Hartree-Fock-Bogoliubov calculations with $T=1$ plus $T=0$ pairing correlations

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(Received 15 March 1976)

Hartree-Fock-Bogoliubov calculations have been performed for even-even $N \neq Z$ isotopes using the Kuo-Brown reaction matrix elements for the Hamada-Johnston potential. The possibility of generalized pairing is explored by considering $T=1$, $T=0$ and $T=1$ plus $T=0$ correlations for the axial and triaxial shapes. It is found that only for the nuclei with $N-Z=2$ there is a small contribution by the $T=0$ pairing correlations. Only the $|T_z|=1$ pairing correlations are important for the ground-state solutions.

[NUCLEAR STRUCTURE Even-even $N \neq Z$ isotopes of Ti, Cr, Fe, Ni, and Zn; calculated ground-state energies using $T=1$, $T=0$, and $T=1+T=0$ pairing correlations; quadrupole moments pickup strengths for the lowest-energy solutions. Hartree-Fock and Hartree-Fock-Bogoliubov methods. Kuo-Brown interaction.]

I. INTRODUCTION

The Hartree-Fock-Bogoliubov (HFB) theory,[1] treating the field producing effects and the pairing effects due to the nuclear interactions on the same footing and in a self-consistent manner, has been used for many years now for the nuclear structure studies. All the earlier calculations,[2-8] however, were performed by including only neutron-neutron (n-n) and proton-proton (p-p) pairing correlations and thus completely neglecting neutron-proton (n-p) $T=1$ and $T=0$ pairing correlations. Goswami[9] and Camiz, Covello, and Jean[10] independently formulated a procedure for treating n-p $T=1$ correlations along with n-n and p-p $T=1$ correlations in an approximate way (BCS approximation). Later on an n-p $T=0$ pairing theory[11] and eventually a generalized[12] $T=1$ and $T=0$ pairing theory were reported although no numerical calculations were carried out. The isospin problem and, in particular, the restoration of the isospin invariance, had been studied by Ginocchio and Weneser[13] in the random phase approximation.

A full HFB calculation for $N=Z$ nuclei in the $2s$-$1d$ shell by including generalized $T=1$ and $T=0$ pairing correlations was reported by Goodman and collaborators.[14] These studies showed the importance of the $T=0$ pairing rectifying many of the failures of the Hartree-Fock theory. For example it was found that the $T=0$ pairing restores axial symmetry to the equilibrium shapes of ^{24}Mg and ^{32}S and explains the vibrational nature of ^{36}A. Wolter, Faessler, and Sauer[15] performed some calculations for a few $N \neq Z$ nuclei in the $2s$-$1d$ shell and two nuclei in the $2p$-$1f$ shell. In these calculations, however, the $T=1$ and $T=0$ pairing correlations were considered separately and the possibility of existence of $T=1$ and $T=0$ correlations simultaneously was not explored.

The object of the present work is to study the importance of $T=0$ and $T=1$ pairing correlations for even-even $N \neq Z$ isotopes of Ti, Cr, Fe, Ni, and Zn in a systematic way. The calculations are performed in three steps, namely by including (i) $T=1$ plus $T=0$ correlations simultaneously, (ii) $T=1$ correlations alone, and finally (iii) $T=0$ correlations. A ^{40}Ca core is assumed, and the calculations are carried out for the renormalized Kuo-Brown matrix elements[16] for the Hamada-Johnston interaction. The single-particle energies for neutrons and protons are -6.5, 0.0, -4.5, and 2.5 MeV corresponding to the orbits $1f_{7/2}$, $1f_{5/2}$, $2p_{3/2}$, and $2p_{1/2}$, respectively.[17] The harmonic-oscillator parameter (b) for the entire calculation is 2×10^{-13} cm.

The self-consistent HFB formalism as used in the present calculations is given in Sec. II. Results of the calculations are discussed in Sec. III and Sec. IV is a summary and discussion of the results.

II. SELF-CONSISTENT HFB FORMALISM

The main feature of the formalism is the generalized Bogoliubov transformation:

$$c^{\dagger}_{\alpha\tau} = \sum_{k\mu} \left(u_{\alpha\tau,k\mu} a^{\dagger}_{k\mu} + v_{\alpha\tau,k\mu} a_{\bar{k}\mu} \right), \tag{1a}$$

$$c_{\bar{\alpha}\tau} = \sum_{k\mu} \left(u^{*}_{\bar{\alpha}\tau,\bar{k}\mu} a_{\bar{k}\mu} + v^{*}_{\bar{\alpha}\tau,\bar{k}\mu} a^{\dagger}_{k\mu} \right). \tag{1b}$$

This linear canonical transformation relates the single-particle creation ($a^\dagger_{k\mu}$) and annihilation ($a_{k\mu}$) operators in the shell model basis ($k \equiv n_k l_k j_k m_k, \mu = \pm\frac{1}{2}$, the z component of the nucleon isotopic spin) to the quasiparticle creation ($c^\dagger_{\alpha\tau}$) and annihilation ($c_{\alpha\tau}$) operators which are convenient for the description of the pairing phenomena. The bar denotes the time reversed state, i.e. $|\bar{k},\mu\rangle = (-)^{j_k - m_k + l_k}|n_k l_k j_k - m_k, \mu\rangle$. The ground state of the nucleus is approximated by the vacuum for the quasiparticles

$$c_{\alpha\tau}|\Phi_{\mathrm{HFB}}\rangle = 0 . \tag{2}$$

The transformation coefficients u and v are, in general, complex. The quasiparticles defined in Eq. (1) are required to be fermions and the resulting conditions on u and v are equivalent to requiring the transformation defined in Eq. (1) to be unitary. Further, if one imposes the restriction of time reversal symmetry on the quasiparticles one obtains

$$u_{\bar{\alpha}\tau,\bar{k}\mu} = u^*_{\alpha\tau,k\mu} , \tag{3a}$$

$$v_{\alpha\tau,k\mu} = -v^*_{\bar{\alpha}\tau,\bar{k}\mu} . \tag{3b}$$

The quasiparticle transformation (1) can be written explicitly in the isotopic spin space as

$$\begin{bmatrix} c^\dagger_1 \\ c^\dagger_2 \\ \bar{c}_1 \\ \bar{c}_2 \end{bmatrix} = \begin{bmatrix} u_{1p} & u_{1n} & -v_{1p} & -v_{1n} \\ u_{2p} & u_{2n} & -v_{2p} & -v_{2n} \\ v_{1p} & v_{1n} & u_{1p} & u_{1n} \\ v_{2p} & v_{2n} & u_{2p} & u_{2n} \end{bmatrix} \begin{bmatrix} a^\dagger_p \\ a^\dagger_n \\ \bar{a}_p \\ \bar{a}_n \end{bmatrix} , \tag{4}$$

where p and n refer to the isotopic spin indices for the proton and neutron, respectively. Since this transformation mixes the particle creation and annihilation operators, the ground-state wave function $|\Phi_{\mathrm{HFB}}\rangle$ defined in Eq. (2) above will not conserve the particle number. This forces us to impose the constraints that the number of protons and neutrons be conserved on the average

$$\langle\Phi_{\mathrm{HFB}}|\hat{N}_p|\Phi_{\mathrm{HFB}}\rangle = \langle\Phi_{\mathrm{HFB}}|\sum_k a^\dagger_{k1/2}a_{k1/2}|\Phi_{\mathrm{HFB}}\rangle = Z , \tag{5a}$$

$$\langle\Phi_{\mathrm{HFB}}|\hat{N}_n|_{\mathrm{HFB}}\rangle = \langle\Phi_{\mathrm{HFB}}|\sum_k a^\dagger_{k-1/2}a_{k-1/2}|\Phi_{\mathrm{HFB}}\rangle = N . \tag{5b}$$

These constraints are imposed in the calculation through two Lagrange multipliers λ_p and λ_n in the Hamiltonian which takes the form

$$H = \sum_{\substack{kl \\ \mu\nu}} \langle k\mu|\epsilon - \delta_{kl}\delta_{\mu\nu}(\lambda_p\delta_{\mu\,1/2} - \lambda_n\delta_{\mu,-1/2})|l\nu\rangle a^\dagger_{k\mu}a_{l\nu} + \frac{1}{4}\sum_{\substack{klmn \\ \mu\nu\rho\sigma}} \langle k\mu l\nu|V_a|m\rho n\sigma\rangle a^\dagger_{k\mu}a^\dagger_{l\nu}a_{n\sigma}a_{m\rho} , \tag{6}$$

where ϵ is the single-particle energy for a nucleon outside the ^{40}Ca core and V is the effective two-body interaction between the nucleons outside the core. The suffix a indicates that the matrix elements are evaluated between antisymmetric two-particle states.

To determine the transformation coefficients u and v, and therefore the ground-state wave function $|\Phi_{\mathrm{HFB}}\rangle$, the Hamiltonian (6) is expressed in terms of the quasiparticle operators and on ignoring the residual quasiparticle interaction results in the HFB equations

$$\begin{bmatrix} \epsilon + \Gamma - \lambda & \Delta \\ \Delta^+ & -\epsilon - \Gamma + \lambda \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = E \begin{bmatrix} u \\ v \end{bmatrix} , \tag{7}$$

where Γ and Δ are the Hartree-Fock (HF) and the pairing potentials, respectively, and E represents the quasiparticle energy. Explicit expressions for the elements of Γ and Δ are:

$$\Gamma_{k\mu,l\nu} = \sum_{\substack{mn \\ \rho\sigma}} \langle k\mu m\rho|V_a|l\nu n\sigma\rangle\rho_{n\sigma m\rho} , \tag{8}$$

and

$$\Delta_{k\mu,\bar{l}\mu} = \sum_{mn} \langle k\mu\bar{l}\mu|V_a|m\mu\bar{n}\mu\rangle\chi_{m\mu,\bar{n}\mu} , \tag{9}$$

$$\Delta_{k\mu,\bar{l}-\mu} = \sum_{mn} \left(\langle k\bar{l}\,T=1|V_a|m\bar{n}T=1\rangle \mathrm{Re}\chi_{m\mu,\bar{n}-\mu} + i\langle k\bar{l}\,T=0|V_a|m\bar{n}T=0\rangle \mathrm{Im}\chi_{m\mu,\bar{n}-\mu}\right) . \tag{10}$$

The single-particle density matrix ρ and the pairing tensor χ appearing in the above expressions are defined as:

$$\rho_{k\mu,l\nu} = \langle\Phi_{\mathrm{HFB}}|a^\dagger_{l\nu}a_{k\mu}|\Phi_{\mathrm{HFB}}\rangle = \sum_{\alpha\tau} v_{\alpha\tau,l\nu}v^*_{\alpha\tau,k\mu} \tag{11}$$

and

$$\chi_{k\mu,\bar{l}\nu} = \langle\Phi_{\mathrm{HFB}}|a_{\bar{l}\nu}a_{k\mu}|\Phi_{\mathrm{HFB}}\rangle = \sum_{\alpha\tau} u_{\alpha\tau,l\nu}v^*_{\alpha\tau,k\mu} . \tag{12}$$

The energy of the ground state $|\Phi_{\mathrm{HFB}}\rangle$ is given by

$$E_{\mathrm{HFB}} = E^{\mathrm{HF}}_{\mathrm{HFB}} + E^{\mathrm{pair}}_{\mathrm{HFB}} , \tag{13}$$

where

$$E^{\mathrm{HF}}_{\mathrm{HFB}} = \sum_{\substack{kl \\ \mu\nu}} (\epsilon + \tfrac{1}{2}\Gamma)_{k\mu,\,l\nu}\rho_{l\nu,k\mu} \tag{13a}$$

and

$$E^{\mathrm{pair}}_{\mathrm{HFB}} = \frac{1}{2}\sum_{\substack{kl \\ \mu\nu}} \Delta_{k\mu,\,\tilde{l}\nu}\chi^{\dagger}_{\tilde{l}\nu,\,k\mu}\,. \tag{13b}$$

In the present work the calculations are performed with the harmonic-oscillator expansion basis limited to the $2p$-$1f$ shell assuming ^{40}Ca as an inert core. Parity is therefore a good quantum number for the quasiparticles. As is clear from the above formalism, time reversal symmetry has been imposed on the quasiparticles. Axial symmetric solutions are obtained by carrying the summation in (1) over the states $|k\mu\rangle$ with the same value of m_k. For triaxial solutions the summation over $|k\mu\rangle$ is restricted to odd value of $m_k - \frac{1}{2}$. This restriction is dictated by the time reversal symmetry. It is obvious from Eq. (1) that if one wants to include np pairing correlations, χ_{np} should be complex. In the present work the calculations are performed with the completely general form (4) of the quasiparticle transformation with complex u and v coefficients. $|T_z| = 1$ and $T = 0$ calculations are performed with $\chi_{np} = 0$, and $\chi_{nn} = \chi_{pp} = \mathrm{Re}\chi_{np} = 0$, respectively.

III. CALCULATIONS AND RESULTS

The results of the self-consistent HF and HFB calculations for axial (prolate and oblate) and triaxial shapes of $N \neq Z$ isotopes of Ti, Cr, Fe, Ni, and Zn are presented in Tables I–IV. For the two-body interaction for the nucleons outside the ^{40}Ca inert core the Kuo-Brown[16] renormalized matrix elements of the Hamada-Johnston potential are employed. The single-particle energies for the extra core nucleons are the same as used earlier by the authors.[17] All the minimum energy solutions for the prolate, oblate, and triaxial shapes are listed for the HF case. The HFB calculations have been performed by including $|T_z| = 1$, $T = 0$, and $T = 1$ (nn, pp, np) plus $T = 0$ pairing correlations for each of the three different shapes mentioned above. However, the results are presented only for those HFB cases for which the pairing correlations are nonzero, as otherwise the solutions are identical to the HF solutions.

In Table I the HF energy minima along with the gap between the last occupied and the first unoccupied neutron and proton states are listed for prolate, oblate, and triaxial shapes. In Table II the HFB energy minima along with the pairing energies for different shapes and pairing modes are reported. It is found that ^{46}Ti, ^{48}Ti, and ^{50}Ti favor prolate, triaxial, and prolate shapes, respectively. The neutron gaps are much smaller than the proton gaps. A mixed mode solution for ^{46}Ti in the oblate shape indicates the presence of a small contribution from the $T = 0$ np pairing correlations. Inclusion of the $T = 0$ np correlations alone, however, gives a higher-energy solution. Inclusion of $T = 1$ plus $T = 0$ correlations simultaneously should be preferred over either of the pairing modes alone for the purpose of cal-

TABLE I. Comparison of the HF energy (E_{HF}) for oblate, prolate, and triaxial shapes. The corresponding neutron (G_n) and proton (G_p) HF gaps are listed. All the energies are in MeV.

Nucleus	E_{HF} Oblate	Prolate	Triaxial	Oblate G_n	Oblate G_p	Prolate G_n	Prolate G_p	Triaxial G_n	Triaxial G_p
^{46}Ti	−50.94	−53.85	−53.84	0.90	2.04	2.29	3.02	2.29	3.02
^{48}Ti	−67.36	−68.95	−69.12	0.61	2.38	0.43	2.38	0.85	2.30
^{50}Ti	−83.72	−82.27	−83.72	1.92	2.40	0.06	1.96	1.92	2.40
^{50}Cr	−91.07	−96.50	−96.31	0.79	0.62	1.14	2.99	1.25	2.82
^{52}Cr	−112.04	−114.96	−112.28	3.76	0.83	2.43	2.86	1.91	1.34
^{54}Cr	−127.27	−128.60	−129.79	0.44	0.69	0.04	2.80	1.11	2.83
^{54}Fe	−141.00	−141.66	−141.65	4.41	0.89	2.41	1.10	2.40	1.10
^{56}Fe	−157.24	−159.74	−159.95	0.39	0.04	1.69	1.20	1.36	2.00
^{58}Fe	−175.74	−176.05	−177.71	1.39	0.77	1.05	1.29	1.96	2.79
^{58}Ni	−188.85	−188.73	−188.73	0.16	4.69	1.70	2.56	1.22	2.56
^{60}Ni	−208.78	−207.73	−209.24	0.37	3.62	1.15	3.28	1.05	2.75
^{62}Ni	−229.14	−222.91	−229.13	3.03	3.83	2.32	0.26	3.03	3.83
^{64}Ni	−245.10	−242.85	−245.10	2.53	3.00	1.20	3.37	2.52	3.00
^{62}Zn	−235.69	−234.97	−238.45	0.76	0.18	1.21	1.67	1.91	2.00
^{64}Zn	−255.94	−255.96	−259.55	0.10	0.10	2.20	0.61	2.26	1.00
^{66}Zn	−278.57	−276.04	−279.08	1.94	0.43	0.81	1.23	2.38	1.64
^{68}Zn	−296.11	−294.60	−296.29	2.32	1.17	2.10	0.08	2.46	0.98

TABLE II. Comparison of the HFB solutions obtained by performing the calculation in different pairing modes. Solutions for which pairing is absent are not listed. All the energies are given in MeV.

Nucleus	Pairing mode	E_{HFB} Oblate	E_{HFB} Prolate	E_{HFB} Triaxial	E^{pair} Oblate	E^{pair} Prolate	E^{pair} Triaxial
^{46}Ti	$T=1+T=0$	−51.61	−53.85	−53.79	−3.43	−0.29	−0.53
	$T=1$	−51.61	−53.85	−53.79	−3.30	−0.28	−0.53
	$T=0$	−51.10			−0.31		
^{48}Ti	$T=1+T=0$	−68.36	−69.93	−70.03	−3.78	−2.58	−2.69
	$T=1$	−68.36	−69.93	−70.03	−3.92	−2.59	−2.70
^{50}Ti	$T=1+T=0$	−84.04	−84.98	−84.95	−3.62	−3.20	−3.49
	$T=1$	−84.04	−84.98	−84.96	−3.79	−3.19	−3.49
^{50}Cr	$T=1+T=0$	−92.82	−96.66	−96.67	−4.98	−1.26	−1.44
	$T=1$	−92.80	−96.66	−96.67	−5.01	−1.28	−1.44
	$T=0$	−91.28			−0.57		
^{52}Cr	$T=1+T=0$	−112.80	−115.07	−114.87	−2.08	−0.41	−0.64
	$T=1$	−112.79	−115.06	−114.87	−2.10	−0.41	−0.65
^{54}Cr	$T=1+T=0$	−129.05	−130.53	−130.46	−4.76	−2.92	−2.96
	$T=1$	−129.04	−130.53	−130.47	−4.80	−2.94	−2.96
^{54}Fe	$T=1+T=0$	a	−141.79	a		−1.06	
	$T=1$	−141.59	−141.79	−141.71	−1.81	−1.12	−1.23
^{56}Fe	$T=1+T=0$	−159.63	−159.97	−160.34	−4.21	−2.69	−2.11
	$T=1$	−159.62	−159.97	−160.34	−4.28	−2.69	−2.11
^{58}Fe	$T=1+T=0$	−177.05	−176.96	−177.56	−4.66	−4.23	−1.69
	$T=1$	−177.01	−176.94	−177.57	−4.69	−4.33	−1.69
^{58}Ni	$T=1+T=0$	−190.06	a	−188.64	−2.08		−1.00
	$T=1$	−190.06	−188.73	−188.64	−2.08	−0.60	−1.01
^{60}Ni	$T=1+T=0$	−209.84	−208.13	−208.06	−2.21	−2.12	−2.21
	$T=1$	−202.69 [b]	−208.13	−208.06	−11.21	−2.14	−2.22
^{62}Ni	$T=1+T=0$	−229.13	−226.45		−0.00	−2.14	
	$T=1$	−225.19 [b]	−226.44		−6.94	−2.18	
^{64}Ni	$T=1+T=0$	−245.09	−243.29	a	−0.01	−1.74	
	$T=1$	−246.00	−243.28	−245.00	−0.43	−1.87	−1.15
^{62}Zn	$T=1+T=0$	−237.37	−235.21	−238.30	−4.03	−2.17	−0.87
	$T=1$	−237.31	−235.17	−238.30	−3.98	−2.68	−0.87
	$T=0$	−236.25			−1.52		
^{64}Zn	$T=1+T=0$	−260.08	b	b	−1.91	−6.18	
	$T=1$	−257.66 [b]	b	b	−5.82	−6.05	
^{66}Zn	$T=1+T=0$	−279.36	−277.39	−278.91	−2.30	−5.40	−2.69
	$T=1$	−279.36	−277.38	−278.92	−2.30	−5.52	−2.69
^{68}Zn	$T=1+T=0$	−296.50	a	−296.50	−2.27		−2.27
	$T=1$	−296.50	−296.22	−296.51	−2.27	−3.05	−2.30

[a] No convergence.
[b] The solution converged to a spherical shape when the iterations were started with a deformed guessed wave function.

culating the intrinsic properties of this nucleus for the oblate shape. The lowest-energy solution for this nucleus is, however, prolate axial which has a large proton HF gap, thus prohibiting *pp* and *np* pairing. Results for ^{48}Ti and ^{50}Ti are quite similar with almost degenerate prolate axial and triaxial solutions without any *np* pairing correlations.

Another mixed mode solution is obtained for ^{50}Cr for the oblate shape for which both the neutron and the proton HF gaps are small and almost the same. The mixed mode solution is degenerate with the $|T_z| = 1$ mode solution. Like in the case of ^{46}Ti, the $T = 0$ solution is a little higher in energy. All the Cr isotopes have prolate axial lowest-energy solutions, with almost degenerate triaxial solutions. Although the pairing energies for the $T = 1$ plus $T = 0$ mode differ from those of the $|T_z| = 1$ mode, pairing potential Δ in the former case has no significant Δ_{np} components in the final solution. Very similar results are obtained for the Fe isotopes with ^{54}Fe favoring a prolate shape whereas ^{56}Fe and ^{58}Fe have triaxial solutions slightly lower than the prolate and oblate solutions, respectively.

All the Ni isotopes favor an oblate shape with

TABLE III. Multipole mass moments (Q_{LM}) and the pickup strengths for the minimum energy solution. For axial shapes $Q_{LM} = (Q_{20}, Q_{40})$ and for triaxial shapes $Q_{LM} = (Q_{20}, Q_{22}, Q_{40})$ are given columnwise. For each nucleus the neutron pickup strengths are given in the first row and the proton pickup strengths in the second row. Experimental values for the pickup strengths are given in parentheses below the corresponding theoretical values.

Nucleus	Solution	Pairing mode	Q_{LM} (fm)	Pickup strengths $j = \frac{1}{2}$	$j = \frac{3}{2}$	$j = \frac{5}{2}$	$j = \frac{7}{2}$
^{46}Ti	HFB (prolate)	$T = 1$	100.24	0.121	0.572	0.195	3.111
			898.08		(0.52) [a]		(2.7) [a]
				0.103	0.477	0.090	1.330
					(0.35) [b]	(0.48) [b]	(1.43) [b]
^{48}Ti	HFB (triaxial)	$T = 1$	102.80	0.302	1.052	0.303	4.340
			1.24		(0.50) [a]		(5.1) [a]
			662.88	0.103	0.526	0.075	1.306
					(0.24) [b]		(1.95) [b]
^{50}Ti	HFB (prolate)	$T = 1$	102.40	0.485	1.607	0.362	5.546
			443.20		(0.48) [a]		(5.1), [a] (5.2) [c]
				0.106	0.571	0.062	1.261
							(1.8) [b]
^{50}Cr	HFB (prolate)	$T = 1$	142.48	0.523	1.091	0.585	3.801
			539.36				(3.4) [d]
				0.118	0.827	0.179	2.876
							(4.3) [e]
^{52}Cr	HFB (prolate)	$T = 1$	147.80	0.666	1.229	0.723	5.382
			226.08	(0.88) [f]			(5.76) [f]
				0.105	0.890	0.148	2.857
							(3.7) [g]
^{54}Cr	HFB (prolate)	$T = 1$	135.96	0.803	2.070	1.138	5.989
						0.133	(6.1) [f]
			169.60	0.090	0.893		2.884
							(4.5) [h]
^{54}Fe	HFB (prolate)	$T = 1$	164.56	0.729	1.349	0.616	5.306
					(0.16) [i]		(5.88) [i]
			−91.84	0.614	1.282	0.484	3.620
					(0.1) [i]	(0.4) [i]	(5.6) [i]
^{56}Fe	HFB (triaxial)	$T = 1$	140.84	0.912	2.237	1.206	5.655
			77.92		(1.43) [j]	(0.93) [j]	
			−217.44	0.368	1.491	0.298	3.852
^{58}Fe	HFB (triaxial)	$T = 1$	129.72	1.003	2.712	1.809	6.476
			110.68		(1.61) [j]	(2.05) [j]	
			−236.32	0.283	1.528	0.295	3.894
^{58}Ni	HFB (oblate)	$T = 1$	−167.84	1.023	2.553	1.261	5.163
			819.04	0.724	2.425	0.700	4.152
^{60}Ni	HFB (oblate)	$T = 1$	−159.55	1.028	3.560	0.188	7.223
			502.15	0.508	2.480	0.252	4.760
^{62}Ni	HFB (oblate)	$T = 1$	−157.97	2.000	4.000	0.003	7.997
			202.88	0.648	3.112	0.206	4.034
^{64}Ni	HFB (oblate)	$T = 1$	−115.92	1.801	3.903	2.392	7.903
			262.40	0.408	2.620	0.251	4.721
^{62}Zn	HFB (triaxial)	$T = 1$	−146.08	1.435	2.937	1.290	6.338
			89.52	1.074	2.824	0.667	5.435
			−46.88				
^{64}Zn	HFB (oblate)	$T = 1$	−27.48	1.979	3.995	0.044	7.983
			−49.44	(0.9) [k]	(2.0) [k]	(3.2) [k]	
				1.006	3.467	0.227	5.300
				(0.57) [l]	(1.94) [l]	(1.36) [l]	(8.0) [l]
^{66}Zn	HFB (oblate)	$T = 1$	−102.40	1.834	3.900	2.394	7.872
			−138.08	(0.9) [k]	(2.71) [k]	(4.3) [k]	
				0.854	2.972	0.318	5.856
				(0.45) [l]	(2.0) [l]	(1.09) [l]	(8.0) [l]

TABLE III *(Continued)*

Nucleus	Solution	Pairing mode	Q_{LM} (fm)	Pickup strengths $j=\frac{1}{2}$	$j=\frac{3}{2}$	$j=\frac{5}{2}$	$j=\frac{7}{2}$
^{68}Zn	HFB(oblate)	$T=1$	−78.12	1.854	3.934	4.252	7.957
			−470.72	(1.2) [k]	(3.4) [k]	(5.0) [k]	
				0.432	2.852	0.166	6.550

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no np pairing correlations. The ^{64}Ni oblate $T=1$ plus $T=0$ mode solution is a little different from the $|T_z|=1$ mode solution because it was obtained with a lower accuracy due to a very slow convergence, rather than because of the presence of np pairing correlations. This was checked by examining the Δ_{np} components in the final solution obtained.

The ^{62}Zn nucleus again possesses a mixed mode $T=1$ plus $T=0$ solution in the oblate shape. The $T=0$ mode solution is a little higher but the pairing energy is −1.52 MeV, the maximum pairing energy for this mode among all the nuclei considered here. The lowest-energy solution is triaxial however, with no np pairing correlations.

The intrinsic mass multipole moments

$$Q_{LM}=\langle\Phi_{\mathrm{HFB}}\left|\sum_{i=1}^{A} r_i^L Y_{LM}(\Omega_i)\right|\Phi_{\mathrm{HFB}}\rangle$$

and the spectroscopic pickup strengths

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

are presented in Table III for the lowest-energy solution for each nucleus. The coefficients C_{jm}^{α} in the above expression are the components of the orthogonal matrix which diagonalizes the density matrix ρ and $V_{\alpha m}{}^2$ are the occupation probabilities of the deformed orbits, obtained by such a diagonalization. The spectroscopic factors contain the information about the wave function which can be related to the experimental data obtained from the one-nucleon transfer reaction. However, many of the experimental results do not satisfy the condition

$$\sum_j S_j = n\,,$$

where n is the number of neutrons (or protons) outside the ^{40}Ca core. Also the experimental values are not very precise because of the parameter-dependent distorted-wave Born-approximation analysis. Sometimes, some strengths are missing due to insufficient excitation energy. In some cases this results in very unreasonable strengths.

TABLE IV. Comparison of HF and HFB gaps for the ground-state shapes.

Nucleus	HF gaps G_p	HF gaps G_n	HFB gaps G_p	HFB gaps G_n
^{46}Ti	3.02	2.29	3.02	2.44
^{48}Ti	2.30	0.85	2.61	3.10
^{50}Ti	1.96	0.06	2.77	2.88
^{50}Cr	2.99	1.14	2.99	1.88
^{52}Cr	2.86	2.43	2.86	2.58
^{54}Cr	2.80	0.04	2.83	2.48
^{54}Fe	1.10	2.41	1.89	2.58
^{56}Fe	2.00	1.36	2.39	2.37
^{58}Ni	4.69	0.16	4.99	2.21
^{60}Ni	3.62	0.37	3.65	3.52
^{62}Ni	3.03	3.83	3.48	4.62
^{64}Ni	2.53	3.00	2.68	3.15
^{62}Zn	2.00	1.91	2.13	2.13
^{64}Zn	0.10	0.10	3.26	3.87
^{66}Zn	0.43	1.94	2.19	2.41
^{68}Zn	1.17	2.32	2.49	2.12

Keeping these limitations of the values deduced from the experimental data from one-nucleon transfer reactions in mind, the agreement between the calculated values from the present work and the experimental values is fairly good. One important conclusion that can be drawn from these values for the Zn isotopes is that ^{56}Ni is not a closed shell as is assumed in some shell model calculations since the $1f_{7/2}$ orbit is not completely filled for the protons.

In Table IV a comparison of the HF and HFB gaps is made for the purpose of studying the stability of the various HF and HFB solutions. Since all the HFB solutions in this table correspond to the $|T_z|=1$ pairing mode, the gaps have been labeled as neutron and proton gaps. It is clear that if the HF gap is more than 2 MeV there are hardly any pairing correlations and the gap stays the same when the HFB calculation is performed. For smaller HF gaps, the increase in the gaps ranges up to 3 MeV, when pairing correlations are included, making the solutions stable against any excitations. With a few exceptions the HFB gaps are always more than 2.5 MeV.

IV. SUMMARY AND CONCLUSIONS

The importance of neutron-proton pairing correlations in $N\neq Z$ isotopes of Ti, Cr, Fe, Ni, and Zn is systematically studied within the framework of the Hartree-Fock-Bogoliubov theory. Complete HFB calculations are carried out by including $|T_z|=1$, $T=0$, and $T=1$ (nn,pp,np) plus $T=0$ pairing correlations. It is found that for nuclei with $N-Z=2$ (except for ^{54}Fe and ^{58}Ni) there is a small contribution of the $T=0$ np pairing correlations. However, even in these cases the $|T_z|=1$ mode dominates over the $T=0$ mode and the $T=1$ np correlations are completely absent. It is therefore suggested that if the small contribution of $T=0$ correlations is to be included in the intrinsic ground states for these nuclei, both the $T=1$ and $T=0$ pairing correlations should be included simultaneously. For nuclei with $N-Z>2$ the np pairing correlations are completely absent. Unlike the case of $N=Z$ nuclei where $T=0$ pairing was found[17] to be more important than $|T_z|=1$ pairing in the excited states, the $T=0$ pairing correlations are not significant for the $N\neq Z$ nuclei in the $2p$-$1f$ shell. This is particularly so for $N-Z>2$ nuclei.

The gound-state shapes for the first half of the $2p$-$1f$ shell nuclei are found to be prolate (except for ^{48}Ti and ^{58}Fe which favor asymmetric triaxial shape), whereas the nuclei in the second half (Ni and Zn isotopes) favor an axial oblate shape. Further, on including the pairing correlations (mostly $|T_z|=1$) an increase in the gaps of up to 3 MeV from ground state to the first excited state over the corresponding gap in the HF solution of the same shape is observed. Keeping in mind the limitations of the values of the experimental spectroscopic strengths the agreement between the calculated and the experimental values ranges from good to fair.

The authors are grateful to Professor A. L. Goodman for his continued interest in this work.

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