# Particle-number-conserving theory for nuclear pairing

L. Y. Jia (贾力源)*

*Department of Physics, University of Shanghai for Science and Technology, Shanghai 200093, People's Republic of China*
*and Department of Physics, Hebei Normal University, Shijiazhuang, Hebei 050024, People's Republic of China*

(Received 13 May 2013; revised manuscript received 15 September 2013; published 3 October 2013)

A new microscopic theory for nuclear pairing is proposed through the generalized density matrix formalism. Instead of the variation principle, we start from the Heisenberg equations of motion for density matrix operators $K_{12} \equiv a_2 a_1$. The theory generalizes the well-known particle-particle random-phase approximation. Its analytical equations are as simple as that of the BCS theory and can be solved within a similar computer time if the model space is not too large. The current theory conserves the exact particle number and is valid at arbitrary pairing strength (including those below the BCS critical strength). It is also of interest to other mesoscopic systems such as ultrasmall metallic grains.

DOI: 10.1103/PhysRevC.88.044303 PACS number(s): 21.60.Ev, 21.10.Re, 21.30.Fe, 27.40.+z

## I. INTRODUCTION

The BCS theory was first proposed as a microscopic theory for superconductivity [1]. Later it was adopted in nuclear physics for treating pairing correlations [2,3]. After fifty years, it is still one of the "standard" treatments [4], mainly because of its simplicity and the convenience in adding higher-order correlations [for example, by quasiparticle random-phase approximation (QRPA)]. However, there are two main disadvantages of the theory applied to finite nuclei, as compared to macroscopic quantum systems. First, by introducing quasiparticles, it destroys particle-number conservation. This is often a problem because the effective number of particles involved in nuclear pairing is never very large. Second, for the nuclear system with finite level spacing, the BCS theory requires a minimum pairing strength. Below that strength it gives only trivial (vanishing) solutions, while in reality pairing always has an effect.

A common improvement is to use the "pair condensate" [Eq. (1), with definite particle number] as the variational ground state [5] instead of the BCS "quasiparticle vacuum". Usually the criteria to determine the variational parameters is minimizing the energy in the variation principle [5–10].

In this work we propose a new criteria for determining the wave function (1). Instead of the variation principle, we start from the Heisenberg equations of motion (EOM) for density matrix operators $K_{12} \equiv a_2 a_1$. The current theory generalizes the well-known particle-particle random-phase approximation (pp-RPA) describing pairing vibrations at magic nuclei [11–14].

We note that the pairing Hamiltonian could be solved exactly by direct numerical diagonalization in spaces with fixed seniority [15,16] or by the Monte Carlo algorithm [17–19]. And there exist exact algebraic solutions for a special class [20,21] of the pairing Hamiltonian following Richardson's method [22]. The advantage of the current EOM method should be its simplicity and the convenience for treating higher-order correlations along the same line, as explained in the text.

This work is an application of the generalized density matrix (GDM) formalism that was originally introduced in Refs. [23–26] and recently reconsidered in Refs. [27–29]. Until now its treatment of nuclear pairing correlations is limited to the conventional BCS and has the above discussed disadvantages. Here we explore the possibility of using the pair condensate (1) as the ground state, instead of the BCS quasiparticle vacuum. The manuscript is organized as following. In Sec. II we set up the GDM formalism in a general way, but solve in this work only the lowest-order (mean-field) equations. We show that the theory is correct in the limits of strong and weak pairing. Then in Sec. III the theory is applied to the calcium isotopes with comparisons to the exact shell-model results and those of BCS and the variation principle. Finally Sec. IV summarizes the work and discusses further directions.

## II. FORMALISM

In the presence of pairing correlations, we assume that the ground state of the $2N$-particle system is an $N$-pair condensate

$$|\phi_N\rangle = \frac{1}{\sqrt{\chi_N}}(P^\dagger)^N|0\rangle, \tag{1}$$

where $\chi_N$ is a normalization factor that will be specified later [see Eq. (23)], and $P^\dagger$ is the pair creation operator

$$P^\dagger = \frac{1}{2}\sum_1 v_1 a_1^\dagger a_{\tilde{1}}^\dagger. \tag{2}$$

In Eq. (2) the summation runs over the entire single-particle space (we label the single-particle levels by the Arabic numerals 1, 2, ...). $|\tilde{1}\rangle$ is the time-reversed level of the single-particle level $|1\rangle$. The pair structures $v_1$ are parameters to be determined by the theory.

With the antisymmetrized fermionic Hamiltonian

$$H = \sum_{12} \epsilon_{12}\, a_1^\dagger a_2 + \frac{1}{4}\sum_{1234} V_{1234}\, a_1^\dagger a_2^\dagger a_3 a_4, \tag{3}$$

*liyuan.jia@usst.edu.cn

 

we calculate the Heisenberg equations of motion for the density matrix operators $R_{12} \equiv a_2^\dagger a_1$ and $K_{12} = a_2 a_1$,

$$[R_{12}, H] = [f\{R\}, R]_{12} - (K\Delta^\dagger\{K\})_{12} + (\Delta\{K\}K^\dagger)_{12}, \tag{4}$$

$$[K_{12}, H] = \Delta\{K\}_{12} + (Kf^T\{R\})_{12} + (f\{R\}K)_{12} - (\Delta\{K\}R^T)_{12} - (R\Delta\{K\})_{12}, \tag{5}$$

where the self-consistent fields are defined as

$$W\{R\}_{12} = \sum_{34} V_{1432} R_{34}, \quad f\{R\} = \epsilon + W\{R\}, \tag{6}$$

$$\Delta\{K\}_{12} = \frac{1}{2}\sum_{34} V_{1234} K_{43}. \tag{7}$$

The quantities $W\{R\}$, $f\{R\}$, and $\Delta\{K\}$ are square matrices with dimensions equal to that of the single-particle space; their matrix elements are operators given by Eqs. (6) and (7). Terms on the right-hand side of Eqs. (4) and (5) are read as matrix multiplications; for example, $[f\{R\}, R]_{12} = (f\{R\}R)_{12} - (Rf\{R\})_{12} = \sum_3 f\{R\}_{13}R_{32} - \sum_3 R_{13}f\{R\}_{32}$.

On the right-hand side of Eqs. (4) and (5) we have used the factorization

$$a_4^\dagger a_3^\dagger a_2 a_1 \doteq a_4^\dagger a_1 \cdot a_3^\dagger a_2 - a_4^\dagger a_2 \cdot a_3^\dagger a_1 + a_4^\dagger a_3^\dagger \cdot a_2 a_1, \tag{8}$$

$$a_4^\dagger a_3 a_2 a_1 \doteq a_4^\dagger a_1 \cdot a_3 a_2 - a_4^\dagger a_2 \cdot a_3 a_1 + a_4^\dagger a_3 \cdot a_2 a_1, \tag{9}$$

generalizing Eq. (11) in Ref. [28]. In the presence of the pair condensate, terms like $a_4^\dagger a_3^\dagger \cdot a_2 a_1$ are not small. As before, "$\doteq$" is used when an equation holds in the collective subspace but not in the full many-body space. For details we refer the reader to Ref. [28], where the approximations (8) and (9) have been explained at length.

The method assumes that the Hamiltonian and the density matrix operators can be expanded as Taylor series of the bosonic mode operators (collective coordinate $\alpha$ and momentum $\pi$) within the collective subspace (see Ref. [28] for details),

$$H \doteq \sum_{ml} \Lambda^{(m,2l)} \frac{1}{2} \frac{\{\alpha^m, \pi^{2l}\}}{m!(2l)!}, \tag{10}$$

and

$$R_{12} = a_2^\dagger a_1 \doteq \sum_{mn} r_{12}^{(mn)} \frac{1}{2} \frac{\{\alpha^m, \pi^n\}}{m!n!}, \tag{11}$$

$$K_{12} = a_2 a_1 \doteq \sum_{mn} k_{12}^{(mn)} \frac{1}{2} \frac{\{\alpha^m, \pi^n\}}{m!n!}. \tag{12}$$

In Eq. (12) $K_{12}$ destroys two particles, hence it connects the collective subspace with $2N$ particles to that with $2N-2$ particles. The first term $k^{(00)} \equiv \kappa$ is the usual "pair transfer amplitude" between the ground states of neighboring even-even nuclei. Higher-order terms $k^{(mn)}$ represent the transfer amplitudes between the collectively excited states (with phonons). Strictly speaking, the generalized density matrices ($r_{N,12}$, $k_{N,12}$), the mode operators ($\alpha_N$, $\pi_N$), and the bosonic Hamiltonian parameters $\Lambda_N^{(m,2l)}$ should have the label of particle number $2N$, and the GDM equations should be solved simultaneously for all the nuclei between two magic numbers, in a way similar to that in Ref. [30]. However, in this work we will drop the label $N$, assuming neighboring even-even nuclei have similar collective modes ($\alpha_N \approx \alpha_{N-1}$, $\pi_N \approx \pi_{N-1}$) and density matrices ($r_N \approx r_{N-1}$, $k_N \approx k_{N-1}$). More careful treatment with explicit label $N$ will be discussed in the future.

Substituting the expansions (10)–(12) into the equations of motion (4) and (5), and calculating commutators involving bosonic operators $\alpha$ and $\pi$, we arrive at the GDM set of equations. In this work we consider only the lowest-order (mean-field) equations:

$$0 = [f, \rho] - \kappa\delta^\dagger + \delta\kappa^\dagger, \tag{13}$$

$$\left(\Lambda_N^{(00)} - \Lambda_{N-1}^{(00)}\right)\kappa = f\kappa + \delta - \delta\rho^T - \rho\delta + \kappa f^T, \tag{14}$$

where $\rho \equiv r^{(00)}$, $\kappa \equiv k^{(00)}$, $f = \epsilon + W\{\rho\}$, and $\delta = \Delta\{\kappa\}$ are leading terms in the expansions of respective quantities (6, 7, 11, 12). [$W\{\rho\}$ is defined by replacing $R$ with $\rho$ in Eq. (6); similarly for $\Delta\{\kappa\}$ by replacing $K$ with $\kappa$ in Eq. (7).] $\Lambda_N^{(00)}$, the leading term in the bosonic Hamiltonian (10), is the binding energy of the $N$-pair condensate (1). Usually the difference $\Lambda_N^{(00)} - \Lambda_{N-1}^{(00)}$ is not small and should be kept. Equation (14) generalizes the well-known pp-RPA [12]; the latter results if we put $f = \epsilon$, and $\rho$ to be the Slater determinant ($\rho^2 = \rho$) for the single-particle occupation numbers of the magic nucleus.

On the ground state (1), the density matrices $\rho$ and $\kappa$ are "diagonal":

$$\rho_{12} = \langle\phi_N|a_2^\dagger a_1|\phi_N\rangle = \delta_{12} n_1, \tag{15}$$

$$\kappa_{12} = \langle\phi_{N-1}|a_2 a_1|\phi_N\rangle = \delta_{\bar{1}2} s_1, \tag{16}$$

where $s_1$ and $n_1$ are functions of the pair structure $v$ (2), given later by the recursive formula (24). In a realistic shell-model calculation, usually each single-particle level has distinct spin and parity, thus both the mean fields $f$ and $\delta$ are "diagonal":

$$f_{12} = \delta_{12} e_1, \tag{17}$$

$$\delta_{12} = \delta_{1\bar{2}} g_1. \tag{18}$$

Under Eqs. (15)–(18), Eq. (13) is satisfied automatically, and Eq. (14) becomes

$$\Lambda_N^{(00)} - \Lambda_{N-1}^{(00)} = 2e_1 + g_1 \frac{2n_1 - 1}{s_1}. \tag{19}$$

Equation (19) is the main equation of the theory. It implies that the right-hand side is independent of the single-particle label 1, which gives $\Omega - 1$ constraints for a single-particle space of dimension $2\Omega$ ($\Omega$ time-reversal pairs). These constraints fix the $\Omega - 1$ parameters in Eq. (2) (a common factor in $v_1$ does not matter), which completes the theory.

The theory extends the concept of pairing vibration at magic nuclei [12] to open-shell nuclei: What is the "best" *local* pair structure (2), such that the ground state of the neighboring even-even nucleus can be reached by simply removing one pair from the condensate (1), without adjusting or changing the pair structure? In reality this would be the case if the experimental pair-emission cross section to the ground state is dominant over those to other $0^+$ states.

At last we supply the formula for the recursive calculation of $\rho$ (15) and $\kappa$ (16) in terms of $v$ (2). Introducing

$$P_1^\dagger = a_1^\dagger a_{\bar{1}}^\dagger \tag{20}$$

and

$$t_N^1 = \langle 0|P^{N-1}P_1(P^\dagger)^N|0\rangle, \tag{21}$$

it is easy to deduce the recursive formula

$$t_N^1 = Nv_1\chi_{N-1} - N(N-1)(v_1)^2 t_{N-1}^1, \tag{22}$$

$$\chi_N = \frac{1}{2}\sum_1 v_1 t_N^1, \tag{23}$$

with initial value $t_{N=1}^1 = v_1$. Here $t_N^1$ and $\chi_N$ (1) are polynomials of $v$. Finally the expressions for $n_1$ (15) and $s_1$ (16) are

$$n_1 = \frac{Nv_1 t_N^1}{\chi_N}, \quad s_1 = \frac{t_N^1}{\sqrt{\chi_N\chi_{N-1}}}. \tag{24}$$

The functional forms of $n$ and $s$ in terms of $v$ (2) are "kinematics" of the system (like the "kinematic" Clebsch-Gordan coefficients for rotational symmetry), which can be calculated (and stored or tabulated) once for all in a given model space that is not too large. The main computing-time cost of the method should be that required to solve Eq. (19), which is as simple as the BCS equation. In fact, Eq. (19) behaves better than the BCS one, because it involves essentially a ratio of two polynomials but no square roots.

Of course, in too large a model space the storage of the "kinematics" in a computer would be impossible. Here we do a rough estimation for the computer space needed in practical calculations. With the spherical mean field, a typical large calculation may involve 15 single-particle levels (3 major shells) and 25 pairs of particles (Fermi surface in the middle of the model space). Hence there are $C_{25-1+15-1}^{15-1} \approx 10^{10}$ terms in the polynomial $t_N^1$ (22), and we need to store the $10^{10}$ coefficients as the "kinematics" of the system. This needs roughly 10 gigabytes of computer space, which is within the capacity of a hard disk, even the memory, of modern computers. However, for bigger model spaces, or if one decides to break the rotational symmetry in the mean field and use Nilsson single-particle levels (more nondegenerate levels), the kinematics may be too big to be stored in a computer. In this case the kinematics needs to be calculated on the fly and may become the dominating computing-time cost.

Below we take the pairing Hamiltonian:

$$\epsilon_{12} = \delta_{12}\epsilon_1, \quad V_{1234} = -\delta_{2\bar{1}}\delta_{3\bar{4}}G_{13} \tag{25}$$

in Eq. (3). Consequently the mean fields (17) and (18) become

$$e_1 = \epsilon_1 - G_{11}n_1, \quad g_1 = \frac{1}{2}\sum_2 G_{12}s_2. \tag{26}$$

The theory is correct in the limits of strong and weak pairing. In the degenerate model (limit of strong pairing), Eqs. (22) and (23) imply $t_N = Nv^2(\Omega - N + 1)t_{N-1}$ and $\chi_N = \Omega v t_N$, which in turn give $n = N/\Omega$ and $s = \sqrt{N(\Omega - N + 1)}/\Omega$ according to Eq. (24). They agree with the known results. The right-hand side of Eq. (19) becomes $2\epsilon + (G\Omega s)[(2N/\Omega - 1)/s] = 2\epsilon + G(2N - \Omega)$, which is the correct binding energy difference $\Lambda_N^{(00)} - \Lambda_{N-1}^{(00)}$.

In the limit of weak pairing, keeping only leading-order terms in $G$, we have on the Fermi surface $n_F \approx N_F/\Omega_F$, $s_F \approx \sqrt{N_F(\Omega_F - N_F + 1)}/\Omega_F$ ($N_F$ is the number of pairs on the Fermi surface at zero $G$, and $2\Omega_F$ is the degeneracy at the Fermi surface); $s_1 \approx 0$, $n_1 \approx 1$ or 0 for other single-particle levels below or above the Fermi surface; and the mean fields $e_1 \approx \epsilon_1$, $g_1 \approx G_{1F}\Omega_F s_F$. Consequently Eq. (19) becomes $2\epsilon_F \approx 2\epsilon_1 + G_{1F}\Omega_F(2n_1 - 1)s_F/s_1$, which implies that $s_1 \approx G_{1F}(1 - 2n_1)\sqrt{N_F(\Omega_F - N_F + 1)}/[2(\epsilon_1 - \epsilon_F)]$ for $1 \neq F$. This is the correct first-order perturbation theory result.

In this work the numerical calculations (in Sec. III) are done by MATLAB. We solve Eq. (19) by minimizing the objective quantity

$$\sum_{1\leqslant i\leqslant\Omega}\left[\left(2e_i + g_i\frac{2n_i - 1}{s_i}\right) - \left(2e_{i+1} + g_{i+1}\frac{2n_{i+1} - 1}{s_{i+1}}\right)\right]^2$$

with the MATLAB built-in function "fminunc", resulting in a minimum in the order of magnitude $10^{-14}$. The variables in the minimization are pair structures $v_1$ (2), on which the objective quantity depends through Eqs. (22)–(24), and (26). Other theories (the BCS equation and the variational principle) are numerically solved by the same MATLAB function fminunc.

## III. CALCIUM ISOTOPES

We apply the theory to calcium isotopes, using the well established FPD6 interaction [31] (keeping only the pairing two-body matrix elements), where $^{40}$Ca is taken as an inertia core, and the valence neutrons are distributed in four single-neutron levels $0f_{7/2}$, $1p_{3/2}$, $0f_{5/2}$, and $1p_{1/2}$.

We first consider the nucleus $^{48}$Ca, where the BCS results in only a trivial zero solution due to the "complete filling" of the $0f_{7/2}$ orbit. In the pairing Hamiltonian (25), the single-particle energies $\epsilon$ are fixed by experimental data. From the spectrum of $^{49}$Ca we read $\epsilon_{p_{1/2}} - \epsilon_{p_{3/2}} = 2.023$ MeV, and $\epsilon_{f_{5/2}} - \epsilon_{p_{3/2}} = 3.585$ MeV. The neutron absorption energy of $^{48}$Ca gives $\epsilon_{p_{3/2}} = -5.146$ MeV. $\epsilon_{f_{7/2}}$ is estimated within the single-$j$ degenerate pairing model as $\epsilon_{f_{7/2}} = -9.945 + 0.541 = -9.404$ MeV, where $-9.945$ MeV is the neutron emission energy of $^{48}$Ca and 0.541 MeV is the FPD6 pairing strength for the $0f_{7/2}$ orbit. For the two-body part, an artificial factor $\eta$ is multiplied onto the FPD6 pairing matrix elements ($G_{12} = \eta G_{12}^{\mathrm{FPD6}}$). To see how the theory behaves at different pairing strengths, we do a set of calculations at different values of $\eta$ (from 0.2 to 2.0), the realistic case corresponds to $\eta = 1$.

The results are given in Fig. 1. We see that the GDM calculation reproduces quite well the exact results (by the shell-model code NUSHELLX [32]) of occupation numbers $n_J$ and pair emission amplitudes $s_J$ at all pairing strengths, including those below the critical value ($\eta_c = 1.345$) of BCS. It even gets one detail right: the inversion (around $\eta = 1.6$) of relative positions of the two very close curves for $f_{5/2}$ and $p_{1/2}$.

Next we test the theory in different nuclei. The chain of calcium isotopes is calculated with mass number $42 \leqslant A \leqslant$

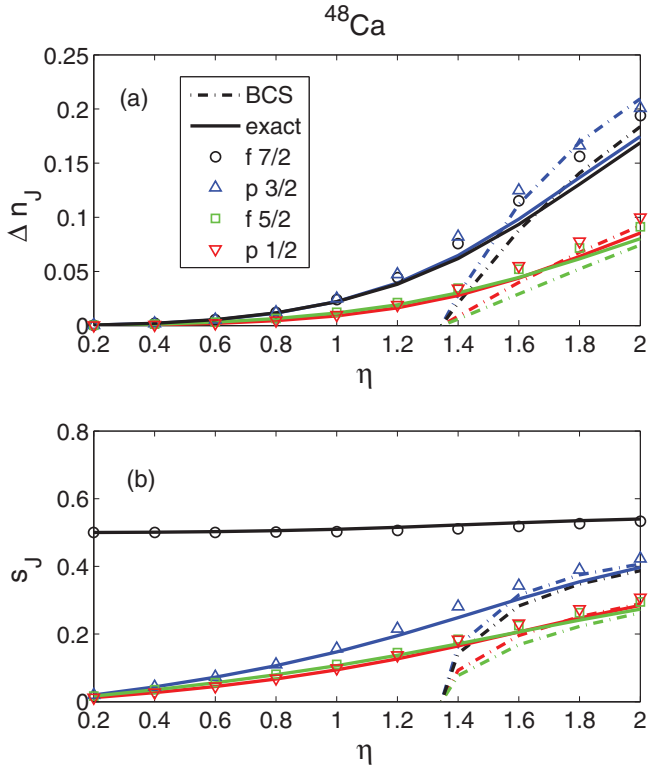


FIG. 1. (Color online) Occupation numbers $n_J$ (15) and pair-emission amplitudes $s_J$ (16) in $^{48}$Ca as a function of pairing strength $\eta$. The upper panel plots $\Delta n_J$, the derivations from the naive Fermi occupation ($\Delta n_J = 1 - n_{f7/2}, n_{p3/2}, n_{f5/2}, n_{p1/2}$). The solid lines and dashed-dotted lines show the exact results (by NUSHELLX) and BCS results, respectively. The symbols show the GDM results, where black circles, blue up-triangles, green squares, and red down-triangles are for single-particle levels $f_{7/2}$, $p_{3/2}$, $f_{5/2}$, and $p_{1/2}$, respectively. The same color convention is used in plotting the solid lines (exact) and dashed-dotted lines (BCS). The plotted BCS $s_J$ is defined as $s_1 = {}_{\rm BCS}\langle\phi_N|a_{\bar{1}}a_1|\phi_N\rangle_{\rm BCS} = \sqrt{n_1(1-n_1)}$.

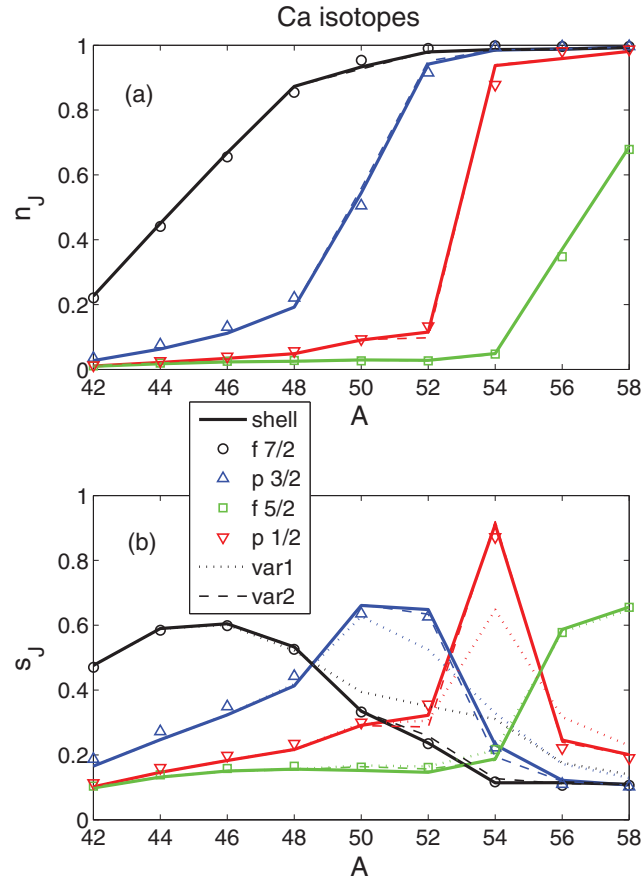


FIG. 2. (Color online) Occupation numbers $n_J$ (15) and pair-emission amplitudes $s_J$ (16) in calcium isotopes ($A$ is the mass number). The solid lines show the shell-model results (by NUSHELLX). The dotted lines and dashed lines show two sets of variational results, as explained in the text. The symbols show the GDM results, where black circles, blue up-triangles, green squares, and red down-triangles are for single-particle levels $f_{7/2}$, $p_{3/2}$, $f_{5/2}$, and $p_{1/2}$, respectively. The same color convention is used in plotting the solid lines (shell), dotted lines (var1), and dashed lines (var2). Note that different single-particle energies are used in Figs. 1 and 2 (see text).

58. For simplicity in this example we fix the single-particle energies $\epsilon$ by the FPD6 ones: $\epsilon_{f_{7/2}} = -8.388$, $\epsilon_{p_{3/2}} = -6.495$, $\epsilon_{f_{5/2}} = -1.897$, and $\epsilon_{p_{1/2}} = -4.478$ MeV. For the two-body part we take the FPD6 pairing matrix elements ($G_{12} = G_{12}^{\rm FPD6}$). The results are shown in Fig. 2. The GDM method reproduces the exact results quite well, even the sudden changes around $A = 54$.

We also compare the GDM method with the variation principle in Fig. 2. The most convenient way to calculate the expectation value of the pairing Hamiltonian (25) on the pair condensate (1) is probably given by the recursive formulas [including Eq. (22)] in the appendix of Ref. [9]. Then the variational parameters $v_1$ (2) are determined by minimizing the average energy. For the occupation numbers $n_J$ (15), we see that the variational results are better in most cases. For the pair-transfer amplitudes $s_J = \langle\phi_{N-1}|a_{J\tilde{M}}a_{JM}|\phi_N\rangle$ (16), we present two sets of variational results. In "var1" the pair structure $v_1$ in $|\phi_{N-1}\rangle$ and $|\phi_N\rangle$ are the same, given by minimizing $\langle\phi_N|H|\phi_N\rangle$; while in "var2" $v_1$ in $|\phi_{N-1}\rangle$ and $|\phi_N\rangle$ are different, given by minimizing $\langle\phi_{N-1}|H|\phi_{N-1}\rangle$ and $\langle\phi_N|H|\phi_N\rangle$, respectively. We see that in general the GDM $s_J$ and the var2 $s_J$ have similar accuracy, both agree well with the exact results; but the less-careful var1 $s_J$ sometimes have considerable errors. Specifically, if we insist on the situation of pairing vibration (removing one pair without adjusting the pair structure $v_1$), we should use the GDM theory. (We have also done a third variational calculation, by minimizing $\langle\phi_{N-1}|H|\phi_{N-1}\rangle + \langle\phi_N|H|\phi_N\rangle$, insisting that $|\phi_{N-1}\rangle$ and $|\phi_N\rangle$ have the same $v_1$; the result improves var1 $s_J$ but is not as good as that of the GDM method.) The necessary recursive formulas for the variational calculation are given in Appendix.

It is well known that the variation principle gives the best and lowest energy, hence it is natural to ask how far away the GDM solution is from this energy minimum. In Fig. 3 we show the ground state energies by different calculations in calcium isotopes. The curve "corr" shows the pairing correlation energy $E_{\rm corr}$, defined by $E_{\rm corr} = \sum_1 \epsilon_1 n_1^F - E_{\rm shell}$, where $E_{\rm shell}$ is the exact ground state energy of the shell model calculation, and $n_1^F = 1$ or 0 is the occupation number

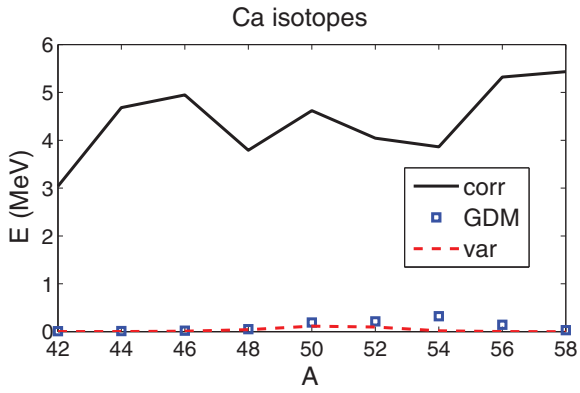


FIG. 3. (Color online) Ground state energies in calcium isotopes ($A$ is the mass number). The black solid line shows the pairing correlation energy. The blue squares and the red dashed line show the ground state energies calculated by the GDM method and the variation principle, respectively, measured from the exact ground state energy. For details please see text.

of the naive Fermi distribution. The curve "var" shows the ground state energy by the variational calculation measured from the exact one, $E_{\rm var} = \langle\phi_N^{\rm var}|H|\phi_N^{\rm var}\rangle - E_{\rm shell}$, where $|\phi_N^{\rm var}\rangle$ is the pair condensate (1) with its pair structure $v_1$ (2) determined by the variation principle. Similarly, the curve "GDM" shows the ground state energy by the GDM method, $E_{\rm GDM} = \langle\phi_N^{\rm GDM}|H|\phi_N^{\rm GDM}\rangle - E_{\rm shell}$, where $v_1$ in $|\phi_N^{\rm GDM}\rangle$ is determined by the GDM equation (19). From Fig. (3) we see that both the variation principle and the GDM method give good ground state energies: the errors are small relative to the pairing correlation energies. In particular, the energy of $|\phi_N^{\rm GDM}\rangle$ is very close to the variational minimum $\langle\phi_N^{\rm var}|H|\phi_N^{\rm var}\rangle$. Thus the latter is relatively flat in certain directions.

## IV. SUMMARY

In summary, we explored the possibility of using the pair condensate (1) instead of the BCS quasiparticle vacuum as the starting point of the GDM formalism. As the lowest-order result, a theory for nuclear pairing is proposed that conserves the exact particle number and is valid at arbitrary pairing strength (including those below the critical point of BCS). It is a generalization of the well-known pp-RPA. Correlations beyond the mean field could be studied solving higher-order equations in the GDM formalism.

Instead of the variation principle, the current pairing theory starts from the Heisenberg equations of motion. It would be interesting to see how the theory behaves in cases when the average energy had a flat minimum and the variational calculation was likely to fail.

We note that the GDM theory (19) reproduces the pair-transfer amplitudes with excellent accuracy directly, while the variational principle needs two calculations for the parent and daughter nuclei, respectively, to achieve the same accuracy (see the "var2" curve in Fig. 2).

Odd-mass nuclei could be calculated consistently. The effective Hamiltonian, $\langle 2N+1|H|2N+1\rangle = \langle 2N|aHa^\dagger|2N\rangle$, was calculated by substituting Eq. (3) into the above expression and then using factorizations similar to Eq. (8), where the density matrices $a^\dagger a$ and $aa$ are known from the neighboring even-even nuclei. Spectroscopic factors, $\langle 2N-1|a|2N\rangle = \langle 2N|a^\dagger a|2N\rangle$, could also be calculated in a similar way. These will be studied in the future.

Another important direction is to consider the current GDM pairing theory in the case when the mean fields are not diagonal in the single-particle basis. This would correspond to the generalization from BCS to Hartree-Fock-Bogoliubov (HFB) theory, and was necessary for *ab initio* mean-field calculations like the modern density-functional-theory–HFB methods. In particular, it might be helpful for treating the ambiguities related to particle-number projection in the latter (see, for example, Ref. [33]).

## ACKNOWLEDGMENT

The author gratefully acknowledges discussions with Prof. Vladimir Zelevinsky.

## APPENDIX: RECURSIVE FORMULAS

Here we provide the necessary recursive formulas for the variational calculations in Sec. III. These formulas exist because operators $P_1^\dagger$ (20), $P_1$, and $\hat{n}_1 = a_1^\dagger a_1$ form a closed algebra (commute among themselves). We introduce

$$a_N^{12} \equiv \langle 0|P^N P_1^\dagger P_2 (P^\dagger)^N|0\rangle, \tag{A1}$$

$$b_N^{12} \equiv \langle 0|P^{N-2} P_1 P_2 (P^\dagger)^N|0\rangle, \tag{A2}$$

where $P^\dagger$ and $P_1^\dagger$ have been defined in Eqs. (2) and (20), $a_N^{12}$ and $b_N^{12}$ are real symmetric matrices, and $b_N^{11} = 0$. It is easy to derive the recursive formulas

$$a_N^{12} = v_2 N t_N^1 - (v_2)^2 N(N-1) b_N^{12}, \tag{A3}$$

$$b_N^{1\neq 2} = v_2 N t_{N-1}^1 - (v_2)^2 N(N-1) a_{N-2}^{12}, \tag{A4}$$

where $t_N^1$ has been calculated in Eq. (22). Then the expectation value of the pairing Hamiltonian (25) on the pair condensate (1) is

$$\langle\phi_N|H|\phi_N\rangle = \sum_1 \epsilon_1 n_1 + \frac{1}{4}\sum_{12} G_{12}\frac{a_N^{12}}{\chi_N}, \tag{A5}$$

where $\chi_N$ and $n_1$ have been calculated in Eqs. (23) and (24). In Eq. (A5) the summation runs over the entire single-particle space. Equations (A1)–(A5) have been given in the appendix of Ref. [9] in a slightly different form.

The var2 curve of Fig. 2 plots the quantity

$$\bar{s}_1 \equiv \langle\bar{\phi}_{N-1}|P_1|\phi_N\rangle, \tag{A6}$$

where $|\bar{\phi}_{N-1}\rangle$ and $|\phi_N\rangle$ have different pair structures, $\bar{v}_1$ and $v_1$. To calculate $\bar{s}_1$ we introduce

$$T_N^1 \equiv \langle 0|\bar{P}^{N-1} P_1 (P^\dagger)^N|0\rangle, \tag{A7}$$

$$\bar{T}_N^1 \equiv \langle 0|P^{N-1} P_1 (\bar{P}^\dagger)^N|0\rangle, \tag{A8}$$

$$X_N \equiv \langle 0|\bar{P}^N (P^\dagger)^N|0\rangle. \tag{A9}$$

It is easy to derive the recursive formulas

$$T^1_N = v_1 N X_{N-1} - (v_1)^2 N(N-1)\bar{T}^1_{N-1}, \quad \text{(A10)}$$

$$\bar{T}^1_N = \bar{v}_1 N X_{N-1} - (\bar{v}_1)^2 N(N-1) T^1_{N-1}, \quad \text{(A11)}$$

$$X_N = \frac{1}{2}\sum_1 \bar{v}_1 T^1_N = \frac{1}{2}\sum_1 v_1 \bar{T}^1_N, \quad \text{(A12)}$$

with initial values $T^1_{N=1} = v_1$ and $\bar{T}^1_{N=1} = \bar{v}_1$. Consequently $\bar{s}_1$ is

$$\bar{s}_1 = \frac{T^1_N}{\sqrt{\bar{\chi}_{N-1}\chi_N}}. \quad \text{(A13)}$$


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