Deformed nuclei in the Lipkin-Nogami approach

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(Received 05 July 1978)

The Lipkin-Nogami version of the spherical BCS method is extended to study the effects of pairing correlations on the ground-state properties of nuclei with permanent deformation. The Kuo-Brown effective interaction is used to study the even-even nuclei in the $2p$-$1f$ shell. Considerable changes in the pairing energies compared with the deformed BCS and full Hartree-Fock-Bogoliubov methods are obtained. The neutron-pair separation energies and the projected spectra show improved agreement with the data.

[NUCLEAR STRUCTURE Lipkin-Nogami method with deformed basis applied to even Ti isotopes. Effective Kuo-Brown Interaction; projected spectra.]

In an attempt to correct the ground-state energy of a nucleus in the Bardeen-Cooper-Schrieffer (BCS) approximation[1] for the fluctuations in the number of nucleons due to pairing correlations, the present authors recently applied[2] the Lipkin-Nogami version[3-7] of the BCS approximation to study the Ni, Zn, and Ge isotopes. Unlike the previous studies[3-7] a realistic interaction was used and the method was extended to be applicable to nuclei having both neutrons and protons outside the closed core. The method was limited to spherical shapes only. Nuclei in the $2p$-$1f$ shell, however, are known[8] to possess deformed Hartree-Fock (HF) and Hartree-Fock-Bogoliubov (HFB) solutions which are lower in energy than the spherical BCS solutions. The purpose of the present paper is to extend and apply the Lipkin-Nogami method to nuclei having deformed solutions. The method is termed as modified deformed BCS approximation (MDBCS).

As before[2] the modified Hamiltonian is written as

$$\mathcal{H} = H - \lambda_1 N - \lambda_2 N^2 , \tag{1}$$

where H is the shell-model Hamiltonian describing the n particles outside the core, i.e.,

$$H = \sum_i \epsilon_i a_i^\dagger a_i + \frac{1}{4} \sum_{ijkl} \langle ij \,|V_A|\, kl\rangle a_i^\dagger a_j^\dagger a_l a_k , \tag{2}$$

where ϵ_i represents the single-particle energy in a state $|i\rangle \equiv |j_i m_i \tau\rangle$ and $\langle ij\,|V_A|\,kl\rangle$ represents the antisymmetrized matrix elements between two-particle states. N represents the particle number operator. The Lagrange multiplier λ_1 is determined by the constraint

$$\langle N\rangle = n , \tag{3}$$

where the expectation value $\langle N\rangle$ is calculated with respect to the BCS ground-state wave function which is approximated by the vacuum of quasiparticles ($A_\alpha^\dagger$) defined by

$$A_\alpha^\dagger = U_\alpha C_\alpha^\dagger + V_\alpha C_{\bar\alpha} , \tag{4}$$

where $C_\alpha^\dagger$ represents a Hartree-Fock deformed particle state $|\alpha\rangle$ given by

$$|\alpha\rangle = C_\alpha^\dagger |0\rangle = \sum_i D_{\alpha i} |i\rangle , \tag{5}$$

and $|\bar\alpha\rangle = T|\alpha\rangle$ is the time reversed state. The HF transformation coefficients $D_{\alpha i}$ are obtained by self-consistently diagonalizing the HF Hamiltonian

$$\langle jm\tau\,|h_{\rm HF}\,|j'm\tau\rangle = \epsilon_j \delta_{jj'} + \sum_{\substack{j_1 j_2 \\ m_1 \tau'}} \langle jm\tau, j_1 m_1 \tau'\,|V_A\,|j'm\tau, j_2 m_1 \tau'\rangle \times \sum_{\alpha=1}^{n_\tau} D^{\tau'}_{\alpha, j_1 m_1} D^{\tau'}_{\alpha, j_2 m_1} , \tag{6}$$

where an axial symmetry is implied for the HF orbitals and the superscript on D coefficients stands for the z component of the isotopic spin. The parameter λ_2 is determined using three different conditions as described in Ref. 2. The resulting values of λ_2 are labeled I, II, and III, respectively. The first condition

$$\langle \mathcal{H} N^2\rangle = \langle \mathcal{H}\rangle \langle N^2\rangle , \tag{7}$$

gives

$$\lambda_2^{\mathrm{I}} = -\frac{1}{4}\frac{\sum_{\alpha,\beta,i,j} D_{\alpha i}^{\,2}\langle i\bar{i}\,|V_A|\,j\bar{j}\rangle D_{\beta j}^{\,2} U_\alpha V_\alpha^{\,3} U_\beta^{\,3} V_\beta - \sum_{\alpha,i} D_{\alpha i}^{\,2} D_{\alpha i}^{\,2}\langle i\bar{i}\,|V_A|\,i\bar{i}\rangle U_\alpha V_\alpha^{\,3} U_\alpha^{\,3} V_\alpha}{\sum_{\alpha\neq\beta}(U_\alpha V_\alpha U_\beta V_\beta)^2}. \tag{8}$$

The second condition,

$$\langle \mathcal{H} H\rangle = \langle \mathcal{H}\rangle\langle H\rangle, \tag{9}$$

leads to

$$\lambda_2^{\mathrm{II}} = \frac{1}{4}\frac{\sum_{\alpha,\beta,i,j}(D_{\alpha i}^{\,2}\langle i\bar{i}\,|V_A|\,j\bar{j}\rangle D_{\beta j}^{\,2})^2 (V_\alpha^{\,2} U_\beta^{\,2})^2 - \sum_{\alpha,i}(D_{\alpha i}^{\,2}\langle i\bar{i}\,|V_A|\,i\bar{i}\rangle D_{\alpha i}^{\,2})^2 (V_\alpha^{\,2} U_\alpha^{\,2})^2}{\sum_{\alpha,\beta,i,j} D_{\alpha i}^{\,2}\langle i\bar{i}\,|V_A|\,j\bar{j}\rangle D_{\beta j}^{\,2} U_\alpha V_\alpha^{\,3} U_\beta^{\,3} V_\beta - \sum_{\alpha,i} D_{\alpha i}^{\,2} D_{\alpha i}^{\,2}\rangle i\bar{i}\,|V_A|\,i\bar{i}\rangle U_\alpha V_\alpha^{\,3} U_\alpha^{\,3} V_\alpha}. \tag{10}$$

λ_2^{III} is obtained by combining (8) and (10), i.e.,

$$\lambda_2^{\mathrm{III}} = \frac{1}{4}\left[\frac{\sum_{\alpha,\beta,i,j}(D_{\alpha i}^{\,2}\langle i\bar{i}\,|V_A|\,j\bar{j}\rangle D_{\beta j}^{\,2})^2 (V_\alpha^{\,2} U_\beta^{\,2})^2 - \sum_{\alpha,i}(D_{\alpha i}^{\,2}\langle i\bar{i}\,|V_A|\,i\bar{i}\rangle D_{\alpha i}^{\,2})^2 (V_\alpha^{\,2} U_\alpha^{\,2})^2}{\sum_{\alpha\neq\beta}(U_\alpha V_\alpha U_\beta V_\beta)^2}\right]^{1/2}. \tag{11}$$

The BCS transformation coefficients U and V and the parameters λ_1 and λ_2 are determined self-consistently by solving the gap equations

$$V_\alpha^\tau = \frac{1}{\sqrt{2}}\left(1 + \frac{e_\alpha^\tau - \lambda^\tau}{E_\alpha^\tau}\right)^{1/2}, \tag{12}$$

$$U_\alpha^\tau = [1 - (V_\alpha^\tau)^2]^{1/2}, \tag{13}$$

where

$$E_\alpha^\tau = [(\Delta_\alpha^\tau)^2 + (e_\alpha^\tau - \lambda^\tau)^2]^{1/2}, \tag{14}$$

$$e_\alpha^\tau = \sum_{ij} D_{\alpha i}^\tau \Gamma_{ij}^\tau D_{j\alpha}^\tau, \tag{15}$$

$$\Delta_\alpha^\tau = \sum_{ij} D_{\alpha i}^\tau \Delta_{ij}^\tau D_{j\alpha}^\tau, \tag{16}$$

$$\Gamma_{ij}^\tau = \epsilon_j^\tau \delta_{ji} + \sum_{k,l,\tau'} \langle i\tau, k\tau'\,|V_A|\,j\tau, l\tau'\rangle \times \sum_\alpha D_{k\alpha}^{\tau'} D_{\alpha l}^{\tau'} (V_\alpha^{\tau'})^2, \tag{17}$$

$$\Delta_{ij}^\tau = -\frac{1}{2}\sum_{kl}\langle i\tau\bar{j}\tau\,|V_A|\,k\tau\bar{l}\tau\rangle \sum_\alpha D_{k\alpha}^\tau D_{\alpha l}^\tau V_\alpha^\tau U_\alpha^\tau, \tag{18}$$

and

$$\lambda^\tau = \lambda_1^\tau + 2\lambda_2^\tau(n_\tau + 1). \tag{19}$$

The ground-state energy is given by

$$E = \frac{1}{2}\sum_{\alpha\tau}[(\langle\alpha\,|\epsilon\,|\alpha\rangle + e_\alpha^\tau)V_\alpha^{\tau\,2} + \Delta_\alpha^\tau U_\alpha^\tau V_\alpha^\tau] - 4\sum_\tau \lambda_2^\tau \sum_\alpha (U_\alpha^\tau V_\alpha^\tau)^2. \tag{20}$$

The last term represents the correction to the ground-state energy for the fluctuations in the number of particles due to pairing correlations.

The calculations are performed using the renormalized Kuo-Brown matrix elements for the Hamada-Johnston potential. A ^{40}Ca Core is assumed and the basis states are limited to $2p_{1/2}$, $2p_{3/2}$, $1f_{5/2}$, and $1f_{7/2}$ harmonic oscillator states. The single particle energies (ϵ) are taken to be -8.35, -2.85, -6.28, and -4.22 MeV for neutrons and -1.07, 4.83, 0.72, and 2.43 MeV for protons corresponding to $1f_{7/2}$, $1f_{5/2}$, $2p_{3/2}$, and $2p_{1/2}$ orbitals, respectively. The calculations were performed for all the even-even isotopes of Ti, Cr, Fe, Ni, and Zn. The results are reported, however, for only the Ti isotopes since the results obtained for the other sets of isotopes are similar in nature. The modified deformed BCS equations are solved using all the three expressions (8), (10), and (11) for λ_2 and the results are labeled I, II, and III, respectively. The ordinary deformed BCS solutions are obtained self-consistently by solving the above gap equations with $\lambda_2 = 0$. Before solving the gap equations for MDBCS or DBCS case, the transformation coefficients D are obtained by performing a self-consistent Hartree-Fock calculation. The calculations were performed for both the prolate and oblate shapes. The results are given only for the prolate shapes which are lower in energy than the corresponding oblate shapes for all the nuclei reported here.

The results for the ground-state energies are displayed in Table I. It is clear that the DBCS is a good approximation to a complete HFB calculation. The changes in the ground-state energies

TABLE I. Comparison of the ground-state energies (E) and the pairing energies for the Ti isotopes obtained by solving the modified deformed BCS equations using three different expressions (8), (10), and (11) for λ_2 labeled as I, II, and III, respectively. The results are compared with those of HFB and ordinary deformed BCS calculations. The pairing energies are given in the parentheses. All the energies are given in MeV.

Nucleus	MDBCS I	MDBCS II	MDBCS III	DBCS	HFB	Experiments
^{44}Ti	−28.60	−28.60	−28.60	−28.60	−28.60	−33.425
	(− 0.00)	(− 0.00)	(− 0.00)	(− 0.00)	(− 0.00)	
^{46}Ti	−51.36	−50.98	−51.70	−50.77	−50.77	−56.146
	(− 2.14)	(− 1.51)	(− 2.51)	(− 0.46)	(− 0.58)	
^{48}Ti	−71.46	−70.88	−71.92	−70.57	−70.63	−76.649
	(− 3.79)	(− 3.25)	(− 4.16)	(− 2.93)	(− 2.85)	
^{50}Ti	−90.85	−89.76	−91.27	−89.41	−89.46	−95.741
	(− 6.20)	(− 4.56)	(− 6.62)	(− 3.31)	(− 3.64)	

TABLE II. Comparison of the parameter λ_2 obtained using different approximations. The superscripts n and p denote neutron and proton, respectively.

Nucleus	λ_2^n I	λ_2^n II	λ_2^n III	λ_2^p I	λ_2^p II	λ_2^p III
^{44}Ti	0.000	0.000	0.000	0.000	0.000	0.000
^{46}Ti	0.360	0.177	0.493	0.000	0.000	0.000
^{48}Ti	0.255	0.094	0.371	0.000	0.000	0.000
^{50}Ti	0.241	0.078	0.319	0.410	0.132	0.440

TABLE III. Comparison of neutron-pair separation energies ($-\Delta E_{NP}$) obtained from different approximations and the corresponding experimental values. All the energies are given in MeV.

Nucleus	$-\Delta E_{NP}$ I	II	III	DBCS	HFB	Experiment
^{46}Ti	22.76	22.38	23.10	22.17	22.17	22.72
^{48}Ti	20.10	19.90	20.22	19.80	19.86	20.50
^{50}Ti	19.39	18.88	19.35	18.84	18.83	19.09

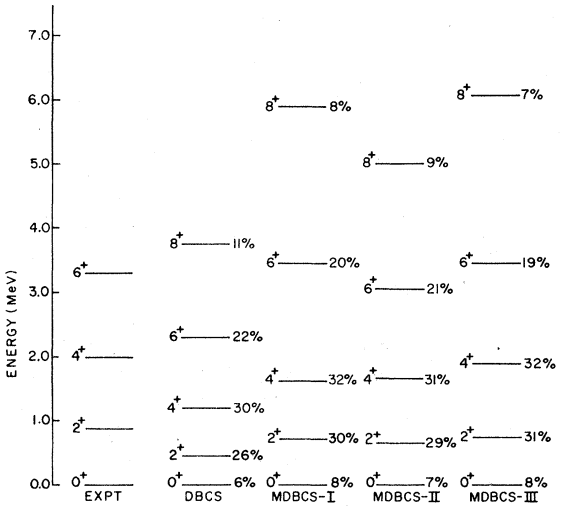

FIG. 1. Comparison of experimental [see C. Lederer, J. Hollander, and I. Perlman, Table of Isotopes (Wiley, New York, 1967)] and calculated spectrum of ^{46}Ti with DBCS and MDBCS in three different approximations. The percentages give the probability of each angular momentum state in the DBCS and MDBCS wave functions.

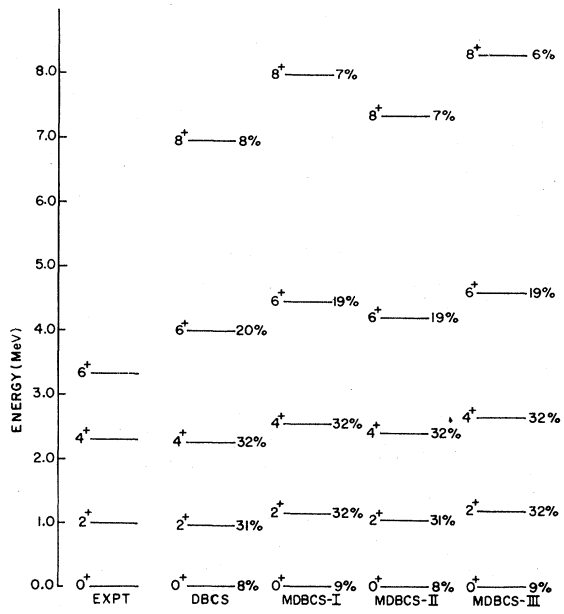

FIG. 2. Comparison of experimental [see C. Lederer, J. Hollander, and I. Perlman, Table of Isotopes (Wiley, New York, (1967)] and calculated spectrum of ^{48}Ti with DBCS and MDBCS in three different approximations. The percentages give the probability of each angular momentum state in the DBCS and MDBCS wave functions.

in the MDBCS approximation compared to the DBCS approximation are not negligible, and there is considerable change in pairing energies. This reflects a change in the wave function. This is in agreement with the conclusion reached in the spherical case[2] with realistic interaction. For a phenomenological interaction, however, the changes in the spherical wave functions for Ni isotopes due to the introduction of parameter λ_2 were insignificant.[5] In the present calculations the contribution to the energy due to the fluctuation of particle number is largest for approximation III unlike in the spherical solutions[2] where the contribution was largest for approximation II. The values of the parameter λ_2 using different approximations are shown in Table II.

Neutron-pair separation energies are compared with the experimental values in Table III to check the quality of the ground-state energies obtained in the MDBCS approximation. The neutron-pair separation energy is defined as

$$\Delta E_{\mathrm{NP}}(N,Z) = E(N,Z) - E(N-2,Z).$$

The experimental values are those of Mattauch, Thiele, and Wapstra.[9] Unlike the spherical solutions, there is a definite improvement in the neutron-pair separation energies in the MDBCS approximations I and III as compared to the DBCS approximation.

In order to test the wave functions obtained in the MDBCS approximations, projection of good angular momentum states was carried out following the procedure laid out in Ref. 10 and the results are displayed in Figs. 1 and 2 for ^{46}Ti and ^{48}Ti, respectively. The spectrum for ^{44}Ti is not presented since the DBCS and MDBCS wave functions are identical for this nucleus due to the absence of pairing correlations. The figures indicate that MDBCS leads to a definite improvement in the calculated spectrum of ^{46}Ti whereas for ^{48}Ti the two approximations give almost identical results.

From the results of this paper it seems that the Lipkin-Nogami modification of the BCS approximation does lead to improved agreement with experiments for deformed nuclei when realistic interaction is used.

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