We have also studied the deformation dependence of the pairing-energy obtained from various projection methods. As the deformation increases, the pairing is expected to drop. In particular, for superdeformed shapes the pairing is quite weak and the results become quite sensitive to the treatment of the pairing-energy. In Fig. 5, the pairing-energy is presented as a function of the deformation parameter, $\kappa$ for three different pairing-interactions shown in the three panels of the figure. As is clear from the figure, the pairing-energy drops with increasing deformation obtained from all the methods. However, the HFB pairing-energy goes to zero at around $\kappa = 5G$ with monopole- and (monopole plus quadrupole)-interactions shown in the upper two panels of Fig. 5. In the case of full delta-interaction, the HFB pairing-energy collapses at a slightly higher deformation value of $\kappa = 5.5G$. The LN pairing-energy has a smooth behaviour as a function of the deformation, which is quite similar to pairing-energy obtained in the PHFB case. However, the LN pairing-energy also goes to zero at higher deformation values, whereas the PHFB pairing-energy is finite for all the studied deformation values.

In Fig. 6, the results of the cranking calculations are presented for a very large deformation value of $\kappa = 5.5$ which is analogous to the deformation of the superdeformed bands. The dynamic moment of inertia ($J^{(2)}$) shown in Fig. 6 is obtained from the calculated
aligned angular-momentum as a function of the rotational frequency. As is evident from Fig. 6 the HFB $J^{(2)}$ is quite large as compared to $J^{(2)}$ obtained from PHFB for all the three pairing interactions. The Lipkin-Nogami $J^{(2)}$ appears to be close to the PHFB $J^{(2)}$ at lower rotational frequencies. However, at higher rotational frequencies it deviates quite a lot from the PHFB $J^{(2)}$ and as a matter of fact it becomes worse than HFB.

V. SUMMARY

In the present study, an attempt has been made to test the quality of the various particle-number projection methods by comparing the pairing-correlations and other related quantities. First of all, it is clear from the present study that the mean-field HFB approach appears to be a better approximation with more realistic pairing-interaction. This to our knowledge is not discussed in the literature. The HFB results for total-energy and the aligned angular-momentum appear to be in better agreement with the PHFB or exact results for the delta-interaction. This is in contrast to what is expected from the BCS theory. The BCS theory is known to be a better approximation for the simple monopole-interaction. This is easy to understand since in BCS theory one only considers the interaction among the particles in the time-reversed states, which is appropriate for the monopole-interaction. But in a more realistic pairing-interaction, one also has particle-particle correlations which do not necessarily operate in time-reversed states. These extra correlations are obviously neglected in the BCS theory. In the HFB theory, on the other hand, all the particle-particle correlations are considered in a self-consistent manner. We would also like to point out that we have considered all the terms arising from the pairing-interaction. In most of the studies, the exchange term arising from the pairing-interaction ($\Gamma$) is not considered since it contributes to the already fitted Hartree-Fock potential. This contribution turns out to be largest with the delta-interaction. In the absence of this term, the agreement between HFB and PHFB is better for the monopole-pairing.

The usefulness of a projection method is evaluated from its description of the pairing-correlations. The mean-field HFB approach suffers from a fundamental problem that it leads to a sharp phase transition from a superfluid to an unpaired phase. This is clear from the results presented in the present work, the HFB pairing-energy at critical points goes to zero. The major test of a projection method is how well it cures for this transitional problem. The PAV method is obviously not meant to solve this transitional problem, since it uses the HFB solution to start with. It suffers from the same problems as that of HFB.

The LN method which is used quite extensively appears to improve the pairing-energy somewhat, but is also seen to breakdown in the weak pairing limit. It is observed that as a function of the pairing-strength it does have a non-zero pairing-correlations at $G = 0.4$, which is a critical point in the HFB case. However, it should be noted that the pairing-correlations derived from LN are quite weak as compared to the PHFB case. As a function of the rotational frequency, the LN pairing-energy has a similar behaviour, it does not approach zero at the HFB critical frequency, but goes to zero at a slightly higher frequency. It can be, therefore, concluded from the present study that Lipkin-Nogami method is marginally better than the HFB approach.

The pairing-energy calculated from the PHFB method is seen to be finite for all the studied cases. As already mentioned, the calculated total-energy and the aligned-angular
momentum from the PHFB method are in complete agreement with the exact solutions of the model Hamiltonian. We consider that the PHFB method is an ideal candidate to replace the Lipkin-Nogami method in the nuclear structure studies. It is to be noted that one of the, often stated, advantages of the LN method is its computational simplicity \[15, 17\]. The LN method, apart from the evaluation of the \( \lambda_2 \) Lagrangian parameter, is exactly same as that of HFB approach. The PHFB equations have also same structure as that of HFB, except that one needs to evaluate the projected-fields. The evaluation of these projected-fields requires some extra work.

We would like to caution that a simple model Hamiltonian has been employed in the present work and the question arises whether the conclusions drawn here can be extrapolated to a realistic Hamiltonian and model space. First of all, we would like to mention that the present model Hamiltonian is not totally unrealistic as it contains most of the essential elements of a realistic Hamiltonian. The important difference is in the model configuration space. In the present work, we have employed the model space of a single-j shell and a realistic model space contains several major shells. Due to this major difference, the computation of the projected-fields may take a longer time. We are presently implementing the PHFB method in a realistic configuration space and our initial estimate is that the projected calculations may increase the numerical work by a factor of three to four as compared to the normal HFB case.

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VI. APPENDIX

We shall derive here general expressions for particle-number projected averages and their variation, valid at zero and finite temperature. The approach is also applicable to other projections. Let \( R \) be an arbitrary many-body density operator. The average of an operator \( O \) with respect to \( R \) will be denoted as

\[
\langle O \rangle_R = \text{Tr}[OR],
\]

where the trace is taken in the full grand canonical ensemble. For a Hamiltonian \( H \) satisfying \([H, \hat{N}] = 0\), the average projected-energy is given by

\[
E^N = \frac{\langle HP^N \rangle_R}{\langle P^N \rangle_R} = \int d\phi y^N(\phi) H(\phi),
\]

where

\[
y^N(\phi) = \frac{e^{-i\phi \hat{N}} \langle e^{i\phi \hat{N}} \rangle_R}{\int d\phi e^{-i\phi \hat{N}} \langle e^{i\phi \hat{N}} \rangle_R}, \quad H(\phi) = \frac{\langle He^{i\phi \hat{N}} \rangle_R}{\langle e^{i\phi \hat{N}} \rangle_R},
\]

13
with \( \int d\psi \hat{V}(\phi) = 1 \). Eq. (64) reduces to (28) in the pure limit \( R = |\Phi\rangle\langle\Phi| \).

Let us consider now a density of the form

\[
R = e^{-\beta K}/\text{Tr}[e^{-\beta K}],
\]

(66)

where \( K \) is an hermitian one-body operator. In a fermion system, the most general one-body \( K \) can be written as

\[
K = \sum_{i,j} \mathcal{K}^{ij}_{11} c_i^\dagger c_j + \frac{1}{2}(\mathcal{K}^{20}_{i1} c_i^\dagger + \mathcal{K}^{02}_{ij} c_i c_j) = k_0 + \frac{1}{2}Z\dagger KZ,
\]

(67)

with \( k_0 = \frac{1}{2}\text{Tr}\mathcal{K}^{11} \) and \( \mathcal{K}^{20}, \mathcal{K}^{02} \) antisymmetric matrices. For \( K \) hermitian, \( \mathcal{K}^\dagger = \mathcal{K} \), i.e., \( (\mathcal{K}^{11})^T = (\mathcal{K}^{11})^* \), \( \mathcal{K}^{02} = -(\mathcal{K}^{20})^* = (\mathcal{K}^{20})^\dagger \). The norm in (66) is

\[
\text{Tr}[e^{-\beta K}] = e^{-\beta k_0} \det[1 + e^{-\beta \mathcal{K}}]^{1/2}. \]

(68)

It is convenient to define a generalized density matrix \( \mathcal{R} \), of elements \( \mathcal{R}_{mn} = \langle Z^*_n Z_m \rangle_R \), that comprises both the standard density matrix and the pairing tensors and is a function of \( \mathcal{K} \):

\[
\mathcal{R} \equiv \begin{pmatrix} \rho & \kappa \\ \bar{\kappa} & 1 - \rho \end{pmatrix} = [1 + e^{\beta \mathcal{K}}]^{-1},
\]

(69)

where \( \rho_{ij} = \langle c_j^\dagger c_i \rangle_R \), \( \kappa_{ij} = \langle c_j c_i \rangle_R \), \( \bar{\kappa}_{ij} = \langle c_j^\dagger c_i^\dagger \rangle_R \), For \( K \) hermitian, \( \mathcal{R}^\dagger = \mathcal{R} \), i.e., \( \rho^T = \rho^* \), \( \bar{\kappa} = -\kappa^* = \kappa^\dagger \). All averages with respect to \( R \) can be expressed in terms of \( \mathcal{R} \). In particular, for an operator \( O \) of the form (32),

\[
\langle O \rangle_R = \text{Tr}[O^{11} \rho + \frac{1}{2}(O^{20} \bar{\kappa} + O^{02} \kappa)] = o_0 + \frac{1}{2}\text{Tr}[O\mathcal{R}].
\]

Let us write now the particle-number operator \( \hat{N} = \sum_i c_i^\dagger c_i \) as

\[
\hat{N} = n_0 + \frac{1}{2}Z\dagger N Z, \quad N = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},
\]

(70)

with \( 2n_0 \) the dimension of the single particle space. As the product of exponentials of one-body operators is the exponential of a one-body-operator, we have \( e^{i\phi \hat{N}} e^{-\beta K} = e^{-\beta K(\phi)} \), with \( K(\phi) \) a one-body operator determined by (18)

\[
K(\phi) = k_0(\phi) + \frac{1}{2}Z\dagger \mathcal{K}(\phi)Z,
\]

(71)

\[
e^{-\beta \mathcal{K}(\phi)} = e^{i\phi \hat{N}} e^{-\beta \mathcal{K}} = e^{i\phi \hat{N}} \mathcal{R}(1 - \mathcal{R})^{-1},
\]

(72)

and \( k_0(\phi) = k_0 - i\phi n_0/\beta \). Eqs. (66)–(72) lead then to

\[
\langle e^{i\phi \hat{N}} \rangle_R = e^{i\phi n_0} \frac{\det[1 + e^{-\beta \mathcal{K}(\phi)}]^{1/2}}{\det[1 + e^{-\beta \mathcal{K}}]^{1/2}} = \det[e^{i\phi/2 \mathcal{C}(\phi)}]^{1/2},
\]

(73)

\[
\mathcal{C}(\phi) = 1 + (e^{i\phi \hat{N}} - 1)\mathcal{R},
\]

(74)
which enables the evaluation of \( y^N(\phi) \). Besides, by means of Wick’s theorem, \( H(\phi) \) can be expressed in terms of the elements of the non-hermitian density matrix determined by

\[
R(\phi) = e^{i\phi N} R(e^{i\phi N})_R = e^{-\beta K(\phi)}/\text{Tr}[e^{-\beta K(\phi)}],
\]

\[
\mathcal{R}(\phi) \equiv \left( \begin{array}{cc} \rho(\phi) & \kappa(\phi) \\ \bar{\kappa}(\phi) & 1 - \rho^T(\phi) \end{array} \right) = [1 + e^{\beta K(\phi)}]^{-1} = e^{i\phi N} \mathcal{R} C^{-1}(\phi),
\]

where \( \rho(\phi) = \langle c_i^+c_i \rangle_R(\phi), \kappa(\phi) = \langle c_j c_i \rangle_R(\phi), \bar{\kappa}(\phi) = \langle c_j^+ c_i^+ \rangle_R(\phi) \). In the case \([3]\),

\[
H(\phi) = \text{Tr}\{[e + \frac{1}{2} \Gamma(\phi)]\rho(\phi) + \frac{1}{4} \{\Delta(\phi)\bar{\kappa}(\phi) + \bar{\Delta}(\phi)\kappa(\phi)\}\},
\]

with \( \Gamma_{ij}(\phi) = \sum_{k,l} \bar{v}_{ikjl} \rho_{kl}(\phi), \Delta_{ij}(\phi) = \frac{1}{2} \sum_{k,l} \bar{v}_{ikjl} \kappa_{kl}(\phi), \bar{\Delta}_{ij}(\phi) = \frac{1}{2} \sum_{k,l} \bar{v}_{klij} \bar{\kappa}_{kl}(\phi) \). Let us now evaluate the variation of \([64]\) with respect to \( \mathcal{R} \). We have

\[
\delta (e^{i\phi N})_R = \frac{1}{2} (e^{i\phi N})_R \text{Tr}\{C^{-1}(\phi) [e^{i\phi N} - 1] \delta \mathcal{R}\},
\]

\[
\delta \mathcal{R}(\phi) = e^{i\phi N} C^{-1}(\phi) (\delta \mathcal{R}) C^{-1}(\phi), \quad \bar{\Delta}(\phi) = 1 + \mathcal{R}(e^{i\phi N} - 1),
\]

\[
\delta H(\phi) = \frac{1}{2} \text{Tr}[\mathcal{H}(\phi) \delta \mathcal{R}(\phi)] = \frac{1}{2} \text{Tr}[C^{-1}(\phi) \mathcal{H}(\phi) e^{i\phi N} \bar{C}^{-1}(\phi) \delta \mathcal{R}],
\]

where \( \mathcal{H}(\phi) \) is defined by \( \frac{1}{2} \mathcal{H}_{nm}(\phi) = \partial H(\phi)/\partial \rho_{nm}(\phi) \), i.e.,

\[
\mathcal{H}(\phi) = \left( \begin{array}{cc} h(\phi) & \Delta(\phi) \\ \bar{\Delta}(\phi) & -h^T(\phi) \end{array} \right),
\]

\[
h_{ij}(\phi) = -\partial h(\phi)/\partial \rho_{ji}(\phi), \quad \frac{1}{2} \Delta_{ij}(\phi) = -\partial H(\phi)/\partial \rho_{ji}(\phi), \quad \frac{1}{2} \bar{\Delta}_{ij}(\phi) = -\partial H(\phi)/\partial \bar{\rho}_{ji}(\phi).
\]

Eqs. \([77]-[78]\) are valid for any many-body Hamiltonian. In the case \([76]\), \( h(\phi) = e + \Gamma(\phi) \) and \( \Delta(\phi), \bar{\Delta}(\phi) \) coincide with the previous definitions. We finally obtain

\[
\delta E^N = \frac{1}{2} \text{Tr}[\mathcal{H}^N \delta \mathcal{R}],
\]

where \( \mathcal{H}^N \), defined by \( \frac{1}{2} \mathcal{H}_{nm}^N = \partial E^N/\partial \mathcal{R}_{nm} \), is given by

\[
\mathcal{H}^N = \int d\phi y^N(\phi) C^{-1}(\phi) [(e^{i\phi N} - 1)(H(\phi) - E^N) + \mathcal{H}(\phi) e^{i\phi N} \bar{C}^{-1}(\phi)]
\]

\[
= \left( \begin{array}{cc} h^N & \Delta^N \\ \bar{\Delta}^N & -(h^N)^T \end{array} \right).
\]

For \( H \) hermitian, \( (\mathcal{H}^N)^\dagger = \mathcal{H}^N \). The first term \( C^{-1}(\phi)(e^{i\phi N} - 1)(H(\phi) - E^N) \) arises from the variation of \( y^N(\phi) \).

Eq. \([79]\) holds for arbitrary variations \( \delta \mathcal{R} \). For unitary variations \( \delta \mathcal{R} = i[\delta \mathcal{W}, \mathcal{R}] \), Eq. \([79]\) leads to \( \delta E^N = -\frac{1}{2} i \text{Tr}\{[\mathcal{H}^N, \mathcal{R}] \delta \mathcal{W}\} \). Stability against these variations leads then to the necessary condition

\[
[\mathcal{H}^N, \mathcal{R}] = 0,
\]

which has the same form as the standard HFB condition \([3]\) except that the HFB matrix \( \mathcal{H} \) has been replaced by \( \mathcal{H}^N \).
All previous expressions hold actually in any basis of single particle or quasiparticle states, after appropriate transformation of $\mathcal{N}$. The matrix $\mathcal{K}$ can be diagonalized with a transformation (3), i.e., $Z' = \mathcal{W}^\dagger Z$, with $(Z')^\dagger = (\alpha^\dagger, \alpha)$. We may then write $\mathcal{K} = \mathcal{W} \mathcal{K}' \mathcal{W}^\dagger$, with $\mathcal{K}'$ diagonal, and

$$
\mathcal{R} = \mathcal{WR}' \mathcal{W}^\dagger, \quad \mathcal{R}' = \begin{pmatrix} f & 0 \\ 0 & 1 - f \end{pmatrix},
$$

(82)

with $f_k = \langle \alpha_k^\dagger \alpha_k \rangle_R = (1 + e^{\beta E_k})^{-1}$ and $E_k$ the positive eigenvalues of $\mathcal{K}$.

$T = 0$ limit. For $T = \beta^{-1} \to 0$, $f_k \to 0$ (assuming $E_k \neq 0$) and $R \to |0\rangle\langle 0|$, with $|0\rangle$ the vacuum of the quasiparticles $\alpha_k$. In this limit,

$$
\mathcal{R}' \to \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathcal{R} \to \begin{pmatrix}VV^\dagger & UV^\dagger \\ UU^\dagger \end{pmatrix}^*,
$$

(83)

implying $\rho = (VV^\dagger)^*$, $\kappa = (UV^\dagger)^* = \bar{\kappa}^\dagger$, and $\mathcal{R}^2 = \mathcal{R}$, i.e., $\rho^2 + \kappa \bar{\kappa} = \rho$, $\rho \kappa = \kappa \rho^T$. Using these relations, we obtain the simplified expressions

$$
\det\left[e^{i\phi/2} C(\phi)\right]^{1/2} \to \det\left[e^{i\phi} D(\phi)\right]^{1/2}, \quad D(\phi) = e^{i\phi} \rho + e^{-i\phi} (1 - \rho),
$$

$$
\mathcal{R}(\phi) \to \begin{pmatrix} e^{i\phi} D^{-1}(\phi) \rho & e^{i\phi} D^{-1}(\phi) \kappa \\ e^{-i\phi} \bar{\kappa} D^{-1}(\phi) & 1 - e^{i\phi} [D^{-1}(\phi) \rho]^T \end{pmatrix},
$$

(84)

with $C^{-1}(\phi) = 1 + (e^{-i\phi N} - 1) \mathcal{R}(\phi)$, $\bar{C}^{-1}(\phi) = 1 - e^{-i\phi N} \mathcal{R}(\phi) (e^{i\phi N} - 1)$. With the replacements $C(\phi) = e^{i\phi} D^{-1}(\phi)$, $\bar{C}(\phi) = \bar{\kappa}^\dagger(\phi)$, $\bar{\Delta}(\phi) = \bar{\Delta}^\dagger(\phi)$, Eq. (84) leads to Eqs. (26)–(28).

For $T = 0$ variations that preserve the idempotent condition $\mathcal{R}^2 = \mathcal{R}$, we may employ a simplified matrix $\mathcal{H}^N$, which can be directly derived from the above expressions. Its elements are

$$
h^N = \int d\phi y^N(\phi) D^{-1}(\phi) \{i \sin \phi (H(\phi) - E^N) \\
+ [h(\phi) - i \sin \phi (e^{i\phi} \kappa \bar{\Delta}(\phi) + e^{-i\phi} \Delta(\phi) \bar{\kappa})] D^{-1}(\phi)\},
$$

$$
\Delta^N = \int d\phi y^N(\phi) e^{-i\phi} D^{-1}(\phi) \Delta(\phi), \quad \bar{\Delta}^N = \int d\phi y^N(\phi) e^{i\phi} \bar{\Delta}(\phi) D^{-1}(\phi).
$$

(85)

In the case of Hamiltonian (1), with the previous replacements these expressions lead to Eqs. (22)–(25).
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FIGURES

FIG. 1. The results of the total energy ($E_{tot}$) and the pair-energy ($E_{pair}$) as a function of the strength of the pairing-interaction ($G$) using various particle-number projection methods.

FIG. 2. The results of the total energy ($E_{tot}$), the pair-energy ($E_{pair}$) and the alignment ($J_x$) for six-particles in a deformed $j = 11/2$ orbital using the monopole interaction. The results are obtained with Hartree-Fock-Bogoliubov (HFB), projection after variation (PAV), Lipkin-Nogami (LN) and projected HFB (PHFB) approaches.

FIG. 3. The results of the total energy ($E_{tot}$), the pair-energy ($E_{pair}$) and the alignment ($J_x$) using the monopole plus quadrupole pairing interaction.

FIG. 4. The results of the total energy ($E_{tot}$), the pair-energy ($E_{pair}$) and the alignment ($J_x$) using the full delta-interaction.

FIG. 5. The results of the pair-energy ($E_{pair}$) as a function of the deformation parameter ($\kappa$). (a) gives the results with monopole-pairing, (b) presents the results with (monopole plus quadrupole)-interaction and (c) gives the results with full delta-interaction.

FIG. 6. The dynamic moment of inertia for $\kappa = 5.5$. (a) gives the results with monopole-pairing, (b) presents the results with (monopole plus quadrupole)-interaction and (c) gives the results with full delta-interaction.
