

Generalized pairing in $N = Z$ even-even $2p-1f$ shell nuclei

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Hartree-Fock-Bogoliubov calculations have been performed for self-conjugate even-even nuclei in the $2p-1f$ shell using the central Yukawa interaction and Kuo-Brown reaction matrix elements for the Hamada-Johnston potential. The possibility of generalized pairing correlations is studied by considering $T=0$, $T=1$, and $T=0+T=1$ correlations and comparing the ground-state properties for axial and triaxial shapes. It is found that for nuclei studied neither the correlations $T=0$ nor $T=1$ play any important role in the ground state. In general $T=0+T=1$ pairing yields results which are identical with those obtained with either $T=0$ or $T=1$. In the excited states, however, the $T=0$ correlations are found to be more important than the $T=1$ correlations.

NUCLEAR STRUCTURE ^{44}Ti , ^{48}Cr , ^{52}Fe , ^{56}Ni , ^{60}Zn ; calculated binding energies, quadrupole moments, pickup strengths. Hartree-Fock-Bogoliubov method with generalized pairing.

I. INTRODUCTION

Employing the generalized Bogoliubov-Valatin transformation, the Hartree-Fock-Bogoliubov (HFB) theory was first formulated for nuclei by Baranger.¹ In this formalism the Hartree-Fock (HF) field and the pairing field are treated on the same footing and in a self-consistent manner. The resulting HFB equations were first treated numerically by Dietrich, Mang, and Pradal² and Gunye and Das Gupta³ for some rare-earth and $2s-1d$ shell nuclei. Later on some extensive and sophisticated calculations⁴⁻⁶ were reported for $1p$, $2s-1d$, and $2p-1f$ shell nuclei using both phenomenological and realistic nucleon-nucleon interactions. All of these calculations, however, consider only $T_z=1$ (i.e., neutron-neutron and proton-proton) pairing correlations. A general conclusion of these calculations is that this type of pairing correlation is not important for the ground state description of $N=Z$ nuclei. However, $T_z=1$ pairing is found to be significant for $N \neq Z$ nuclei.

In an effort to improve the situation for $N=Z$ even-even nuclei, generalized $T=1$ pairing theory^{7,8} and $T=0$ pairing theory were formulated.⁹ This eventually led to a generalized $T=0$ and $T=1$ pairing theory,¹⁰ which was first applied by Goodman and collaborators¹¹ in a full HFB calculation to $2s-1d$ shell $N=Z$ nuclei. It was found that the $T=0$ $n-p$ pairing correlations play an important part in the properties of these nuclei. Wolter *et al.*¹² performed similar calculations for two $N=Z$ nuclei in the $2p-1f$ shell, though the possibility of incorporating both $T=0$ and $T=1$ pairing

correlations simultaneously was not explored. In the above work, pairing is permitted between nucleons in time-reversed orbitals ($\alpha-\bar{\alpha}$ pairing). Since neutrons and protons are not restricted by the Pauli exclusion principle they may occupy identical spatial orbitals, thereby creating $\alpha-\alpha$ pairing correlations. A completely generalized pairing theory has been derived including $\alpha-\alpha$ ($T=0$) pairing as well as $\alpha-\bar{\alpha}$ ($T=0$ plus $T=1$) pairing.¹³

The object of the present work is to study the importance of the $T=0$ ($\alpha-\bar{\alpha}$) pairing in all the $N=Z$ even-even nuclei in the $2p-1f$ shell assuming ^{40}Ca as an inert core. The calculations are carried out for the renormalized Kuo-Brown matrix elements for the Hamada-Johnston interaction and the central Yukawa (CY) interaction described earlier.⁶ The single-particle energies for neutrons and protons are -6.5 , 0.0 , -4.5 , and -2.5 MeV, corresponding to the active orbits $1f_{7/2}$, $1f_{5/2}$, $2p_{3/2}$, and $2p_{1/2}$, respectively. The harmonic-oscillator parameter (b) for the entire calculation is 2.0×10^{-13} cm.

A brief review of the HFB self-consistent formalism as applied in the present calculation is given in Sec. II to make the paper self-contained, and it will also be employed for interpreting the results. Section III is devoted to describing the results of the calculation for axial and triaxial shapes. The conclusions are presented in Sec. IV.

II. SELF-CONSISTENT HFB FORMALISM

The Hamiltonian of a nucleus in the second quantized form may be written as

$$H = \sum_{\substack{k\bar{l} \\ \mu\nu}} \langle k\bar{l} | \epsilon | l\nu \rangle a_{k\mu}^\dagger a_{l\nu} \\ + \frac{1}{4} \sum_{\substack{k\bar{l}m\bar{n} \\ \mu\nu\rho\sigma}} \langle k\bar{l}l\nu | V_A | m\rho n\sigma \rangle a_{k\mu}^\dagger a_{l\nu}^\dagger a_{n\sigma} a_{m\rho}, \quad (1)$$

where $a_{k\mu}^\dagger$ ($a_{k\mu}$) denotes a creation (annihilation) operator for a nucleon in the shell-model state $|n_{k\bar{l}j_k} m_{k\mu}\rangle$ with μ as the z component of isotopic spin, and the rest of the symbols have their usual meaning.

The pairing correlations are introduced through the transformation¹

$$C_{\alpha\tau}^\dagger = \sum_{k>0, \mu} (U_{\alpha\tau, k\mu} a_{k\mu}^\dagger + V_{\alpha\tau, \bar{k}\mu} a_{\bar{k}\mu}), \quad (2)$$

where the transformation coefficients $U_{\alpha\tau, k\mu}$ and $V_{\alpha\tau, \bar{k}\mu}$ are, in general, complex. Since the above transformation does not conserve particle number it is necessary to impose the constraints

$$\langle \hat{N}_p \rangle = \sum_{k, \mu > 0} \langle a_{k\mu}^\dagger a_{k\mu} \rangle = Z, \quad (3)$$

$$\langle \hat{N}_n \rangle = \sum_{k, \mu < 0} \langle a_{k\mu}^\dagger a_{k\mu} \rangle = N, \quad (4)$$

and the Hamiltonian (1) is modified to the form

$$H' = H - \lambda_n \hat{N}_n - \lambda_p \hat{N}_p, \quad (5)$$

where λ_p and λ_n are the Lagrange multipliers.

Upon assuming time-reversal invariance and requiring that $\langle \hat{T} \rangle = 0$ for $N=Z$ nuclei, Eq. (2) in the isospin space may be explicitly written as

$$\begin{pmatrix} C_1^\dagger \\ C_2^\dagger \\ \bar{C}_1 \\ \bar{C}_2 \end{pmatrix} = \begin{pmatrix} U_{1,1} & 0 & -V_{1,1} & -V_{1,2} \\ 0 & U_{2,2} & -V_{1,2}^* & -V_{2,2} \\ V_{1,1} & V_{1,2} & U_{1,1} & 0 \\ V_{1,2}^* & V_{2,2} & 0 & U_{2,2} \end{pmatrix} \begin{pmatrix} a_p^\dagger \\ a_n^\dagger \\ \bar{a}_p \\ \bar{a}_n \end{pmatrix}, \quad (6)$$

where the unitarity condition for the transformation has been assumed. In the absence of Coulomb interaction between the protons, $U_{1,1} = U_{2,2}$ and $V_{1,1} = -V_{2,2}$. For pure $|T_x|=1$ pairing, $V_{1,2} = 0$, and for pure $T=0$ pairing, $V_{1,1} = V_{2,2} = 0$.

The coefficients of the above transformation are determined by solving the HFB equations:

$$\begin{pmatrix} \mathcal{K} - \lambda & \Delta \\ \Delta^\dagger & -\mathcal{K} + \lambda \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ V \end{pmatrix}, \quad (7)$$

where

$$\mathcal{K}_{k\mu, l\mu} = \epsilon_{k\mu, l\mu} + \Gamma_{k\mu, l\mu} \quad (8a)$$

and

$$\Gamma_{k\mu, l\mu} = \sum_{m\bar{n}\nu} \langle k\mu m\nu | V_A | l\mu n\nu \rangle \rho_{n\nu, m\nu} \quad (8b)$$

are diagonal in isospin space, and

$$\Delta_{k\mu, \bar{l}\mu} = -\Delta_{k-\mu, \bar{l}-\mu} \\ = \sum_{m\bar{n}} \langle k\bar{l} T=1 | V_A | m\bar{n} T=1 \rangle \chi_{m\mu, \bar{n}\mu}, \quad (9)$$

$$\Delta_{k\mu, \bar{l}-\mu} = \Delta_{k\mu, \bar{l}-\mu}^{T=1} + i\Delta_{k\mu, \bar{l}-\mu}^{T=0}, \quad (10)$$

$$\Delta_{k\mu, \bar{l}-\mu}^{T=1} = \sum_{m\bar{n}} \langle k\bar{l} T=1 | V_A | m\bar{n} T=1 \rangle \text{Re}\chi_{m\mu, \bar{n}-\mu}, \quad (11)$$

$$\Delta_{k\mu, \bar{l}-\mu}^{T=0} = \sum_{m\bar{n}} \langle k\bar{l} T=0 | V_A | m\bar{n} T=0 \rangle \text{Im}\chi_{m\mu, \bar{n}-\mu}. \quad (12)$$

The single-particle density matrix ρ and the pairing tensor χ are defined as

$$\rho_{k\mu, l\mu} = \langle a_{l\mu}^\dagger a_{k\mu} \rangle = \sum_{\alpha\tau} V_{\alpha\tau, l\mu} V_{\alpha\tau, k\mu}^*, \quad (13)$$

$$\chi_{k\mu, l\nu} = \langle a_{l\nu}^\dagger a_{k\mu} \rangle = \sum_{\alpha\tau} U_{\alpha\tau, l\nu} V_{\alpha\tau, k\mu}^*. \quad (14)$$

The energy of the ground state Φ_0 (the quasiparticle vacuum) is

$$E_{\text{HFB}} = E_{\text{HFB}}^{\text{HF}} + E_{\text{HFB}}^{\text{pair}}, \quad (15)$$

where

$$E_{\text{HFB}}^{\text{HF}} = \text{Tr}[(\epsilon + \frac{1}{2}\Gamma)\rho], \quad (15a)$$

$$E_{\text{HFB}}^{\text{pair}} = \frac{1}{2} \text{Tr}[\Delta\chi^\dagger]. \quad (15b)$$

III. DISCUSSION OF SELF-CONSISTENT RESULTS

The results of self-consistent HF and HFB calculations of the axial and triaxial shapes of $N=Z$ nuclei in the $2p-1f$ shell are presented in Tables I through III. The calculations, as mentioned before, have been performed for two different interactions, namely CY and HJ. The HF and HFB solutions for axial (both prolate and oblate) shapes are reported for each nucleus while only those triaxial solutions are reported which were found to be lower in energy than the axial solutions for a particular nucleus. In each of the above cases, however, the HFB solutions are reported by including $T=1$ and $T=0$ as well as $T=1$ plus $T=0$ pairing correlations. Requiring axial symmetry restricts the summation

TABLE II. Self-consistent HF and HFB results for the central Yukawa interaction. For an explanation of this table, see Table I.

Nucleus	Shape	E_{HF} (G)	E_{HFB} (E_{HFB}^{HF})		$Q_{LM}(f \frac{1}{m})$ HFB		λ (MeV)		
			T=1	T=0	T=1	T=0	T=1	T=0	
^{44}Ti	p	-34.96 (3.99)	-34.96 (-0.00)	24.53	24.54	24.53	24.54	-9.41	-9.02
		-32.90 (1.62)	-33.02 (-0.00)	428.50 -14.52	428.54 -10.73	428.50 -14.52	428.41 -10.73	-9.07	-8.88
^{48}Cr	p	-73.65 (2.47)	-73.65 (-0.00)	34.34	34.35	34.35	34.35	-10.16	-10.22
		-69.30 (0.58)	-71.49 (-3.68)	274.75 -13.61	274.86 -10.67	274.86 -13.61	274.76 -14.39	-10.19	-10.25
^{52}Fe	p	-74.04 (3.10)	-74.03 (-0.00)	38.42	38.42	38.42	38.42	-11.03	-11.53
		-116.06 (2.51)	-116.06 (-0.00)	309.00	309.00	309.00	309.00	-10.93	-11.55
^{56}Ni	p	-113.79 (2.19)	-113.79 (-0.00)	4.09	4.09	4.09	4.09	-11.58	-11.37
		-163.35 (5.42)	-163.35 (-0.00)	25.75	25.75	25.75	25.75	-10.79	-8.82
^{60}Zn	p	-161.50 (3.35)	-161.50 (-0.00)	0.01	0.004	0.004	0.004	-11.45	-10.98
		-209.03 (3.70)	-209.03 (-0.00)	25.70	25.71	25.72	25.72	-11.95	-11.86

TABLE III. Comparison of $\langle \vec{T}^2 \rangle$ for the states where pairing correlations are important. $\langle \vec{T}^2 \rangle = 0$ for the $T=0$ mode.

Nucleus	Shape	Interaction	$\langle \vec{T}^2 \rangle$	
			$T=1$ plus $T=0$	$T=1$
^{44}Ti	oblate	HJ	1.552	1.552
		CY	1.831	1.833
^{48}Cr	oblate	HJ	0.0008	
		CY	1.857	2.819
^{52}Fe	oblate	HJ	0.0001	
		CY	0.0015	
^{60}Zn	oblate	HJ	0.0001	

in (2) over states $|k\rangle$ with the same value of m_k . For triaxial solution, the summation in (2) is carried out over the states $|k\rangle$ with odd values of $m_k - \frac{1}{2}$ to preserve time-reversal symmetry.

The intrinsic shapes for triaxial nuclei are characterized by the multipole moment Q_{20} , Q_{40} , Q_{22} , and Q_{44} , where

$$Q_{LM} = \left\langle \sum_{i=1}^A r_i^L Y_{LM}(\Omega_i) \right\rangle. \quad (16)$$

For axial nuclei, $Q_{22} = Q_{42} = Q_{44} = 0$. The pickup strengths are defined by

$$S_j = \sum V_{\alpha m}^2 (C_{jm}^\alpha)^2, \quad (17)$$

where C_{jm}^α 's are the components of the orthogonal matrix which diagonalizes the density matrix ρ defined in (13), and $V_{\alpha m}^2$'s are the corresponding elements of the diagonal ρ , representing the occupation probability of the deformed orbits.

For both the interactions the lowest axial solution for ^{44}Ti , ^{48}Cr and ^{52}Fe is prolate HF. However, for ^{48}Cr and ^{52}Fe with the HJ interaction and for ^{48}Cr and with the CY interaction the triaxial HF solutions are even lower in energy than the prolate HF solutions. In all the attempts to obtain triaxial solution for ^{44}Ti the final solution converged to an axial shape. The lowest-energy axial and triaxial HFB solutions for the above-mentioned nuclei are identical with the corresponding HF solutions, indicating the absence of pairing in the ground state. In the higher oblate solutions listed in Tables I and II, however, the presence of pairing correlations is obvious. For both the interactions, the oblate HFB solution for ^{44}Ti with $T=1$ pairing is slightly lower than the one with $T=0$ pairing. Including both $T=1$ and $T=0$ pairing simultaneously results in a solution identical with the one obtained by including only $T=1$ pairing. For ^{48}Cr and ^{52}Fe , on the other hand, the oblate

HFB solution with $T=0$ pairing is slightly lower than the one with $T=1$ pairing. A mixed $T=1$ plus $T=0$ oblate solution degenerate with the $T=0$ mode is obtained for ^{48}Cr and ^{52}Fe with the CY interaction.

In Ref. 12, employing the Yale interaction, the HFB ground-state solution for ^{48}Cr is prolate with $T=0$ pairing. The Yale interaction¹² produces a HF spectrum which is compressed with respect to the HF spectrum for the HJ interaction. In particular, the Yale interaction creates a HF gap of 0.58 MeV, which is quite small, thereby favoring large pairing. The HJ interaction yields a HF gap of 2.67 MeV, which is prohibitively large, thereby preventing pairing.

For ^{56}Ni the CY interaction favors a spherical shape, whereas the HJ interaction favors an oblate shape. In both cases, however, the pairing is absent for all the $T=1$, $T=0$, and $T=1$ plus $T=0$ modes. Unlike ^{44}Ti , ^{48}Cr , and ^{52}Fe , there is no pairing even in the higher-energy solutions. As in the case of ^{44}Ti , the triaxial solution does not exist for this nucleus.

There is appreciable lowering of energy for ^{60}Zn for the oblate shape with the HJ interaction when pairing is included. Both the $T=1$ and $T=0$ pairing correlations are found to be equally strong with the $T=0$ solution slightly lower than the $T=1$ solution. The $T=1$ plus $T=0$ mode solution is identical with the $T=0$ mode solution. The lowest-energy solution for this nucleus with the HJ interaction is, however, triaxial HF. The results for the oblate solution with the CY interaction are not reported, as no convergence was obtained. The triaxial solution with the CY interaction was found to be higher than the axial prolate solution and is not reported. For both the interactions, the higher prolate solutions do not show any pairing.

As mentioned earlier, the inclusion of $T=0$ plus $T=1$ pairing results, in general, in a solution identical to the one obtained by including either $T=1$ or $T=0$ pairing. To further check this conclusion, one can make a comparison of the value of $\langle \vec{T}^2 \rangle$ in various cases. Assuming $\langle \vec{T} \rangle = 0$, one obtains

$$\langle \vec{T}^2 \rangle = 2 \sum_{\alpha} (\rho_{\alpha\beta, \alpha\beta} - \rho_{\alpha\beta, \alpha\beta}^2) - 2 \sum_{\alpha\beta} (\text{Im}\chi_{\alpha\beta, \beta\alpha})(\text{Im}\chi_{\alpha\beta, \beta\alpha}).$$

The second term on the right is identical to the first for $T=0$ pairing, making $\langle \vec{T}^2 \rangle = 0$. The values of $\langle \vec{T}^2 \rangle$ are listed in Table III for the different cases where pairing correlations are important. From this table it is clear that for ^{44}Ti , the $T=0$

TABLE IV. Comparison of pickup strengths (neutron plus proton) calculated from intrinsic wave functions corresponding to solutions with minimum energies for the central Yukawa (CY) and Hamada-Johnston (HJ) interactions.

Nucleus	Interaction	Type of solution	Pickup strengths			
			$j = \frac{1}{2}$	$j = \frac{3}{2}$	$j = \frac{5}{2}$	$j = \frac{7}{2}$
^{44}Ti	CY	HF (prolate)	0.21	0.80	0.29	2.69
	HJ	HF (prolate)	0.20	0.82	0.25	2.73
^{48}Cr	CY	HF (triaxial)	0.42	1.41	0.59	5.57
	HJ	HF (triaxial)	0.37	1.45	0.62	5.56
^{52}Fe	CY	HF (prolate)	0.00	0.41	0.08	11.50
	HJ	HF (triaxial)	0.76	2.71	1.21	7.31
^{56}Ni	CY	HF (spherical)	0.00	0.00	0.00	16.00
	HJ	HF (oblate)	1.48	4.86	1.19	8.47
^{60}Zn	CY	HF (prolate)	0.96	3.03	0.33	15.72
	HJ	HF (triaxial)	2.27	5.22	2.21	10.29

plus $T=1$ oblate solution is a pure $T=1$ solution for both the interactions. For all other cases, with the single exception of ^{48}Cr which has a mixed mode solution for the CY interaction, $T=0$ plus $T=1$ solutions are essentially pure $T=0$ solutions.

Comparing the results of the CY and HJ interactions, one notices that although qualitatively the results are similar in the beginning of the $2p-1f$ shell, there are quantitative differences. For ^{56}Ni even the shape of the lowest energy solution for the CY interaction is different from that for the HJ interaction. These differences are more obvious in Table IV, where the pickup strengths are compared. The numbers are surprisingly close for ^{44}Ti and ^{48}Cr but are very different for ^{52}Fe , ^{56}Ni , and ^{60}Zn .

IV. CONCLUSIONS AND SUMMARY

The motivation behind this work was to study the importance of $T=0$ pairing correlations in $N=Z$ nuclei in the $2p-1f$ shell as these correlations play an important role in $N=Z$ nuclei in the $2s-1d$ shell. The study has been carried out by including $T=0$, $T=1$, and $T=1$ plus $T=0$ pairing correlations. It is found that neither the $T=0$ nor the $T=1$ correlations are important for the ground state. In the excited states, however, the $T=0$ correlations are found to be more important than the $T=1$ correlations. For ground-state bands the inclusion of $T=1$ and $T=0$ pairing correlations simultaneously yields results which are identical with those obtained with either $T=1$ or $T=0$, with the exception of ^{48}Cr (oblate) for the CY interaction.

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