Self-Consistent Study of Nuclear Shapes

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Self-consistent Hartree-Fock (HF) and Hartree-Fock-Bogoliubov (HFB) calculations have been performed for the even Ti, Cr, and Fe isotopes. The residual two-body interaction is assumed to be a central potential with a Yukawa radial dependence and an exchange mixture which has been adjusted to fit the low-lying shell-model states of O_{10}^{18} and F_9^{18}. It is found that the HF minima occur for prolate shapes, and hence the HFB calculations are done only for prolate deformations. The HFB calculation yields normal solutions for $N=Z$ nuclei and spherical shapes for $Z<N=28$ nuclei. The effect of pairing on the ground-state properties is also studied. The value of the mass quadrupole moment for the HFB solution is smaller than that for the HF solutions for all the nuclei under consideration. A spherical BCS calculation has been performed to estimate the effect of deformation on pairing energy in the HFB calculation. We construct the excited states for the $Z<N=28$ nuclei from the spherical BCS ground-state solutions in the random-phase approximation. This gives the values for the $0^+\rightarrow 2^+$ energy separation and the $B(E2)$ rates which are in good agreement with experiment.

I. INTRODUCTION

THE Hartree-Fock (HF) and the spherical BCS approximations in the study of nuclear shapes are quite well known. It is also known that in the HF approach the field-producing part of the interaction is treated self-consistently, but the pairing part is neglected. On the other hand, the usual spherical BCS approach completely ignores the possibility of the self-consistent field being deformed, although it takes proper account of the pairing effect through the Bogoliubov-Valatin transformation. In order to treat the pairing part and the field-producing part of the nuclear interaction on the same footing, a very general formalism has been developed in the recent years.[1] This is known as the Hartree-Fock-Bogoliubov (HFB) approximation. In this procedure, the HF equations are generalized by introducing the general Bogoliubov transformation, and the HFB equations thus obtained, when solved self-consistently, are expected to give more realistic shapes for the nuclei.

In the present work, even-even ($N-Z\geq 0$) nuclei in the range $22\leq Z\leq 26$ are considered, and the *realistic shapes* for these nuclei are determined with the HFB approximation. The nuclear interaction, which is responsible for the HF field and the pairing correlation in the HFB solution, is taken to be a central two-body interaction, with a suitable exchange mixture. HF and spherical BCS calculations are also performed for these nuclei with the same interaction, and the numerical results obtained from these calculations are compared with the HFB results. In the HFB and spherical BCS calculations, the pairing correlation is considered only between identical nucleons.

The following assumptions about the HF and HFB intrinsic wave functions are made:

(a) There exists an axis of symmetry.

(b) Because in this study only even-even nuclei for which $K=0$ are considered, the assumption of time-reversal invariance is valid.

(c) Parity is a good quantum number. [Reflection symmetry about the X-Y plane follows from (a) and (c)].

(d) Invariance under rotation of π about the Y axis. [This with (c) implies reflection symmetry in the X-Z plane.]

(e) Mixing of orbitals is restricted to a single major shell ($2p$-$1f$).

Furthermore, the existence of a spherical core completely filling all the shell-model orbitals up to $2s$-$1d$ major shell is assumed. As usual, the effect of this core is simulated by taking the single-particle energies of Ca_{21}^{41} for the single-particle term in the many-body Hamiltonian. As regards the radial part of the wave function, it is taken to be that of a harmonic oscillator, the size parameter $b=(\hbar/m\omega)^{1/2}$ which has been fixed to yield the average root-mean-square charge radius in the p-f shell. Within a major shell, the variation of b with atomic mass number is very small, and hence an average value (2.05×10^{-13} cm) is taken.

The effective two-body nuclear interaction which has been used here is of the following form:

$$V_{ST}(\gamma)=V_{ST}^0(e^{-\gamma/\beta}/\gamma/\beta), \qquad (1)$$

where V_{ST}^0 is the strength of the interaction in a quantum state characterised by spin and isospin multiplicities S and T, respectively. These strengths have been determined from a two-particle shell-model fit to the spectra of O_{10}^{18} and F_9^{18}, and it is assumed here that the potential thus obtained is a good one for doing self-consistent calculations in the $2p$-$1f$ shell.[2] It should be mentioned here that a two-particle shell-model calculation done with this interaction for Ca_{22}^{42} gives quite good agreement with the experi-

[1] M. Baranger, Phys. Rev. **122**, 992 (1961).

[2] Harish Chandra, Doctoral thesis submitted to Calcutta University, 1969 (unpublished).

mental value for the energy separation between the 0^+ and the first 2^+ level. However, it gives only qualitative agreement for the $T=0$ energy levels of Sc_{21}^{42}. The strengths corresponding to different states are given below:

$$V_{31}^0=-46.9 \text{ MeV}, \quad V_{13}^0=-34.4 \text{ MeV},$$
$$V_{33}^0=+19.4 \text{ MeV}, \quad V_{11}^0=+40.9 \text{ MeV}.$$

The range of the interaction, β, is taken to be equal to the Compton wavelength of the pion. In this calculation, we neglect the Coulomb interaction between protons. For this reason the single-particle shell-model energy spectra for protons and neutrons in the $2p$-$1f$ shell are assumed to be the same. From the single-particle energy spectrum for Ca_{21}^{41} we have

$$\epsilon_{f_{7/2}}=-6.5 \text{ MeV}, \quad \epsilon_{f_{5/2}}=0.0 \text{ MeV},$$
$$\epsilon_{p_{3/2}}=-4.5 \text{ MeV}, \quad \epsilon_{p_{1/2}}=-2.5 \text{ MeV}.$$

In Sec. II of this paper, the self-consistent formalism is described briefly. Section III is mainly devoted to the discussion of the self-consistent results. In Sec. IV are presented the results obtained from a random-phase-approximation (RPA) calculation for even-$Z<N=28$ nuclei with spherical BCS shape, and Sec. V contains the conclusions.

II. SELF-CONSISTENT FORMALISM

A. HF Procedure

Detailed accounts of the HF theory are available in many published works,[3] and hence we shall be very brief here. To start with, we write the many-body Hamiltonian in the second-quantized language as

$$H=\sum_{\alpha\beta}\langle\alpha\,|\,\epsilon\,|\,\beta\rangle a_\alpha^\dagger a_\beta+\tfrac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta\,|\,V_A\,|\,\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma, \tag{2}$$

where ϵ is the single-particle energy term. The matrix elements of the interaction $V(r)$ are taken between the antisymmetric two-particle states.

The HF method consists of finding the single determinantal trial wave-function $\Phi_{\rm HF}$ by minimizing the expectation value $\langle\Phi_{\rm HF}\,|\,H\,|\,\Phi_{\rm HF}\rangle/\langle\Phi_{\rm HF}\,|\,\Phi_{\rm HF}\rangle$,

$$\delta\{\langle\Phi_{\rm HF}\,|\,H\,|\,\Phi_{\rm HF}\rangle/\langle\Phi_{\rm HF}\,|\,\Phi_{\rm HF}\rangle\}=0. \tag{3}$$

This amounts to solving the equation

$$h\,|\,\lambda\rangle=\varepsilon_\lambda\,|\,\lambda\rangle,$$

where

$$\langle\alpha\,|\,h\,|\,\beta\rangle=\langle\alpha\,|\,\epsilon\,|\,\beta\rangle+\sum_{\lambda=1}^{A}\langle\alpha\lambda\,|\,V_A\,|\,\beta\lambda\rangle, \tag{4}$$

which states that the single-particle orbitals $|\,\lambda\rangle$ which make up the determinantal wave function $\Phi_{\rm HF}$ are those that diagonalize the HF Hamiltonian h. These orbitals are expanded in some known representation, which, in our case, is the single-particle shell-model states of the $2p$-$1f$ shell; and the expansion coefficients are treated as variational parameters. The single-particle wave function incorporating the assumptions given in the previous section is written as

$$|\,\lambda m\tau_z\rangle=\sum_j C_{jm}^{\lambda\tau_z}\,|\,jm\tau_z\rangle, \tag{5}$$

where the summation is over shell-model states of the $2p$-$1f$ shell. The expansion coefficients $C_{jm}^{\lambda\tau_z}$ are normalized, and they satisfy the following condition:

$$\sum_j C_{jm}^{\lambda\tau_z}C_{jm}^{\lambda'\tau_z}=\delta_{\lambda\lambda'}. \tag{6}$$

The HF matrix is set up in the $jm\tau_z$ representation in terms of arbitrary expansion coefficients, and the iteration procedure is continued till a self-consistent solution with the desired accuracy is obtained.

B. HFB Procedure

HFB equations, used in our calculations, are obtained as a result of following quasiparticle transformation:

$$A_{im\tau_z}^\dagger=\sum_j\left(u_{jm}^{i\tau_z}a_{jm\tau_z}^\dagger+v_{jm}^{i\tau_z}a_{j\tilde{m}\tau_z}\right) \tag{7a}$$

and

$$A_{im\tau_z}=\sum_j\left(u_{jm}^{i\tau_z}a_{jm\tau_z}+v_{jm}^{i\tau_z}a_{j\tilde{m}\tau_z}^\dagger\right). \tag{7b}$$

Since this transformation is a canonical one, the quasiparticle operators $(A^\dagger, A)$, like the particle operators $(a^\dagger, a)$, obey the fermion anticommutation relations. This leads to the following orthogonality relations satisfied by the expansion coefficients u and v:

$$\sum_j\left(u_{jm}^{i\tau_z}u_{jm}^{k\tau_z}+v_{jm}^{i\tau_z}v_{jm}^{k\tau_z}\right)=\delta_{ik} \tag{8a}$$

and

$$\sum_j\left(u_{jm}^{i\tau_z}v_{jm}^{k\tau_z}-v_{jm}^{i\tau_z}u_{jm}^{k\tau_z}\right)=0. \tag{8b}$$

The ground state of the system is approximated by the vacuum for the quasiparticle operators, and hence

$$A_{im\tau_z}\,|\,\Phi_{\rm HFB}\rangle=0. \tag{9}$$

Since the quasiparticle transformations given by (7) do not conserve the number of particles, the HFB wave function will not normally correspond to any particular nuclear system. In view of this, Eq. (2) is modified to

$$\mathfrak{IC}=H-\mu_n\mathfrak{N}_n-\mu_p\mathfrak{N}_p, \tag{10}$$

where μ_n and μ_p are the chemical potentials, whose values are fixed so that the expectation values of the number operators $\mathfrak{N}_n$ and $\mathfrak{N}_p$ between the ground-

[3] I. Kelson, Phys. Rev. **132**, 2189 (1963); G. E. Brown, *Unified Theory of Nuclear Model and Forces* (North-Holland Publishing Co., Amsterdam, 1967), p. 11.

state wavefunction $\Phi_{\rm HFB}$ becomes equal to the desired number of neutrons and protons, respectively.

The HFB equations are obtained by the method of linearization, which proceeds by evaluating the commutator of $\mathcal{H}$ with $a_\lambda^\dagger$, i.e.,

$$[\mathcal{H}, a_\lambda^\dagger]=(\epsilon_\lambda-\mu)a_\lambda^\dagger+\tfrac{1}{2}\sum_{\alpha\beta\delta}\langle\alpha\beta\,|\,V_A\,|\,\lambda\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta. \tag{11}$$

Here it should be understood that the chemical potential μ is to be subscripted with the value of τ_z for state λ.

Now, using Wick's theorem,[4] we can write

$$a_\alpha^\dagger a_\beta^\dagger a_\delta=\langle a_\alpha^\dagger a_\beta^\dagger\rangle a_\delta+\langle a_\beta^\dagger a_\delta\rangle a_\alpha^\dagger-\langle a_\alpha^\dagger a_\delta\rangle a_\beta^\dagger+N(a_\alpha^\dagger a_\beta^\dagger a_\delta), \tag{12}$$

and this becomes linear in $a^\dagger$ and a when we neglect the normal product appearing as the last term in (12). This corresponds to the neglect of the residual interaction between the quasiparticles. The expectation values of the particle operators are taken with respect to the quasiparticle vacuum, hence, we have

$$[\mathcal{H}, a_\lambda^\dagger]=(\epsilon_\lambda-\mu)a_\lambda^\dagger+\sum_{\alpha\beta\delta}\langle\alpha\beta\,|\,V_A\,|\,\lambda\delta\rangle\langle a_\beta^\dagger a_\delta\rangle a_\alpha^\dagger+\tfrac{1}{2}\sum_{\alpha\beta\delta}\langle\alpha\beta\,|\,V_A\,|\,\lambda\delta\rangle\langle a_\alpha^\dagger a_\beta^\dagger\rangle a_\delta, \tag{13}$$

which in terms of Γ and Δ can be written as

$$[\mathcal{H}, a_{jm\tau_z}^\dagger]=(\epsilon_j-\mu_{\tau_z})a_{jm\tau_z}^\dagger+\sum_{j'}\Gamma_{jj'}^{m\tau_z}a_{j'm\tau_z}^\dagger+\sum_{j'}\Delta_{jj'}^{m\tau_z}a_{j'\bar{m}\tau_z}, \tag{14}$$

where Γ and Δ are defined as

$$\Gamma_{jj'}^{m\tau_z}=\sum_{j_1j_2,m_1\tau_z'}\langle jm\tau_z, j_1m_1\tau_z'\,|\,V_A\,|\,j'm\tau_z, j_2m_1\tau_z'\rangle\times\rho_{j_1j_2}^{m_1\tau_z'} \tag{15a}$$

and

$$\Delta_{jj'}^{m\tau_z}=\tfrac{1}{2}\sum_{j_1j_2,m_1}\langle jm\tau_z, j'\bar{m}\tau_z\,|\,V_A\,|\,j_1m_1\tau_z, j_2\bar{m}_1\tau_z\rangle\times\chi_{j_1j_2}^{m_1\tau_z}. \tag{15b}$$

ρ and χ are, respectively, the density and pairing matrices, defined as

$$\rho_{jj'}^{m\tau_z}=\langle\Phi_{\rm HFB}\,|\,a_{jm\tau_z}^\dagger a_{j'm\tau_z}\,|\,\Phi_{\rm HFB}\rangle \tag{16a}$$

and

$$\chi_{jj'}^{m\tau_z}=\langle\Phi_{\rm HFB}\,|\,a_{jm\tau_z}^\dagger a_{j'\bar{m}\tau_z}^\dagger\,|\,\Phi_{\rm HFB}\rangle. \tag{16b}$$

Expressing $(a^\dagger, a)$ in terms of $(A^\dagger, A)$ and using (9), we have

$$\rho_{jj'}^{m\tau_z}=\sum_i v_{jm}^{i\tau_z}v_{j'm}^{i\tau_z};$$

$$\chi_{jj'}^{m\tau_z}=-\sum_i v_{jm}^{i\tau_z}u_{j'm}^{i\tau_z}. \tag{17}$$

Since ρ and χ are real and symmetric, Γ and Δ are also real and symmetric.

Taking the Hermitian conjugate of (14) and using the symmetry properties of Γ and Δ, one gets, after replacing m with $\bar{m}$, the following expression:

$$-[\mathcal{H}, a_{j\bar{m}\tau_z}]=(\epsilon_j-\mu_{\tau_z})a_{j\bar{m}\tau_z}+\sum_{j'}\Gamma_{jj'}^{m\tau_z}a_{j'\bar{m}\tau_z}-\sum_{j'}\Delta_{jj'}^{m\tau_z}a_{j'm\tau_z}^\dagger. \tag{14'}$$

Writing the operator equation

$$[\mathcal{H}, A_{im\tau_z}^\dagger]=E_{im}^{\tau_z}A_{im\tau_z}^\dagger, \tag{18}$$

and expressing (18) in terms of (14), and then equating the coefficients of annihilation and creation operators separately, one gets the following HFB equations:

$$E_{im}^{\tau_z}u_{j'm}^{i\tau_z}=\sum_j\tilde{\Gamma}_{jj'}^{m\tau_z}u_{jm}^{i\tau_z}+\sum_j\Delta_{jj'}^{m\tau_z}v_{jm}^{i\tau_z}, \tag{19a}$$

$$-E_{im}^{\tau_z}v_{j'm}^{i\tau_z}=\sum_j\tilde{\Gamma}_{jj'}^{m\tau_z}v_{jm}^{i\tau_z}-\sum_j\Delta_{jj'}^{m\tau_z}u_{jm}^{i\tau_z}, \tag{19b}$$

where $E_{im}^{\tau_z}$ is the energy required to create the quasiparticle state $A_{im\tau_z}^\dagger\,|\,\Phi_{\rm HFB}\rangle$, and

$$\tilde{\Gamma}_{jj'}^{m\tau_z}=(\epsilon_{j'}-\mu_{\tau_z})\delta_{jj'}+\Gamma_{jj'}^{m\tau_z}. \tag{20}$$

The HFB equations given by (19) define the excitation energy matrix W as

$$W=\begin{pmatrix}\tilde{\Gamma} & \Delta\\ \Delta & -\tilde{\Gamma}\end{pmatrix}, \tag{21}$$

and the quasiparticle energy eigenvalues are obtained by diagonalizing the energy matrix W.

From the structure of W it is obvious that if

$$\begin{pmatrix}u\\ v\end{pmatrix}$$

is an eigenvector corresponding to energy eigenvalue $+E$, then

$$\begin{pmatrix}-v\\ u\end{pmatrix}$$

is also an eigenvector with energy eigenvalue $-E$. Thus, the real orthogonal matrix U that will diagonalize W is of the following form:

$$U=\begin{pmatrix}u & -v\\ v & u\end{pmatrix}, \tag{22}$$

where the matrix

$$\begin{pmatrix}u\\ v\end{pmatrix}$$

is obtained by arranging the different positive-energy eigenvectors along the column. The quasiparticle trans-

[4] S. S. Schweber, *An Introduction to Relativistic Qnautum Field Theory* (Row, Peterson and Co., Evanston, Ill., 1961), p. 435.

TABLE I. Comparison of ground-state energy (in MeV) obtained from HF, HFB, and spherical BCS calculations for Ti, Cr, and Fe isotopes.

Isotope	$E_{\mathrm{HF}}^{\mathrm{oblate}}$	$E_{\mathrm{HF}}^{\mathrm{prolate}}$	E_{HFB}	E_{BCS}	Isotope	$E_{\mathrm{HF}}^{\mathrm{oblate}}$	$E_{\mathrm{HF}}^{\mathrm{prolate}}$	E_{HFB}	E_{BCS}
Ti_{22}^{44}	−32.58	−34.35	−34.35	−32.61	Cr_{28}^{52}	−108.25	−108.45	−109.34	−109.34
Ti_{24}^{46}	−49.42	−50.99	−51.14	−49.98	Cr_{30}^{54}	−122.66	−124.75	−124.76	−124.09
Ti_{26}^{48}	−65.70	−66.70	−67.07	−66.72	Fe_{26}^{52}	−112.26	−114.30	−114.30	−113.10
Ti_{28}^{50}	−82.08	−82.21	−82.76	−82.77	Fe_{28}^{54}	−134.33	−134.59	−135.37	−135.37
Cr_{24}^{48}	−70.19	−72.53	−72.53	−70.34	Fe_{30}^{56}	−150.50	−152.27	−152.42	−152.08
Cr_{26}^{50}	−89.38	−91.01	−91.05	−90.17	Fe_{32}^{58}	−167.27	−167.48	−168.39	−167.98

formation in terms of U is given as

$$\begin{pmatrix} A^\dagger \\ \bar{A} \end{pmatrix} = \tilde{U} \begin{pmatrix} a^\dagger \\ \bar{a} \end{pmatrix}, \tag{23}$$

where the bar over the annihilation operators signifies the time-reversed state, and $\tilde{U}$ is the transpose of U, i.e.,

$$\tilde{U} = \begin{pmatrix} \tilde{u} & \tilde{v} \\ -\tilde{v} & \tilde{u} \end{pmatrix}. \tag{24}$$

The matrices ρ and χ can be expressed in terms of u and v as

$$\rho = v\tilde{v}, \qquad \chi = -v\tilde{u}. \tag{25}$$

Like the HF equations, the HFB equations are also nonlinear. So a self consistent solution is to be obtained by an iterative process. To carry out the calculation we choose the matrices u and v for an arbitrary deformation, and from them set up the ρ and χ matrices. The energy matrix is expressed in terms of the ρ and χ matrices, and is diagonalized to obtain the new u and v. The new energy matrix is set up in terms of ρ and χ obtained from this set of u and v. This process of iteration is continued till self-consistency with the desired accuracy is obtained. The u and v in each iteration are subjected to the constraint that the expectation values of the number operators for protons and neutrons are always fixed.

III. DISCUSSION OF SELF-CONSISTENT RESULTS

A. Nuclear Shape

The ground-state properties, viz., the quadrupole moment and the ground-state energy, can be easily determined once the self-consistent solution for the stable nuclear shape is obtained. The preference for the prolate shape over the oblate one or vice versa can be established by performing self-consistent calculations for these shapes and comparing their energy minima. The one corresponding to the smaller of the two may be accepted as the most stable ground-state shape.

A comparison of the HF energy for the prolate and oblate shapes is made in Table I. One can see that the HF energy for the prolate shape is smaller than that for the oblate shape (the prolate shape is more strongly bound) for all the even-even nuclei considered here. This shows that the ground-state structure favors prolate deformation.

In view of the above results of the HF approximation for the nuclear shape, the HFB calculations have been performed only for prolate shapes.

B. Structure of HF and HFB Spectra

The single-particle HF and the single-quasiparticle HFB energy spectra are shown in Figs. 1–3. The diagrams in the parts labelled (a) correspond to proton states and those in (b) correspond to proton states. Single-particle and single-quasiparticle states are designated by the projection quantum number m. Since our basis consists of $1f_{7/2}$, $1f_{5/2}$, $2p_{3/2}$, and $2p_{1/2}$ states, the deformed states will be ten in number, provided we do not count as separate ones the degenerate time-reversed states for each type of nucleons. Among these states, four will correspond to $m=\frac{1}{2}$, three to $m=\frac{7}{2}$, two to $m=\frac{5}{2}$, and one to $m=\frac{7}{2}$. In the diagrams, energy levels corresponding to different orthogonal states with same projection quantum number are labelled by different number of primes. In attaching these primes the following convention is followed. We write the single-particle wave function as

$$|m^i\rangle = \sum_j C_{jm}{}^i |jm\rangle, \tag{26}$$

where the superscript i on m stands for the number of primes. The unprimed states ($\frac{1}{2}$, $\frac{3}{2}$, $\frac{5}{2}$, and $\frac{7}{2}$) are those which have maximum probability amplitude for $j=\frac{7}{2}$ (i.e., for a state $|m\rangle$, $C_{j=7/2m}{}^2 > C_{j\neq 7/2m}{}^2$). Similarly states with one prime ($1'/2$, $3'/2$) are those for which the $j=\frac{3}{2}$ amplitude is maximum. The state $1''/2$ has maximum amplitude for $j=\frac{1}{2}$ and for other states ($1'''/2$, $3''/2$, $5'/2$) the $j=\frac{5}{2}$ amplitude is maximum.

Deformed single-quasiparticle states obtained from the HFB calculations are also labelled by different number of primes in a similar way. The only difference

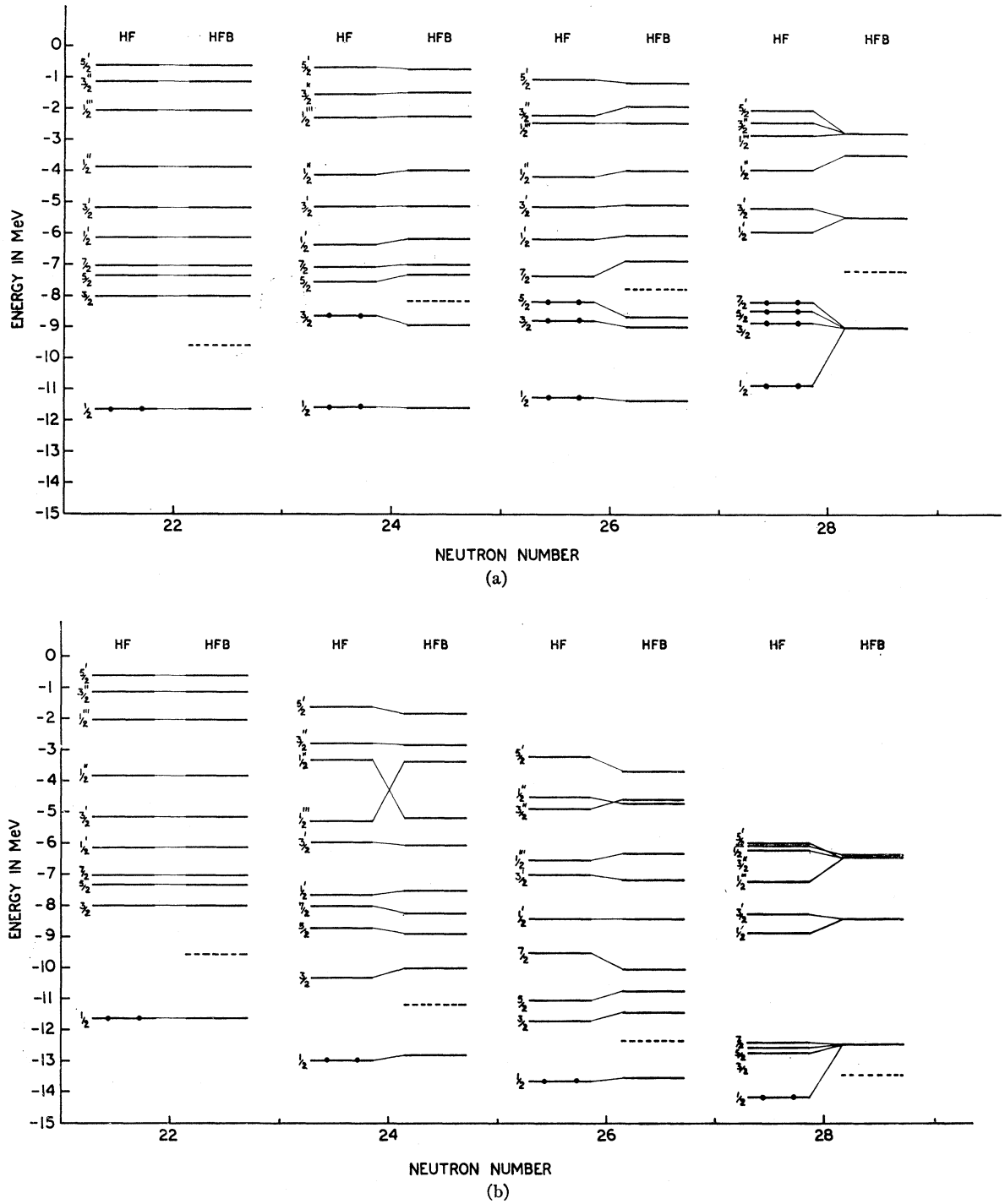


FIG. 1. (a) Self-consistent HF and HFB spectra for neutron states of even Ti isotopes. (b) Self-consistent HF and HFB spectra for proton states of even Ti isotopes.

is that in this case, the component according to whose magnitude states with same projection quantum number are labelled is $u_{jm}{}^{i}$ for the states plotted below the Fermi level, and $u_{jm}{}^{i}$ for the states plotted above it. Since we wish to compare the HF single-particle spectra with the HFB quasiparticle spectra, the HFB spectra are plotted in such a way that the quasiparticle energy levels with occupation probability $\geq 50\%$ are below the Fermi level (as determined by the chemical potential), and those occupation prob-

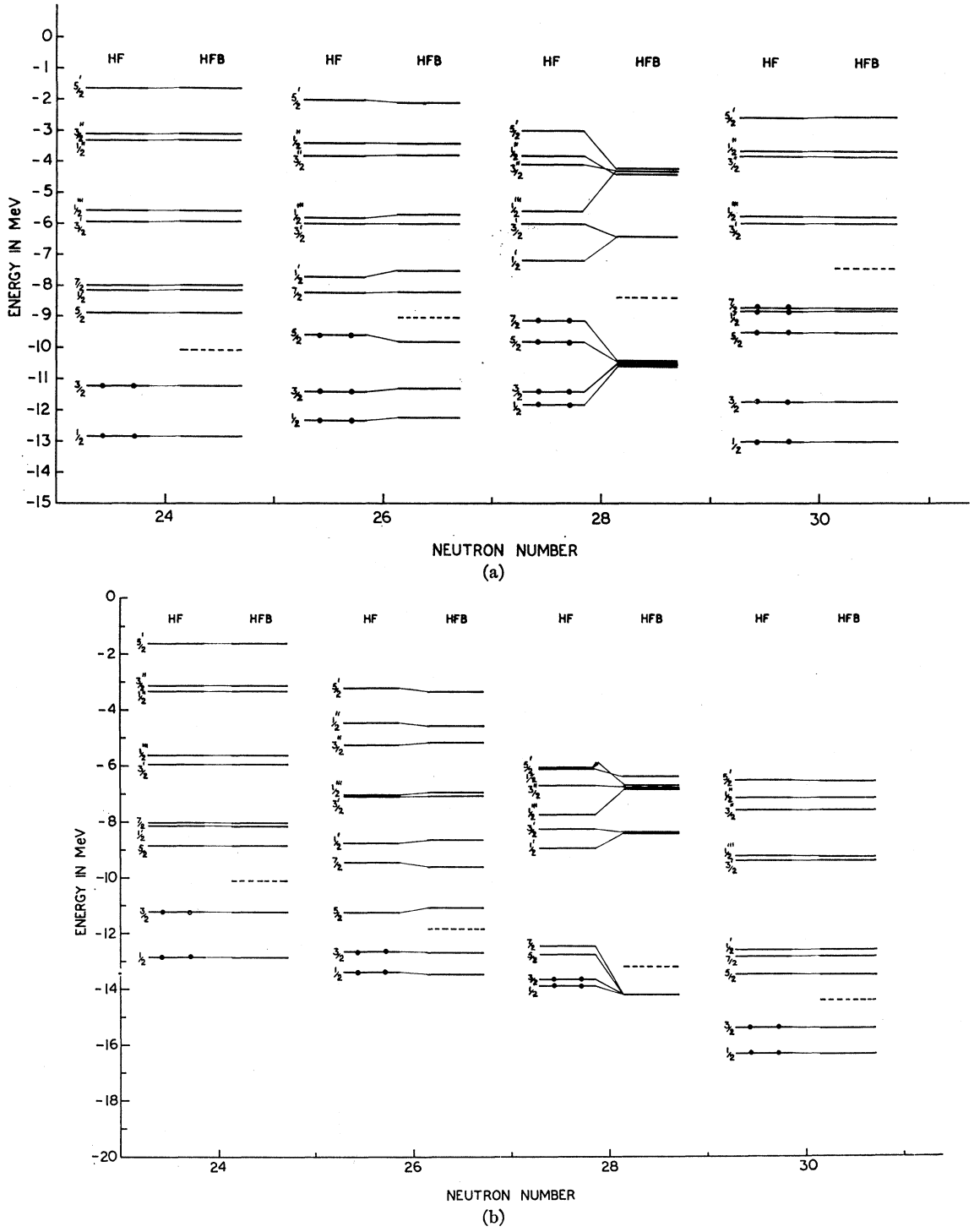
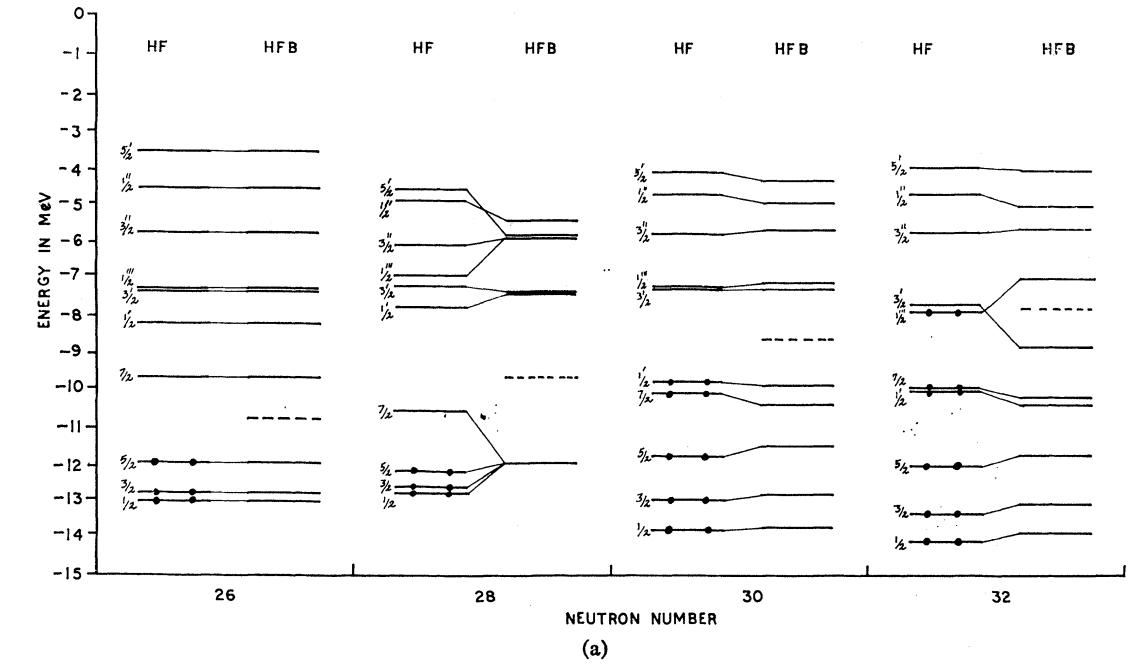
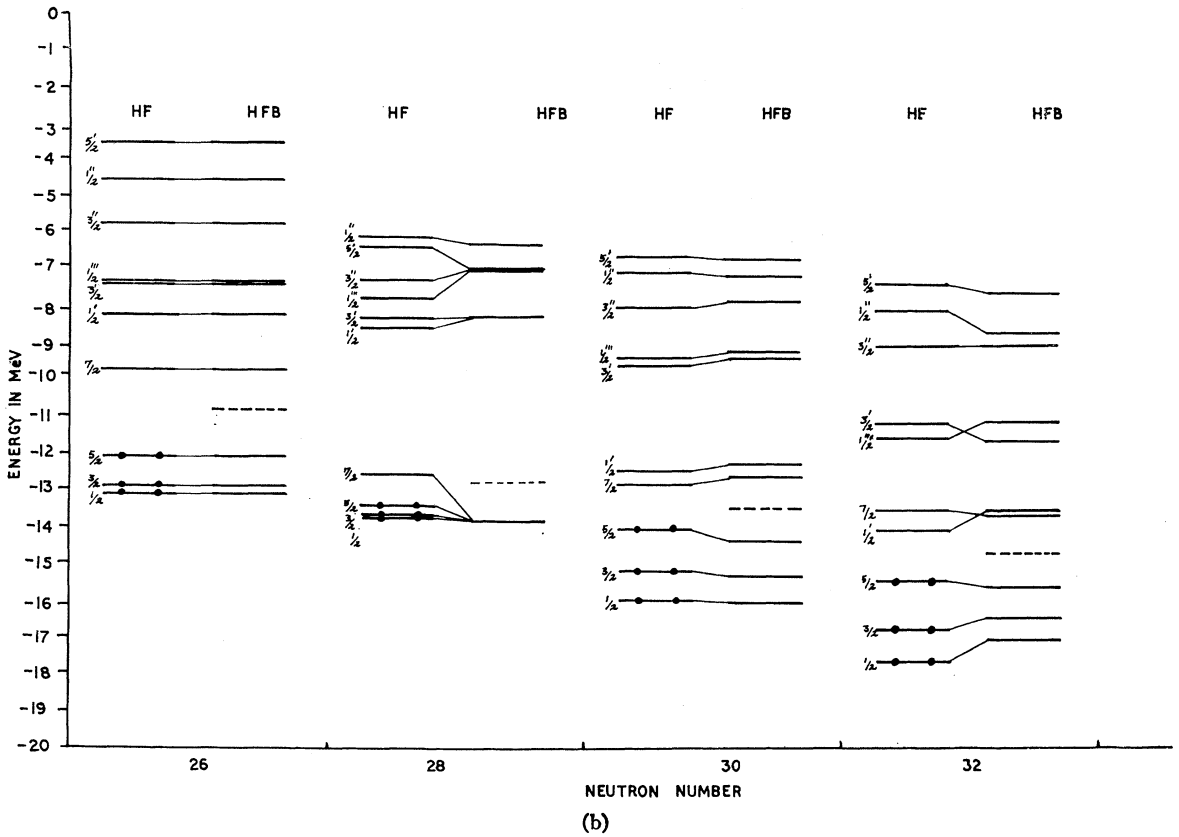


FIG. 2. (a) Self-consistent HF and HFB spectra for neutron states of even Cr isotopes. (b) Self-consistent HF and HFB spectra for proton state of even Cr isotopes.

ability $<50\%$ are above it. An exception to this convention is the quasiparticle spectrum for the proton states of Cr_{28}^{52}. Here the lowest states have an occupation probability of $\approx 49\%$, and if these states were plotted above the Fermi level, then the ordering of the states $m=\frac{1}{2}, \frac{3}{2}, \frac{5}{2}$, and $\frac{7}{2}$, which are very nearly degenerate, would be reversed (i.e., instead of $\frac{1}{2}, \frac{7}{2}$ would occupy the lowest position). To avoid this



(a)



(b)

FIG. 3. (a) Self-consistent HF and HFB spectra for neutron states of even Fe isotopes. (b) Self-consistent HF and HFB spectra for proton states of even Fe isotopes.

reversal, these quasiparticle levels have been plotted below the Fermi level. It is to be noted that the energy of the quasiparticles is measured from the Fermi level, shown by a broken line in each spectrum, and the values of the energy are always taken as positive, whether the energy levels are below the Fermi level or above it.

The quasiparticle spectra shown in Figs. 1–3 can be divided into the following groups:

(a) $N=Z$ nuclei: The HFB spectra for these nuclei do not differ from the HF spectra, i.e., the HFB calculations for these nuclei yield normal solutions.

(b) $Z<N=28$: The effect of pairing is very strong for these nuclei. The HF spectra for these nuclei correspond to deformed shapes and the HFB calculation gives spherical shapes, i.e., the pairing part of the residual interaction is strong enough to make them spherical.

(c) $Z<N\neq 28$: Though the HFB spectra for these nuclei are significantly different from the HF spectra, they correspond to deformed shapes. An exception in this group is Cr_{30}^{54} for which we get an almost normal solution.

It is evident from these diagrams that unlike the well-known HF spectra for the even-even ($N=Z$) nuclei in the first half of the $2s$-$1d$ shell, those for the $2p$-$1f$-shell even-even ($N=Z$) nuclei do not have large gaps between the last occupied and first unoccupied states. However, the fact that the HFB calculations for these nuclei yields normal solutions shows that even the comparatively small energy gap in the HF spectra is quite sufficient to guarantee stability of the HF solutions against pairing correlation. In case of even-$Z<N=28$ nuclei, pairing correlation is present only between proton pairs. For some nuclei in group C (Cr_{30}^{54}, Fe_{30}^{56}) pairing is present only amongst protons whereas in some other nuclei (Ti_{24}^{46}, Ti_{26}^{48}) it is effective only between neutrons. There are few cases (Cr_{26}^{58}, Fe_{32}^{58}) where pairing is effective between neutrons as well as protons. In Cr_{30}^{54} there is no pairing at all amongst neutrons and even amongst protons there is only very little pairing and its effects on the spectrum is not significant. It does modify slightly the values of mass quadrupole moments. It should be mentioned here that in those cases where pairing is present only between one kind of nucleons but absent in the other kind, the HFB spectra for the latter ones are quite different from their respective HF spectra. This change in the HFB spectra is easily understood in terms of the single-particle for these nucleons which gets modified due to the presence of pairing in the other kind of nucleons.

C. Energy Minima for Self-Consistent Shapes

The energy minima corresponding to HF, HFB, and spherical BCS solutions are calculated from the following formulas:

$$E_{\mathrm{HF}}=\langle\Phi_{\mathrm{HF}}\mid H\mid\Phi_{\mathrm{HF}}\rangle=\sum_{k=1/\tau_z}^{\mathrm{occ}}\mathcal{E}(k,\tau_z)+\sum_{\tau_z}T_r^{\tau_z}(\epsilon\rho)_{\tau_z}\quad(27)$$

and

$$E_{\mathrm{HFB}}=\langle\Phi_{\mathrm{HFB}}\mid H\mid\Phi_{\mathrm{HFB}}\rangle=E_{\mathrm{HFB}}^{\mathrm{HF}}+E_{\mathrm{HFB}}^{\mathrm{pair}},\quad(28a)$$

where

$$E_{\mathrm{HFB}}^{\mathrm{HF}}=2\sum_{\tau_z}T_r^{\tau_z}(\epsilon\rho)_{\tau_z}+\sum_{\tau_z}T_r^{\tau_z}(\Gamma\rho)_{\tau_z}\quad(28b)$$

and

$$E_{\mathrm{HFB}}^{\mathrm{pair}}=\sum_{\tau_z}T_r^{\tau_z}(\Delta\chi)_{\tau_z}.\quad(28c)$$

Similarly

$$E_{\mathrm{BCS}}=\langle\Phi_{\mathrm{BCS}}\mid H\mid\Phi_{\mathrm{BCS}}\rangle=E_{\mathrm{BCS}}^{\mathrm{HF}}+E_{\mathrm{BCS}}^{\mathrm{pair}},\quad(29a)$$

where

$$E_{\mathrm{BCS}}^{\mathrm{HF}}=2\sum_{j\tau_z}(j+\tfrac{1}{2})\epsilon_j v_{j\tau_z}^2+\sum_{j\tau_z}(j+\tfrac{1}{2})\Gamma_j^{\tau_z}v_{j\tau_z}^2\quad(29b)$$

and

$$E_{\mathrm{BCS}}^{\mathrm{pair}}=\sum_{j\tau_z}(j+\tfrac{1}{2})\Delta_j^{\tau_z}u_{j\tau_z}v_{j\tau_z}.\quad(29c)$$

$\mathcal{E}(k,\tau_z)$ appearing in (37) is the single-particle HF energy and the summation is over all the occupied HF states. The symbol T_r stands for the trace of the matrix appearing in the brackets following it. Γ, Δ, ρ, and χ of Eq. (28) are defined in Sec. II. u, v and Γ, Δ of Eq. (29) are defined in the Appendix. $E_{\mathrm{HFB}}^{\mathrm{HF}}$, $E_{\mathrm{BCS}}^{\mathrm{HF}}$, $E_{\mathrm{HFB}}^{\mathrm{pair}}$, and $E_{\mathrm{BCS}}^{\mathrm{pair}}$ give the HF and pairing contribution to the energy minima for the HFB and the spherical BCS solutions. These terms are calculated with a view to estimating the effect of deformation and pairing on the self consistent energy minima. The numerical values of E_{HF} (hereafter by E_{HF} we mean $E_{\mathrm{HF}}^{\mathrm{prolate}}$), E_{HFB}, and E_{BCS} are displayed in Table I. From these it is evident that the energy minimum corresponding to HFB shape is always lower than the HF minimum for all such cases where pairing is effective. This implies that, when pairing is effective, there is a definite gain in the binding energy of the nuclear system. However, the *effective* change in the binding energy due to pairing is not large and hence the average binding energy per particle of the system can very well be estimated by simple HF calculation. A comparison of the E_{HFB} with E_{BCS} reveals that the self-consistent HFB minimum is lower than the spherical BCS energy minimum for all the even-even nuclei, except those with neutron number 28, for which E_{HFB} is equal to E_{BCS}. The effect of pairing on E_{HFB} can be studied by comparing E_{HF} with $E_{\mathrm{HFB}}^{\mathrm{HF}}$. The values of $E_{\mathrm{HFB}}^{\mathrm{HF}}$ are given in Table II and we find that in the presence of pairing the contribution to the binding energy from

TABLE II. Pairing and HF contribution to the ground-state energy (in MeV) calculated from HFB and BCS methods for Ti, Cr, and Fe isotopes.

Isotope	$E_{\mathrm{HFB}}^{\mathrm{HF}}$	$E_{\mathrm{BCS}}^{\mathrm{HF}}$	$E_{\mathrm{HFB}}^{\mathrm{pair}}$	$E_{\mathrm{BCS}}^{\mathrm{pair}}$	Isotope	$E_{\mathrm{HFB}}^{\mathrm{HF}}$	$E_{\mathrm{BCS}}^{\mathrm{HF}}$	$E_{\mathrm{HFB}}^{\mathrm{pair}}$	$E_{\mathrm{BCS}}^{\mathrm{pair}}$
Ti_{22}^{44}	−34.35	−28.72	−0.00	−3.89	Cr_{28}^{52}	−106.78	−106.78	−2.56	−2.56
Ti_{24}^{46}	−49.98	−45.30	−1.16	−4.68	Cr_{30}^{54}	−124.68	−119.44	−0.08	−4.65
Ti_{26}^{48}	−65.35	−62.49	−1.72	−4.23	Fe_{26}^{52}	−114.30	−108.83	−0.00	−4.27
Ti_{28}^{50}	−80.92	−80.93	−1.84	−1.84	Fe_{28}^{54}	−133.30	−133.30	−2.07	−2.07
Cr_{24}^{48}	−72.53	−64.97	−0.00	−5.37	Fe_{30}^{56}	−150.98	−147.87	−1.44	−4.21
Cr_{26}^{50}	−90.02	−85.33	−1.03	−4.84	Fe_{32}^{58}	−165.14	−163.33	−3.25	−4.65

HF field reduces. However, this decrease is more than compensated by the pairing contribution. In Table II, we have also displayed the HF contribution to the energy minimum ($E_{\mathrm{BCS}}^{\mathrm{HF}}$) for the spherical BCS solution and it is seen that this quantity is considerably smaller than $E_{\mathrm{HFB}}^{\mathrm{HF}}$, except when HFB yields spherical shape. A comparison of $E_{\mathrm{HFB}}^{\mathrm{pair}}$ with $E_{\mathrm{BCS}}^{\mathrm{pair}}$ given in Table II shows that for the deformed cases the magnitude of the former one is always smaller and is zero for $N=Z$ nuclei. The reason for the large pairing energy in case of spherical BCS approximation is the $(2j+1)$-fold degeneracy of the partially occupied single-particle shell-model states.

D. Quadrupole Moment

The neutron and proton mass quadrupole moments have been separately evaluated by calculating the expectation value of

$$Q=(16\pi/5)^{1/2}r^2Y_0^2(\theta,\varphi), \tag{30}$$

for the HF and HFB wave functions and they are given in Table III.

A comparison of $\langle Q\rangle_{\mathrm{HF}}$ and $\langle Q\rangle_{\mathrm{HFB}}$ shows that these are identical for $N=Z$ nuclei which again demonstrates the absence of pairing in these cases. For Cr_{30}^{54}, as it is expected, the value of $\langle Q\rangle_{\mathrm{HFB}}$ is only slightly smaller than $\langle Q\rangle_{\mathrm{HF}}$.

For nuclei with $Z<N=28$, the mass quadrupole moment for the HFB shape is very small as compared to the HF value. A comparison of the HFB and HF spectra for these nuclei shows that the HFB solutions favor spherical shapes. This is further supported by the numbers displayed in Table II. The very small value of the quadrupole moment obtained for the HFB shape is due to the computational inaccuracy in the calculations.

For $Z<N\neq 28$ nuclei, the presence of pairing always decreases $\langle Q\rangle_{\mathrm{HFB}}$ as compared to the HF value.

IV. RPA RESULTS

In Sec. III, we have seen that the HFB approximation yields spherical shapes for even-$Z<N=28$ nuclei. Hence, excited states for these nuclei can be described in terms of the residual interaction between the quasiparticles of spherical BCS approximation. The first 2^+ excited states for these nuclei can be studied in the RPA.[5] The RPA equations for a system of neutrons and protons are given in the Appendix of this paper.

The excitation energy for the first 2^+ states and reduced transition probability $B(E2)$ between the ground state and the first excited state for these nuclei are given in Table IV, together with the corresponding experimental values. On comparison of these numbers we find that there is good agreement for the excitation energy of the first 2^+ state and for the $B(E2, 0^+\rightarrow 2^+)$ rate agreement is excellent for an effective charge of $0.5e$ or $0.6e$ for neutrons.

TABLE III. Comparison of mass quadrupole moment evaluated from HF and HFB calculations for Ti, Cr, and Fe isotopes. Values are given in units of b^2 ($=4.2\times10^{-26}$ cm^2).

Isotope	$(QP)_{\mathrm{HF}}$	$(QN)_{\mathrm{HF}}$	$(QP)_{\mathrm{HFB}}$	$(QN)_{\mathrm{HFB}}$	Isotope	$(QP)_{\mathrm{HF}}$	$(QN)_{\mathrm{HF}}$	$(QP)_{\mathrm{HFB}}$	$(QN)_{\mathrm{HFB}}$
Ti_{22}^{44}	9.97	9.97	9.97	9.97	Cr_{28}^{52}	9.69	3.98	0.30	0.21
Ti_{24}^{46}	9.79	13.74	9.65	11.81	Cr_{30}^{54}	13.60	12.38	13.55	12.36
Ti_{26}^{48}	8.57	11.94	8.67	9.40	Fe_{26}^{52}	10.42	10.42	10.44	10.44
Ti_{28}^{50}	6.91	4.02	0.08	0.07	Fe_{28}^{54}	8.09	2.83	0.21	0.15
Cr_{24}^{48}	13.87	13.87	13.88	13.88	Fe_{30}^{56}	12.57	11.89	11.58	11.40
Cr_{26}^{50}	12.26	12.04	11.56	11.46	Fe_{32}^{58}	13.06	15.03	12.86	10.17

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TABLE IV. First 2^+ excitation energies (in MeV) and $B(E_2, 0^+\rightarrow 2^+)$ values in units of $10^{-50}\ e^2\ \mathrm{cm}^4$ for even $-Z<N=28$ nuclei.

Isotope	$(E2)_{\text{theoret}}$	$(E2)_{\text{expt}}$	e_n	e_p	$B(E2, 0^+\rightarrow 2^+)_{\text{theoret}}$	$B(E2, 0^+\rightarrow 2^+)_{\text{expt}}$
Ti_{28}^{50}	1.07	1.55	0.5	1.5	3.87	(3.2±0.8)
			0.6	1.6	4.61	
Cr_{28}^{52}	1.02	1.43	0.5	1.5	5.53	(6.7±0.7)
			0.6	1.6	6.54	
Fe_{28}^{54}	1.25	1.41	0.5	1.5	4.92	(5.1±0.5)
			0.6	1.6	5.80	

V. CONCLUSIONS

The main motivation of this paper has been to make a comparison between the HF and HFB self-consistent solutions for the even Ti, Cr, and Fe isotopes. HFB calculation for all these nuclei was performed only with prolate deformations. From the results we have presented here, it is seen that for $N=Z$ nuclei HFB yields normal solutions. For nuclei with $Z<N=28$, the pairing effect is very strong and, as a consequence, the deformed HF shape becomes spherical in the HFB approximation. In all other cases pairing is not so strong and HFB yields deformed shapes. A comparison of the spherical BCS minimum with the corresponding HFB energy minimum shows that the BCS solution is unfavorable for all the cases except for the even $Z<N=28$ nuclei.

The effect of pairing on the binding energy and mass quadrupole moment has been estimated. It is found that the over-all binding energy for the HFB shape is larger than the HF value for all the nuclei where pairing is effective. It is also found that, in the presence of pairing the HF contribution to the binding energy for the HFB shape is small as compared to the binding energy for the HF shape. But the pairing contribution to it is more than sufficient to compensate for this decrease. The presence of pairing always decreases the mass quadrupole moment as compared to the HF value.

RPA results for the spherical nuclei, performed with the effective interaction described in Sec. I, are in good agreement with experimental results.

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APPENDIX: RPA EQUATIONS FOR A SYSTEM OF EVEN NUMBER OF NEUTRONS AND PROTONS

A. BCS Equations

The modified Hamiltonian given by Eq. (10) is

$$\mathcal{H}=\sum_{\alpha}(\epsilon_\alpha-\mu)a_\alpha^\dagger a_\alpha+\tfrac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta\,|\,V_A\,|\,\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma. \tag{A1}$$

We shall adopt the following convention for the symbols:

The Greek letters α, β, γ, δ denote the set of quantum numbers $jm\tau_z$, while the letters a, b, c, d denote all the other quantum numbers except the projection quantum number.

Pairing correlation in the BCS wave function is introduced by performing the following Bogoliubov-Valatin transformation on this Hamiltonian:

$$C_\alpha^\dagger=u_a a_\alpha^\dagger-v_a a_{\bar\alpha},\qquad C_\alpha=u_a a_\alpha-v_a a_{\bar\alpha}^\dagger, \tag{A2a}$$

where $\bar\alpha$ is obtained from α by changing m_a to $-m_a$ and then multiplying it by a phase factor of $(-1)^{j_a-m_a}$. The coefficients u_a and v_a satisfy following condition:

$$u_a^2+v_a^2=1. \tag{A2b}$$

The BCS vacuum corresponding to the quasiparticle operator is given by

$$|\,\Phi_{\text{BCS}}\rangle=\prod_{\frac{1}{2}\alpha}(u_a+v_a a_\alpha^\dagger a_{\bar\alpha}^\dagger)\,|\,0\rangle, \tag{A3}$$

so that

$$C_\alpha\,|\,\Phi_{\text{BCS}}\rangle=0, \tag{A4}$$

and the transformed Hamiltonian takes the following form, after the coefficients of the term containing two quasiparticle creation and annihilation operators have been set equal to zero:

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_{11}+H_{\text{int}}, \tag{A5}$$

where

$$\mathcal{H}_0=\langle\Phi_{\rm BCS}\mid\mathcal{H}\mid\Phi_{\rm BCS}\rangle \tag{A6}$$

and

$$\mathcal{H}_{11}=\sum_\alpha E_a C_\alpha^\dagger C_\alpha. \tag{A7}$$

The last term in the Eq. (A5) is the residual interaction between the quasiparticles and is given by

$$H_{\rm int}=\tfrac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta\mid V_A\mid\gamma\delta\rangle N(a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma), \tag{A8}$$

where the symbol N, as usual, stands for the normal product. The quasiparticle energy E_a appearing in Eq. (A7) is given by

$$E_a=[(\epsilon_{j_a}-\mu_{\tau_z{}^a}+\Gamma_a)^2+\Delta_a{}^2]^{1/2}, \tag{A9a}$$

where

$$\Gamma_a=[1/(2j_a+1)]\sum_b\sum_J(2J+1)G(abab J)v_b{}^2 \tag{A9b}$$

and

$$\Delta_a=\tfrac{1}{2}\sum_{j_b}[(2j_b+1)/(2j_a+1)]^{1/2}\times G(aabb\,J=0\;T=1)u_b v_b. \tag{A9c}$$

$G(abcdJ)$ and $G(abcdJT)$ are related through the Clebsch-Gordan coefficients in the following way:

$$G(abcdJ)=\sum_T\begin{bmatrix}\frac{1}{2} & \frac{1}{2} & T\\ \tau_z{}^a & \tau_z{}^b & T_z\end{bmatrix}\begin{bmatrix}\frac{1}{2} & \frac{1}{2} & T\\ \tau_z{}^c & \tau_z{}^d & T_z\end{bmatrix}G(abcdJT), \tag{A10a}$$

and $G(abcdJT)$ is related to the antisymmetric coupled matrix element.

$$G(abcdJT)=N(ab)N(cd)\langle abJT\mid V_A\mid cdJT\rangle, \tag{A10b}$$

where

$$N(ab)=(1+\delta_{j_a j_b})^{1/2}. \tag{A10c}$$

The values of μ are fixed in such a way that the expectation values of the number operator for the BCS ground-state wave function always gives the desired number of neutrons and protons. The number of neutrons and protons in terms of v are

$$N_{\tau_z}=\sum_{j_a}(2j_a+1)v_a{}^2. \tag{A11}$$

If we define a quantity e_a as

$$e_a=\epsilon_{j_a}-\mu_{\tau_z{}^a}+\Gamma_a, \tag{A12}$$

then the expression for u_a and v_a in terms of e_a and E_a can be written as

$$u_a{}^2=\tfrac{1}{2}(1+e_a/E_a),\qquad v_a{}^2=\tfrac{1}{2}(1-e_a/E_a). \tag{A13}$$

The Eqs. (A9), (A11), and (A13) are the BCS equations.

The residual interaction term, when written explicitly in terms of quasiparticles, is made up to 16 terms which can be arranged in the following way:

$$H_{\rm int}=H_{04}+H_{13}+H_{22}+H_{31}+H_{40}, \tag{A14a}$$

where

$$H_{04}=H_{40}{}^\dagger=\tfrac{1}{4}\sum_{\alpha\beta\gamma\delta}v_a v_b u_c u_d\langle\gamma\delta\mid V_A\mid\bar\alpha\bar\beta\rangle\times C_\alpha C_\beta C_\delta C_\gamma, \tag{A14b}$$

$$H_{13}=H_{31}{}^\dagger=\tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}(u_c u_d u_a v_b\langle\gamma\delta\mid V_A\mid\alpha\bar\beta\rangle+v_a v_b v_d u_c\langle\gamma\bar\alpha\mid V_A\mid\bar\beta\bar\delta\rangle)C_\alpha{}^\dagger C_\beta C_\delta C_\gamma, \tag{A14c}$$

and

$$H_{22}=\tfrac{1}{2}\sum_{\alpha\beta\gamma\delta}[(u_a u_b u_c u_d+v_a v_b v_c v_d)\tfrac{1}{2}\langle\alpha\bar\delta\mid V_A\mid\gamma\bar\beta\rangle-(u_a v_b u_c v_d+v_a u_b v_c u_d)\langle\alpha\bar\delta\mid V_A\mid\gamma\bar\beta\rangle]\times C_\alpha{}^\dagger C_\beta{}^\dagger C_\delta C_\gamma, \tag{A14d}$$

where u and v appearing in (A14) are obtained by solving the BCS equations self-consistently.

B. Equations of Motion for RPA

Denoting by $\omega_J{}^n$ the energy of the nth excited state $\mid\Psi_{JMT}{}^n\rangle$ relative to the ground state, the equations of motion are

$$[\mathcal{H}_{11}+H_{\rm int},\,Q_{JMT}{}^{n\dagger}]\mid\Psi_0\rangle=\omega_J{}^n Q_{JMT}{}^{n\dagger}\mid\Psi_0\rangle=\omega_J{}^n\mid\Psi_{JMT}{}^n\rangle, \tag{A15}$$

where

$$Q_{JMT}{}^{n\dagger}=\sum_{j_a\le j_b,T_z=\pm1}[X_{(ab)}{}^n\mathfrak{A}^\dagger(abJM\;T=1\;T_z)-Y_{(ab)}{}^n\mathfrak{A}(abJ\bar M\;T=1\;T_z)] \tag{A16a}$$

and

$$Q_{JMT}{}^n\mid\Psi_0\rangle=0, \tag{A16b}$$

Ψ_0 is the correlated ground-state wave function (i.e., ground state contains quasiparticle pairs) of the even-even system. $\mathfrak{A}^\dagger$ and $\mathfrak{A}$ are the quasiparticle pair creation and annihilation operators, respectively, and they are defined as

$$\mathfrak{A}^\dagger(abJM\;T=1\;T_z)=-(-1)^{j_a+j_b-J}\mathfrak{A}^\dagger(baJM\;T=1\;T_z)=[N(ab)]^{-1}\sum_{m_a}\begin{bmatrix}j_a & j_b & J\\ m_a & m_b & M\end{bmatrix}C_\sigma{}^\dagger C_\beta{}^\dagger \tag{A17a}$$

and

$$\mathfrak{A}(abJ\bar M\;T=1\;T_z)=(-1)^{J-M}[\mathfrak{A}^\dagger(abJ-M\;T=1\;T_z)]^\dagger. \tag{A17b}$$

The magnitude of T_z is always unity. Quasiparticle pair operators with $T_z=0$ will correspond to neutron-proton quasiparticle pair representing an odd-odd system and hence these are excluded in our basic set of states.

In order to solve the equation of motion for the operator (A16a), one calculates the commutator of

$\mathcal{H}_{11}+H_{\text{int}}$ with $\mathcal{A}^\dagger$ and $\mathcal{A}$, retaining only those terms which are linear in $\mathcal{A}^\dagger$ and $\mathcal{A}$. Clearly, the contributions from H_{13} and H_{31} are neglected in this approximation. The commutator for $\mathcal{A}^\dagger$ is evaluated with the help of Eqs. (A7), (A14b), (A14d), and (A17a) and its value is given below:

$$[\mathcal{H}_{11}+H_{\text{int}}, \mathcal{A}^\dagger(mnJM\ T=1\ T_z)]$$
$$=\sum_{j_a\leq j_b, T_z'=\pm T_z}[A_{(mn)(ab)}\mathcal{A}^\dagger(abJM\ T=1\ T_z')$$
$$+B_{(mn)(ab)}\mathcal{A}(abJ\bar{M}\ T=1\ T_z')]. \quad \text{(A18)}$$

The commutator of $\mathcal{A}(mnJ\bar{M}\ T=1\ T_z)$ is obtained by taking the Hermitian conjugate of (A18) and then reversing the sign, changing M to $-M$ and multiplying the result by the phase factor $(-1)^{J-M}$. The coefficient matrix for all the operators $\mathcal{A}^\dagger$ and $\mathcal{A}$ form the RPA matrix R given as

$$R=\begin{pmatrix} A & B \\ -B & -A \end{pmatrix}, \quad \text{(A19)}$$

where A and B are real and symmetric. The matrix elements of A and B are

$$A_{(mn)(ab)}=(E_m+E_n)\delta_{ma}\delta_{nb}$$
$$+[N(ab)N(mn)]^{-1}[(u_au_bu_mu_n+v_av_bv_mv_n)$$
$$\times G(abmnJ\ T=1)\delta_{T_zT_z'}$$
$$+(u_av_bu_mv_n+v_au_bv_mu_n)F(abmnJ\ T=1)$$
$$-(v_au_bu_mv_n+u_av_bv_mu_n)(-1)^{j_m+j_n-J}$$
$$\times F(abnmJ\ T=1)], \quad \text{(A20a)}$$

$$B_{(mn)(ab)}=[N(ab)N(mn)]^{-1}$$
$$\times[-(u_au_bv_mv_n+v_av_bu_mu_n)$$
$$\times G(abmnJ\ T=1)\delta_{T_zT_z'}$$
$$-(u_av_bu_mv_n+v_au_bv_mu_n)(-1)^{j_m+j_n-J}$$
$$\times F(abnmJ\ T=1)$$
$$+(u_av_bv_mu_n+v_au_bu_mv_n)F(abmnJ\ T=1)], \quad \text{(A20b)}$$

where F and G are related through the U coefficients[6,7] in the following way

$$F(abmnJ\ T=1)$$
$$=-\sum_{J'}(-1)^{j_a+j_b+j_m+j_n}[(2J'+1)/(2J+1)]^{1/2}$$
$$\times U(j_aj_bj_nj_m;JJ')G(anmbJ') \quad \text{(A21)}$$

and

$$F(abmnJ\ T=1)=F(mnabJ\ T=1)$$
$$=(-1)^{j_a+j_b+j_m+j_n}F(banmJ\ T=1). \quad \text{(A22)}$$

The amplitudes X and Y of Eq. (A16a) are obtained from the following matrix equations:

$$R\begin{pmatrix} X^n \\ Y^n \end{pmatrix}=\omega_J{}^n\begin{pmatrix} X^n \\ Y^n \end{pmatrix}, \quad \text{(A23)}$$

and they are so normalized that

$$\langle\Psi_0\mid Q_{JMT=1}{}^nQ_{JMT=1}{}^{n\dagger}\mid\Psi_0\rangle$$
$$=\langle\Psi_0\mid[Q_{JMT=1}{}^n, Q_{JMT=1}{}^{n\dagger}]\mid\Psi_0\rangle=1, \quad \text{(A24)}$$

which gives

$$\sum_{j_a\leq j_b,T_z}[(X_{(ab)}{}^n)^2-(Y_{(ab)}{}^n)^2]=1. \quad \text{(A25)}$$

(This normalization condition is obtained by making the approximation that the average number of quasiparticles in the ground-state wavefunction is small and thus be neglected.[5])

C. Transition Probability

The strength of electric quadrupole transition between the first excited state and the ground state is measured by[8]

$$B(E2, 0^+\rightarrow 2^+)=\sum_{M\mu}\mid\langle\Psi_0\mid\mathfrak{M}(E2,\mu)\mid\Psi_2{}^+{}_M\rangle\mid^2, \quad \text{(A26)}$$

where

$$\mathfrak{M}(E2,\mu)=\sum_{\alpha\beta}e_{\tau_z}\langle\alpha\mid r^2Y_\mu{}^2(\theta,\varphi)\mid\beta\rangle a_\alpha{}^\dagger a_\beta. \quad \text{(A27)}$$

Expressing (A27) in terms of quasiparticles and keeping only the relevant terms, we get

$$\mathfrak{M}(E2,\mu)=\sum_{j_a\leq j_b,T_z(\tau_z)=\pm1}e_{\tau_z}\{\langle j_a\mid\mid r^2Y^2\mid\mid j_b\rangle$$
$$\times[(2j_a+1)/5]^{1/2}(u_av_b+v_au_b)[N(ab)]^{-1}$$
$$\times[\mathcal{A}^\dagger(ab2\mu)+(-1)^M\mathcal{A}(ab2-\mu)]\}, \quad \text{(A28)}$$

where

$$\langle j_a\mid\mid r^2Y^2\mid\mid j_b\rangle=(2j_b+1/4\pi)^{1/2}(-1)^{j_a-1/2}$$
$$\times\begin{bmatrix} j_a & j_b & 2 \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{bmatrix}\int_0^\infty R_a(r)R_b(r)r^4dr. \quad \text{(A29)}$$

R_a and R_b are the oscillator radial wave functions. Substituting (A28) in (A26) and using the result

$$\langle\Psi_0\mid\mathcal{A}^\dagger(ab2\mu)+(-1)^\mu\mathcal{A}(ab2-\mu)\mid\Psi_2{}^+{}_M\rangle$$
$$=(-1)^\mu\delta_{M-\mu}(X_{ab}+Y_{ab}), \quad \text{(A30)}$$

we get for $B(E2, 0^+\rightarrow 2^+)$, the following expression:

$$B(E2, 0^+\rightarrow 2^+)=\mid Q_p+Q_n\mid^2, \quad \text{(A31)}$$

where

$$Q_{\tau_z}=e_{\tau_z}\sum_{j_a\leq j_b}(2j_a+1)^{1/2}\langle j_a\mid\mid r^2Y^2\mid\mid j_b\rangle(u_av_b+v_au_b)$$
$$\times[N(ab)]^{-1}(X_{(ab)}+Y_{(ab)}) \quad \text{(A32)}$$

and e_{τ_z} is the effective nucleon charge.

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