

Generalized Pairing in Light Nuclei. I. Solutions of Hartree-Fock-Bogoliubov Equations in $N=Z$ Even-Even Nuclei*

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The Hartree-Fock-Bogoliubov (HFB) equations are solved for the $N=Z$ even-even nuclei in the s - d shell. The possibility of generalized pairing correlations (e.g. both $T=0$ and $T=1$ pairing) is studied in detail. It is found that the two kinds of pairing are mutually exclusive and that the lowest HFB solution for the even-even $N=Z$ nuclei has $T=0$ independent pairs. The validity and the extent of these correlations is further examined by projecting the solutions onto eigenstates of the total number operator. These $T=0$ pairing correlations occur for the axially symmetric prolate Mg^{24} , oblate S^{32} , and prolate Ar^{36} HFB solutions. In studying the relevance of these HFB solutions to the experimental spectra, it is found that the HFB field gives a more consistent description of the structure of $N=Z$ even-even nuclei and that it can resolve the discrepancies and also the failures of the HF field in the upper half of the s - d shell.

I. INTRODUCTION

BECAUSE of the vast amount of experimental data for the s - d shell nuclei this shell has become a testing area for various models of nuclear structure. One of the most-studied models in this shell is related to the idea of the intrinsic state. The intrinsic state is not the actual state of the nucleus, but rather provides a basis from which physical states can be extracted. The intrinsic-state model was first employed using a harmonic-oscillator potential to calculate deformed single-particle orbitals.^{1,2} Recently the connection between the intrinsic structure of nuclei and the basic two-body interaction has been investigated by utilizing the Hartree-Fock (HF) approximation.³ There have been many studies of the self-consistent fields in s - d shell nuclei. Originally the HF calculations⁴⁻⁶ were performed with an effective central two-body interaction, confining the single-particle space to a single major shell, and thus were quite restricted. More recently, complete HF calculations with a renormalized realistic

interaction and an extended shell-model space have been performed.^{7,8} The majority of these works involve the $N=Z$ even-even nuclei.

The $N=Z$ even-even nuclei are singled out for theoretical study because of the following features. The ground-state equilibrium shapes of Ne^{20} , Mg^{24} , Si^{28} , and S^{32} all seem to be deformed. This suggests that these nuclei can be described in terms of deformed intrinsic states. If the Coulomb force is neglected, proton-neutron exchange and time-reversal become symmetries of the self-consistent field; this produces a considerable simplification in the calculations and in the interpretation of the resulting structure.

A significant aspect of these HF calculations is the existence of a large energy gap between occupied and unoccupied single-particle levels.⁹ This single-particle gap is the main factor in determining the extent to which the HF single-determinant approximation is valid. Its presence leads to a fairly good description of the ground-state rotational spectrum by employing projection or cranking techniques. It should, however, be observed that (1) the HF equations give a large number of solutions for each nucleus, most of which do not have a large gap, (2) the HF solutions underestimate the spacing between the ground and the excited rotational bands in the first half of the s - d shell,

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² M. G. Redlich, Phys. Rev. 110, 468 (1958).

³ F. Villars, in *Proceedings of International School of Physics "Enrico Fermi" Course* (Academic Press Inc., New York, 1963).

⁴ I. Kelson, Phys. Rev. 132, 3189 (1963).

⁵ I. Kelson and C. A. Levinson, Phys. Rev. 134, B269 (1964).

⁶ J. Bar-Touv and I. Kelson, Phys. Rev. 138, B1035 (1965).

⁷ M. K. Pal and A. P. Stamp, Phys. Rev. 158, 924 (1967).

⁸ W. H. Bassichis, A. K. Kerman, and J. P. Svenne, Phys. Rev. 160, 746 (1967).

⁹ J. Bar-Touv and C. A. Levinson, Phys. Rev. 153, 1099 (1967).

(3) recent analysis of experimental data in Mg^{25} suggests that the intrinsic structure of Mg^{24} should be axially symmetric¹⁰ while the preferred HF state is triaxial, and (4) the simple HF picture is completely unable to explain the structure of the upper half of the s - d shell. The presence of HF solutions with small gaps suggests that these solutions are unstable with respect to higher correlations and that dynamically correlated intrinsic states may in fact be necessary to explain experiment.

A natural generalization of the HF self-consistent field method can be made by taking into account pairing correlations. This is known as the Hartree-Fock-Bogoliubov (HFB) method. It has been known for some time that $J=0$ pairing among like nucleons is important for describing heavy nuclei, but also all calculations have assumed that the underlying self-consistent field is not affected by the correlations. This same approximation has been assumed for s - d shell nuclei, but since neutrons and protons are filling the same orbitals, it has been necessary to consider the possibility of proton-neutron pairing.

Several groups have studied $T=1$, $J=0$ charge-independent pairing in light nuclei. Also $T=0$ pairing has been studied and shown to lead to a coherent pair field and hence to a considerable energy-gap in the single-quasiparticle spectrum.¹¹ Recently calculations have been reported which consider the possibility of combined $T=0$ and $T=1$ pairing correlations among the nucleons.^{12,13} However, these calculations were incomplete in the sense that pairing was separated inconsistently from the underlying intrinsic field. This is expected to be particularly important when there is a significant diffuseness of the Fermi surface due to pair correlations. To study this effect we use the HFB method since it treats the HF and the pairing fields on an equal basis.

The first group to perform HFB calculations were Dietrich, Mang, and Pradal.¹⁴ They studied the structure of deformed rare-earth nuclei and also of Mg^{24} , assuming only $J=0$ pairing between like nucleons. Recently, Faessler *et al.*¹⁵ have performed similar calculations for the $1p$ and $2s$, $1d$ shells. These calculations for $N=Z$ nuclei show that this kind of pairing is not an important factor.

In this paper we examine the effect of generalized pairing (including $T=0$ charge-independent pairing) on the HFB self-consistent field. In Sec. II we give details of the formalism and discuss an approximation which allows the separation of the single-particle and

the pairing equations. Section III contains a discussion of the nature of the HFB solutions and the effects of particle number nonconservation. A summary and conclusions are given in Sec. IV.

II. HF AND HFB METHODS

A. Equation of Motion, HF, and HFB Factorizations

We start with the Hamiltonian

$$H = \sum e_{i\mu} C_{i\mu}^\dagger C_{i\mu} + \frac{1}{4} \sum \langle i\mu j\nu | V_a | k\rho l\sigma \rangle C_{i\mu}^\dagger C_{j\nu}^\dagger C_{l\sigma} C_{k\rho}, \quad (1)$$

where $C_{i\mu}^\dagger$, $C_{i\mu}$ are creation and annihilation in the n, l, j, m, μ representation (μ denotes the z component of isospin), e_i denotes the single-particle shell-model energy, and V_a is the two-nucleon interaction.

The commutator of $C_{i\mu}^\dagger$ with H is given by

$$[H, C_{i\mu}^\dagger] = e_{i\mu} C_{i\mu}^\dagger + \frac{1}{2} \sum \langle k\rho l\sigma | V_a | i\mu j\nu \rangle C_{k\rho}^\dagger C_{l\sigma}^\dagger C_{j\nu}. \quad (2)$$

The equation-of-motion method consists in linearizing this equation by using Wick's theorem and neglecting the uncontracted normal product

$$C_{k\rho}^\dagger C_{l\sigma}^\dagger C_{j\nu} = N(C_{k\rho}^\dagger C_{l\sigma}^\dagger C_{j\nu}) + \langle C_{l\sigma}^\dagger C_{j\nu} \rangle C_{k\rho}^\dagger - \langle C_{k\rho}^\dagger C_{j\nu} \rangle C_{l\sigma}^\dagger + \langle C_{k\rho}^\dagger C_{l\sigma}^\dagger \rangle C_{j\nu}. \quad (3)$$

The uncontracted normal product is neglected in both HF and HFB methods. This is reasonable if there is a large energy gap in the single- (quasi) particle spectrum in the HFB and HF representation.

The HF factorization consists in writing

$$C_{k\rho}^\dagger C_{l\sigma}^\dagger C_{j\nu} = \langle C_{l\sigma}^\dagger C_{j\nu} \rangle C_{k\rho}^\dagger - \langle C_{k\rho}^\dagger C_{j\nu} \rangle C_{l\sigma}^\dagger, \quad (4)$$

and is equivalent to minimization of the Hamiltonian in a single determinantal wave function.

The HFB factorization consists in including the extra term $\langle C_{k\rho}^\dagger C_{l\sigma}^\dagger \rangle C_{j\nu}$ from Eq. (3). The major consequence of this is nonconservation of particle-number and isospin. HFB factorization is equivalent to minimization of the Hamiltonian in a BCS wave function—a particular combination of determinants.

B. HF Basis

With HF factorization, the equation of motion becomes

$$[H, C_{i\mu}^\dagger] = \sum_k \mathcal{H}_{i\mu, k\mu} C_{k\mu}^\dagger, \quad (5)$$

where

$$\mathcal{H}_{i\mu, k\mu} = e_i \delta_{ik} + \sum \langle k\mu, l\nu | V_a | i\mu, j\nu \rangle \langle C_{l\nu}^\dagger C_{j\nu} \rangle, \quad (6)$$

which for $N=Z$ nuclei is independent of the isospin index μ . The HF representation is obtained by observing

¹⁰ J. Parikh, Phys. Letters **26**, B607 (1968).

¹¹ A. Goswami and L. S. Kisslinger, Phys. Rev. **140**, B26 (1965).

¹² H. T. Chen and A. Goswami, Phys. Letters **24**, B257 (1967).

¹³ A. L. Goodman, G. L. Struble, and A. Goswami, Phys. Letters **26**, B260 (1968).

¹⁴ K. Dietrich, H. J. Mang, and J. H. Pradal, Phys. Rev. **135**, B22 (1964).

¹⁵ A. Faessler *et al.* (to be published).

that, when one assumes HF factorization, an eigenmode of the system can be written

$$C_{\alpha\mu}^\dagger = \sum_i a_i^\alpha C_{i\mu}^\dagger. \quad (7)$$

The coefficients in the transformation are obtained by solving the eigenvalue equation

$$\mathcal{H}C|\alpha\mu\rangle = \epsilon_\alpha C|\alpha\mu\rangle. \quad (8)$$

The ϵ_α are the HF single-particle energies. The HF total energy is given by

$$E_{\text{HF}} = \langle H \rangle_{\text{HF}} = \frac{1}{2} \sum_\alpha (\langle \alpha | t | \alpha \rangle + \epsilon_\alpha), \quad (9)$$

where

$$\langle i\mu | t | j\nu \rangle = e_i \delta_{ij} \delta_{\mu\nu}. \quad (10)$$

Some assumed general properties of the solutions of the HF equations for even-even $N=Z$ nuclei in the s - d shell are (1) symmetry under the exchange of neutron and proton and (2) time-reversal invariance. Here we define the time-reversed single-particle state as

$$|\bar{\alpha}\rangle = \sum_i a_i^\alpha (-1)^{j_i - m_i} |j_i - m_i\rangle. \quad (11)$$

The HF ground state is the lowest-energy solution of the HF equations. This solution has always been found to possess a large gap between occupied and unoccupied single-particle states. This gap does not allow the building up of a pair field in the BCS sense.

In addition to the ground-state solution, other solutions of the HF equations are found which sometimes differ little in energy. Most of these higher solutions have a less conspicuous single-particle gap and therefore are more susceptible to the inclusion of pairing correlations. We shall consider a self-consistent treatment of pairing based on these HF solutions. The pairing correlations are expected to establish the required gap in the single quasiparticle spectrum and thus bring stability to the new self-consistent field.

C. Treatment of Pair Field and HFB Factorization

We have

$$[H, C_{i\mu}^\dagger] = \sum \mathcal{H}C_{i\mu, k\mu} C_{k\mu}^\dagger + \sum \Delta_{i\mu, k\nu} C_{k\nu}, \quad (12)$$

where

$$\Delta_{i\mu, k\nu} = \frac{1}{2} \sum \langle j\rho, l\sigma | V_\alpha | i\mu, k\nu \rangle \langle C_{j\rho}^\dagger C_{l\sigma}^\dagger \rangle. \quad (13)$$

Similarly we can write the analogous equation of motion for $C_{i\mu}$. The HFB method consists in the self-consistent diagonalization of H in the extended single-particle basis of $C_{i\mu}^\dagger, C_{i\mu}$

$$\begin{pmatrix} \mathcal{H} & \Delta \\ \Delta^\dagger & -\tilde{\mathcal{H}} \end{pmatrix} \quad (14)$$

to obtain the eigenmodes of the system.¹⁶ We shall solve the HFB equations under the following constraints:

The different HF bases obtained when Δ is set equal to zero are assumed to make Δ diagonal in the space-spin part of each of the single-particle orbitals. Also, the pairing matrix is assumed to connect a single-particle operator C_α^\dagger to its time-reversal conjugate $C_{\bar{\alpha}}$. (This follows from the assumed time-reversal invariance of the ground state.) With this assumption the HFB matrix is reduced to 4×4 submatrices, each submatrix belonging to one single-particle orbital.

The HFB submatrix which belongs to an HF orbital α can be written as

$$\begin{pmatrix} \epsilon_\alpha & \Delta_\alpha \\ \Delta_\alpha & -\epsilon_\alpha \end{pmatrix}, \quad (15)$$

where

$$\Delta_\alpha = \begin{pmatrix} \Delta_{pp}(\alpha) & \Delta_{pn}(\alpha) \\ \Delta_{np}(\alpha) & \Delta_{nn}(\alpha) \end{pmatrix}, \quad (16)$$

$$\epsilon_\alpha = \begin{pmatrix} \epsilon_\alpha & 0 \\ 0 & \epsilon_\alpha \end{pmatrix}.$$

By a proper choice of phases we set $\Delta^\dagger = \Delta$. Also we can satisfy the equation $\Delta_{np}(\alpha) = \Delta_{np}^{T=1}(\alpha) + i\Delta_{np}^{T=0}(\alpha)$, as pointed out in Ref. 12. This identification of the real and imaginary parts of Δ_{np} allows us to separate the role of the $T=1$ and $T=0$ forces in a simple manner. The success of the HFB method depends crucially on whether there is an energy gap in the quasiparticle spectrum. There exist the following possibilities for having such a gap.

(1) If $\Delta_{np} = 0$, the eigenvalue problem for the matrix (15) reduces to independent BCS equations for the protons and neutrons, where the quasiparticle energies are

$$E_\alpha = [\epsilon_\alpha^2 + \Delta_{pp}^2(\alpha)]^{1/2} \quad (17)$$

with an energy gap of $\Delta_{pp}(\alpha)$. Note that ϵ_α is measured relative to the chemical potential λ . This possibility arises for heavy nuclei with large neutron excess.

(2) If $\Delta_{pp} = \Delta_{nn} = \Delta_{np}^{T=1} = 0$, then the matrix (15) is again reduced to 2×2 matrices with the energy eigenvalue

$$E_\alpha = [\epsilon_\alpha^2 + \Delta_{np}^{T=0}(\alpha)^2]^{1/2} \quad (18)$$

and an energy gap $\Delta_{np}^{T=0}(\alpha)$. This is the case of isospin pairing.¹¹

(3) $\Delta\Delta^\dagger = \text{constant} \times \mathbf{I}$, \mathbf{I} being the unit matrix. Since $\Delta^\dagger = \Delta$,

$$\Delta^2 = |\det \Delta| \mathbf{I}. \quad (19)$$

¹⁶ M. Baranger, in *1962 Cargese Lectures in Theoretical Physics* (W. A. Benjamin, Inc., New York, 1963).

In this case the energy eigenvalue is given by

$$E_\alpha = [\epsilon_\alpha^2 + |\det \Delta_\alpha|]^{1/2}, \quad (20)$$

with an energy gap of $|\det \Delta_\alpha|^{1/2}$. Since the ground state of most $N=Z$ nuclei has $T=0$, one would like the $T=0$ state to be contained in the intrinsic state without confining the solutions to be eigenstates of T^2 . In analogy to HF where one constrains $\langle \mathbf{J} \rangle$ to be zero, we impose the condition $\langle \mathbf{T} \rangle = 0$; that is, on the average, all components of the isospin vanish in the ground state. We thus guarantee more degrees of freedom in the isotopic-spin coordinates, allowing the possibility of intrinsic states with lower energy. The condition (19) then follows. Note that case 2 is a special case of this more general solution. The gap and number equations in the general case are

$$\begin{aligned} \Delta_{pp}(\alpha) &= -\Delta_{nn}(\alpha) \\ &= \sum \langle \alpha \bar{a} T=1 | V_a | \gamma \bar{\gamma} T=1 \rangle [\Delta_{pp}(\gamma)/E_\gamma], \\ \Delta_{np}^{T=1}(\alpha) &= \sum \langle \alpha \bar{a} T=1 | V_a | \gamma \bar{\gamma} T=1 \rangle [\Delta_{np}^{T=1}(\gamma)/E_\gamma], \end{aligned} \quad (21)$$

$$\begin{aligned} \Delta_{np}^{T=0}(\alpha) &= \sum \langle \alpha \bar{a} T=0 | V_a | \gamma \bar{\gamma} T=0 \rangle [\Delta_{np}^{T=0}(\gamma)/E_\gamma], \\ N=Z &= \sum [1 - (\epsilon_\alpha - \lambda)/E_\alpha], \quad \lambda = \text{chemical potential.} \end{aligned} \quad (22)$$

The generalized Bogoliubov transformation corresponding to this simplified HFB problem is

$$\begin{pmatrix} a_{\alpha 1}^\dagger \\ a_{\alpha 2}^\dagger \\ a_{\bar{\alpha} 1} \\ a_{\bar{\alpha} 2} \end{pmatrix} = \begin{pmatrix} u_\alpha & 0 & -v_\alpha & -v_\alpha' \\ 0 & u_\alpha & -v_\alpha'^* & v_\alpha \\ v_\alpha & v_\alpha' & u_\alpha & 0 \\ v_\alpha'^* & -v_\alpha & 0 & u_\alpha \end{pmatrix} \begin{pmatrix} C_{\alpha p}^\dagger \\ C_{\alpha n}^\dagger \\ C_{\bar{\alpha} p} \\ C_{\bar{\alpha} n} \end{pmatrix}, \quad (23)$$

where u_α and v_α are real and v_α' is complex. The occupation probability of the level α is

$$V_\alpha^2 = v_\alpha^2 + |v_\alpha'|^2. \quad (24)$$

Dietrich *et al.*¹⁴ have shown that, to a good approximation, the principal effect of pairing on the HF degrees of freedom is accounted for in the dispersion of occupation numbers across the Fermi surface. This suggests the following procedure for solving the HFB equations. First solve the HF problem with occupation number of 1 or 0 for a particular orbital; then solve the BCS problem separately to extract improved occupation numbers, solve the HF equations again with these new occupations, and repeat the last two steps until convergence is obtained. The HF equations become

$$\mathcal{H}(V^2) | \alpha \rangle = \epsilon_\alpha | \alpha \rangle \quad (25)$$

with

$$| \alpha \rangle = \sum_i a_i^\alpha(V^2) | i \rangle \quad (26)$$

and

$$\mathcal{H}_{i\mu, k\mu}(V^2) = \epsilon_i \delta_{ik} + \sum \langle i\mu, \alpha\nu | V_a | k\mu, \alpha\nu \rangle V_\alpha^2. \quad (27)$$

The ground-state energy in the HFB approximation can be written as a sum of a HF energy and the pairing energy.

$$\langle H \rangle = E_{\text{HF}} + E_{\text{pair}}, \quad (28)$$

$$E_{\text{HF}} = \frac{1}{2} \sum_\alpha (\langle \alpha | t | \alpha \rangle + \epsilon_\alpha) V_\alpha^2, \quad (29)$$

$$E_{\text{pair}} = 2$$

$$\times \sum_{\alpha > 0} [\Delta_{pp}(\alpha) u_\alpha v_\alpha + \Delta_{np}^{T=1}(\alpha) u_\alpha \text{Re} v_\alpha' + \Delta_{np}^{T=0}(\alpha) u_\alpha \text{Im} v_\alpha']. \quad (30)$$

Note that we have used the same notation for the energy and wave functions of the HF Hamiltonian even when occupation numbers other than zero and one have been used.

III. NATURE OF SOLUTIONS OF HFB EQUATIONS

In this section, we study the general nature of the solutions of the HFB equations for s - d shell $N=Z$ nuclei. To study the major features of the HFB field we use a simple central Rosenfeld two-body interaction with a Yukawa radial shape

$$V = V_0 \frac{e^{-r/a}}{r/a} (0.3 + 0.7 \mathbf{d}_1 \cdot \mathbf{d}_2), \quad (31)$$

$$a = 1.35 \text{ F}, \quad V_0 = 50 \text{ MeV}.$$

This force has been used extensively in earlier HF studies. We confine ourselves to the s - d shell and use an oscillator parameter of 1.65 F. The single-particle part of the Hamiltonian has been chosen to be of the form

$$\epsilon_i = e_0 + \alpha_{1,s} \langle i | \mathbf{1} \cdot \mathbf{s} | i \rangle + \alpha_{1^2} \langle i | \mathbf{1}^2 | i \rangle. \quad (32)$$

In particular, we will refer to the two following cases: $\alpha_{1^2} = 0$ MeV, $\alpha_{1,s} = -2.8$ MeV, and $e_0 = -4.2$ MeV used in Ref. 6 and $\alpha_{1^2} = 0.2$, $\alpha_{1,s} = -2.0$ and $e_0 = -3.3$ MeV corresponding to the experimental single-particle energy spectrum of O¹⁷.

A. Tendency to Higher Symmetry

One major feature of pairing correlations is the tendency toward higher symmetry in the intrinsic wave function. For example, it is well known that $J=0$ pairing correlations are responsible for the spherical shape of a large number of open-shell nuclei.¹⁷ For deformed nuclei in the rare-earth region, pairing correlations lead to axial symmetry.¹⁸

¹⁷ A. Bohr and B. R. Mottelson (in numerous communications).

¹⁸ M. Baranger and K. Kumar, Nucl. Phys. A92, 608 (1967).

TABLE I. HFB solutions corresponding to the axially symmetric prolate shape of Mg^{24} , the axially symmetric oblate shape of S^{32} , and the axially symmetric prolate shape of Ar^{36} . The first column gives the HF single-particle energies in the final state of the HFB convergence. The next six columns give the components of the corresponding HF single-particle wave function in the jm representation. This is followed by the BCS amplitudes u_α and $Im(v_\alpha')$ corresponding to the $T=0$ pairing. The last two columns give the order parameter Δ_α and the quasiparticle energy E_α . For each nucleus the bottom row gives the expectation value of the Hamiltonian split into two parts E_{HF} and E_{pair} . The chemical potential λ and the expectation values of the quadrupole Q_{20} and Q_{40} are also given ($\langle Q_{20} \rangle$ and $\langle Q_{40} \rangle$ are given in arbitrary units).

ϵ_α (MeV)	$1d_{5/2}^{5/2}$	$1d_{1/2}^{5/2}$	$1d_{1/2}^{3/2}$	$2s_{1/2}^{1/2}$	$1d_{-3/2}^{5/2}$	$1d_{-3/2}^{3/2}$	u_α	$Im(v_\alpha')$	Δ_α (MeV)	E_α (MeV)
Mg^{24}										
-17.882		0.687	-0.289	-0.676			0.111	-0.994	1.473	6.659
-12.242					0.965	0.262	0.581	0.814	2.494	2.636
-10.369		0.659	0.646	0.385			0.819	0.573	2.793	2.973
-7.000	1						0.994	-0.110	0.987	4.499
-5.419		-0.326	0.707	-0.628			0.998	-0.056	0.673	6.007
-2.599					-0.262	0.965	0.997	-0.081	1.440	8.907
$E_{HF} = -71.508$ MeV	$E_{pair} = -5.832$ MeV	$E_{HFB} = -77.340$ MeV	$\lambda = -11.389$ MeV	$Q_{20} = 15.311$	$Q_{40} = -5.377$					
S^{32}										
-20.281		0.119	0.001	0.993			0.128	0.992	1.512	5.950
-19.840					0.982	0.191	0.142	-0.990	1.554	5.536
-18.025		0.810	0.578	-0.098			0.182	-0.983	1.343	3.747
-16.790	1						0.393	-0.919	2.371	3.278
-12.872					-0.191	0.982	0.891	0.453	2.272	2.810
-9.565		-0.574	0.816	0.068			0.991	0.137	1.398	5.154
$E_{HF} = -173.600$ MeV	$E_{pair} = -5.231$ MeV	$E_{HFB} = -178.831$ MeV	$\lambda = -14.526$ MeV	$Q_{20} = -19.533$	$Q_{40} = -39.001$					
Ar^{36}										
-23.012		-0.616	0.080	0.783			0.001	0.999	0.008	6.979
-21.659					0.989	0.150	0.001	0.999	0.235	5.449
-21.445		0.787	0.091	0.610			0.030	0.999	0.314	5.239
-19.451	1						0.280	0.960	2.065	3.838
-17.159		-0.022	0.993	-0.119			0.456	0.890	1.311	1.616
-15.424					-0.150	0.989	0.844	0.536	1.685	1.861
$E_{HF} = -232.929$ MeV	$E_{pair} = -3.729$ MeV	$E_{HFB} = -236.658$ MeV	$\lambda = -16.215$ MeV	$Q_{20} = 4.046$	$Q_{40} = -3.432$					

In the s - d shell, HF calculations have shown that the ground HF solution corresponds to axially asymmetric shapes for the nuclei Mg^{24} and S^{32} . The HF equations for a given nucleus usually possess several solutions which often differ very little in the HF energy $\langle H \rangle$. The criterion usually adopted in picking the HF ground state (lowest value of $\langle H \rangle$) is not very reasonable since neglected correlations, for example pairing, would lower the energy of other solutions considerably. Moreover, the reliability of the minimum- $\langle H \rangle$ criterion is further affected by (1) second-order HF energy, (2) rotational energy, and (3) zero-point fluctuation energy. In particular, the first effect is found to be large, about 17% of the first-order HF potential energy.⁸ For Mg^{24} and S^{32} there exist axially symmetric

solutions which differ in $\langle H \rangle$ from the axially asymmetric solutions by about 3 MeV (The axially symmetric HF solutions for S^{32} and Ar^{36} , which favor pairing correlations, are different from the ones given in Ref. 6. These HF solutions are given in Table III). The single-particle HF gaps for these axially symmetric solutions are 3.0 MeV for Mg^{24} and 5.3 MeV for S^{32} . The gaps for the triaxial solutions however are 7.4 and 6.6 MeV, respectively. (These values are for $\alpha_{1,s} = -2.8$ MeV.) The single-particle gap for the triaxial solutions turns out to be large enough to exclude pairing in the BCS sense. This does not mean that pairing correlations do not exist in these cases. The BCS equations are well known to have a cutoff in the build-up of the pairing correlations. The fact that the

TABLE II. The spherical solution for Ne^{20} which displays combined $T=0$ and $T=1$ pairing. The axially asymmetric HF solution went to this solution when the pairing correlations were self-consistently included. The single-particle energies are those used in Ref. (6). Each column represents a jm state. The quantities $V^2(\alpha)$, $\Delta(\alpha)$, and E_α are the total occupation, gap parameter, and quasiparticle energy, respectively. (The unit of energy is MeV.) All quantities are defined in Sec. III.

	$d_{5/2}^{-3/2}$	$d_{5/2}^{1/2}$	$d_{5/2}^{5/2}$	$s_{1/2}^{1/2}$	$d_{3/2}^{1/2}$	$d_{3/2}^{-3/2}$
HF energy	-10.654	-10.584	-10.519	-6.235	-4.065	-3.916
$v_p(\alpha)$	0.373	0.272	0.196	0.058	0.069	0.057
$\text{Re}v_{np}(\alpha)$	0.373	0.272	0.196	0.058	0.069	0.057
$\text{Im}v_{np}(\alpha)$	0.142	0.417	0.528	0.000	0.005	0.018
$V^2(\alpha)$	0.300	0.321	0.355	0.007	0.010	0.007
$\Delta_p(\alpha)$	0.783	0.723	0.693	0.570	0.995	0.827
$\Delta_{np}^{T=1}(\alpha)$	0.783	0.723	0.693	0.570	0.995	0.827
$\Delta_{np}^{T=0}(\alpha)$	0.302	1.128	1.891	0.000	0.073	0.266
$\Delta(\alpha)$	1.148	1.523	2.130	0.806	1.409	1.199
E_α	1.255	1.628	2.224	4.991	7.234	7.343
$\langle H \rangle_{\text{HF}} = -34.618$ $E_{\text{pair}} = -5.119$ $E_{\text{total}} = -39.737$ $\lambda = -11.160$						

pairing correlations are small in the axially asymmetric state is basically due to the fact that axial asymmetry has already taken care of a major part of the dispersion of occupation numbers above the Fermi level relative to the axially symmetric solution.¹⁹ The axially asymmetric solution could also be used as a basis for the inclusion of pairing correlations but at the expense of using more elaborate techniques, namely, by number conserving representations. The defect of such an approach is the nonexistence of simple modes of excitation. The HFB solutions corresponding to the axially symmetric shapes are shown in Table I. After the energy gain by pairing correlations is taken into account along with the rotational energy, the energy $\langle H \rangle$ for the axially symmetric state is comparable to that of the triaxial solution. It will be shown in Sec. III C that the paired solution is likely to be closer to the physical intrinsic state on the basis of comparison with experiment. In this sense only pairing restores axial symmetry to Mg^{24} and S^{32} .

Another example of this tendency toward higher symmetry caused by the pairing correlations occurs for the triaxial HF basis of Ne^{20} . The HFB solution is given in Table II. Notice that the dispersion of occupation numbers due to the pairing correlation is such that all the m states of the $d_{5/2}$ orbital are almost equally occupied, i.e., the intrinsic state has become spherical. The small deviation from sphericity is due to the fact that this solution corresponds to combined $T=0$ and $T=1$ pairing and that $T=0$ pairing inherently implies deformation. It is not known whether this solution corresponds to any physical excited state of Ne^{20} .

¹⁹ J. Bar-Touv and I. Kelson, Phys. Rev. **142**, 599 (1966).

B. Prolate Versus Oblate Shapes

Another feature of the lowest axially symmetric HF solution for the s - d shell is that one gets prolate shapes for the lower half of the shell and oblate shapes for Si^{28} and the upper half. For all s - d shell nuclei there are other HF axially symmetric solutions of opposite shape.

However, in analogy to the competition between axially symmetric and asymmetric shapes, these axial solutions may differ little in $\langle H \rangle$, but one, by virtue of a small gap, may allow extensive pairing correlations. This is the case for Ar^{36} where the prolate and oblate HF solutions differ in $\langle H \rangle$ by only 3 MeV. The single-particle gap for the prolate solution is 2.4 MeV compared to 7.4 MeV for the oblate solution. Consequently, the energy gain due to pairing for the prolate state makes $\langle H \rangle$ closer for the two states. Table I displays the HFB solution corresponding to the prolate state. The physical relevance of the paired solution will be discussed in Sec. III F.

C. Effect of Self-Consistency on HF and Pair Fields

In this section, we shall study the effects of the pair field on the HF field and vice versa. Table III shows the HF wave function for the cases of S^{32} and Ar^{36} with zero pairing and for the final self-consistent HFB solution (the l - s force strength is -2.8 MeV). The change in the HF field due to pairing depends very much on the amount of dispersion of the occupation numbers across the Fermi surface, which in its turn depends on the single-particle gap. In Mg^{24} and S^{32} , where the dispersion is rather small, the change in the HF field due to the pair correlations is small. A significant change, however, occurs in the total HF energy of the system, which

TABLE III. Change of HF wave function due to HFB correlations for axially symmetric oblate state of S^{32} and prolate state of Ar^{36} . For each nucleus the left half of the table gives the pure HF single-particle basis. The right half represents the HF single-particle basis in the final HFB solution; e.g., with HFB occupation. O^{ν} single-particle shell-model energies are used.

ϵ_{α} (MeV)	HF				HF (with HFB occupation)					
	$1d_{5/2}^{s/2}$	$1d_{1/2}^{s/2}$	$2s_{1/2}^{1/2}$	$1d_{-3/2}^{s/2}$	$1d_{5/2}^{s/2}$	$1d_{1/2}^{s/2}$	$2s_{1/2}^{1/2}$	$1d_{-3/2}^{s/2}$		
	S^{32}									
-20.416	0.071	0.002	0.997				0.118	0.993		
-20.001				0.978	0.209			0.981	0.193	
-18.269	0.805	0.591	-0.058				0.809	0.581	-0.096	
-16.257		1.				1.				
-12.848				-0.209	0.978		-0.577	0.814	-0.193	0.981
-9.416	-0.589	0.807	0.040							
	$E_{HF} = -177.293$ MeV				$E_{HF} = -172.926$					
	Ar^{36}									
-23.677	0.739	-0.103	-0.666				0.616	-0.080	-0.783	
-22.060				0.980	0.198				0.989	0.150
-21.575	0.673	0.150	0.724				0.787	0.091	0.610	
-18.414		1.				1.				
-17.528	-0.026	0.983	-0.180				-0.022	0.993	-0.119	
-14.897				-0.198	0.980				-0.150	0.989
	$E_{HF} = -235.966$ MeV				$E_{HF} = -232.933$					

TABLE IV. Variation of properties of the self-consistent field with the single-particle $l \cdot s$ force strength $\alpha_{l \cdot s}$ for Mg^{24} . The dispersion is defined as $\sum_{\alpha > \beta} V_{\alpha\beta}^2$. ΔE_{HF} is the reduction of the HF energy due to the dispersion and A is the inertial parameter defined as $A = \hbar^2/2\mathcal{I}$. The unit of energy is the MeV.

$\alpha_{l \cdot s}$	HF gap	Dispersion	Quasiparticle gap	ΔE_{HF}	E_{pair}	A_{HF}	A_{HFB}
-1.2	0.550	0.408	6.144	2.957	-7.426	0.098	0.318
-1.6	1.111	0.367	5.988	3.317	-6.812	0.111	0.305
-2.0	1.712	0.321	5.801	3.472	-6.031	0.123	0.286
-2.4	2.360	0.268	5.595	3.415	-5.108	0.134	0.265
-2.8	3.065	0.208	5.378	3.066	-4.007	0.146	0.242

decreases because of the dispersion of the occupation numbers to the unoccupied single-particle states of lower binding energy. This loss is more than compensated by the large gain in pairing energy. Moreover, there is an extra gain in the energy of rotation due to a decrease in the moment of inertia (see Sec. III F). In Ar^{36} , where the dispersion is particularly large, the resulting changes in the HF and HFB fields single out Ar^{36} from other $N=Z$ even-even nuclei. (See Sec. III F.)

In order to study the effect of the HF field on pairing, we vary the single-particle $l \cdot s$ force strength. As expected, the decrease of the HF single-particle gap brings an increase in the dispersion across the Fermi surface due to pairing and hence an increase in the pairing energy. Table IV shows the variation of various quantities of the self-consistent fields as a function of $l \cdot s$ force strength. In general, the HFB quantities show a relative stability compared to those of the relevant HF fields. In particular, the quasiparticle gap (the unperturbed energy of the $K=2^+$ state) is significantly stable compared to the abrupt changes of the HF single-particle gap.

It is interesting to notice here that the main effect of using the realistic forces and the extension of the shell-model space to include all lower shells is the reduction of the single-particle HF gap.⁷ This is particularly clear for the axially symmetric HF solutions in Mg^{24} and S^{32} considered in this paper. For example, in Mg^{24} the gap is reduced to 0.5 MeV compared to 3.1 MeV used in this paper.²⁰ By using Table IV it is easy to extrapolate the expected changes in the pairing correlations due to the realistic forces. The *most* significant change, except for the obvious increase in pairing due to the lower HF gap, may well occur in the reduction of HF energy-loss due to pairing, which should be much less than we have found.

D. $T=0$ Versus $T=1$ Pairing

One consistent feature of the generalized pairing solutions for the $N=Z$ even-even nuclei is the mutual exclusion of $T=0$ and $T=1$ pairing; i.e., no physical cases show simultaneous $T=0$ and $T=1$ pairing. This

²⁰ A. P. Stamp, Nucl. Phys. **A105**, 627 (1967).

result does not mean that the $T=1$ ($T=0$) pair correlations are identically zero for $T=0$ ($T=1$) pairing, but, being small, such correlations cannot be accounted for in the BCS approximation. It is well known that BCS solutions go to the trivial ($\Delta=0$) solution in the limit of small Δ .

For the even-even nuclei, due to the large separation of the observed $T=0$ and $T=1$ states, isospin conservation should be important and therefore the $T=0$ pairing solutions should be accepted as the physical solutions. The $T=1$ pairing solution gives an isospin intrinsic state from which one can project the various T states. However, it is unlikely that states separated by ~ 9 MeV could be contained in the same intrinsic state.²¹ For this reason, we disregard the $T=1$ pairing solution. In the $T=0$ pairing picture of the ground state, the $T=1$ states are to be generated as two quasiparticle pairs coupled to $T=1$.

E. Projections onto Eigenstates of the Number Operator

As mentioned in II B the HFB vacuum is not an eigenstate of the number operator. The effects of this approximation have been extensively studied in heavy nuclei where only $T_z=1$ pairing occurs.¹⁴ However such studies have not been performed for $T=0$ pairing and realistic systems with small numbers of nucleons.

The canonical HFB approximation has the conceptual advantage of considering the variational problem in two parts, first solving the Euler-Lagrange equations for the HF degrees of freedom, and then solving the pairing part for the best set of occupation parameters for the HF orbitals. When the solutions to the HFB equations give pure $T=0$ or $T_z=1$ solutions, then the pairing equations result from a variation with the trial wave functions

$$\psi_{T=0} = \prod_{\nu > 0; \tau} [u_{\nu} + (-1)^{1/2-\tau} i v_{\nu} C_{\nu\tau}^{\dagger} C_{\bar{\nu}-\tau}^{\dagger}] |0\rangle, \quad (33)$$

$$\psi_{T_z=1} = \prod_{\nu > 0} (u_{\nu} + v_{\nu} C_{\nu 1/2}^{\dagger} C_{\bar{\nu} 1/2}^{\dagger}) \times \prod_{\nu > 0} (u_{\nu} + v_{\nu} C_{\nu -1/2}^{\dagger} C_{\bar{\nu} -1/2}^{\dagger}) |0\rangle. \quad (34)$$

²¹ B. H. Flowers and M. Vujicic, Nucl. Phys. **49**, 586 (1963).

TABLE V. Cranking moment of inertia parameters ($A_i = 1/2g_i$ in MeV) of the axially asymmetric HF solutions and the HFB axially symmetric solutions for Mg^{24} and S^{32} . In each case the first value presented corresponds to O^{17} single-particle energies, and the second to the single-particle energies given in Ref. 6.

	Mg^{24}				S^{32}			
	Nonaxial		Axial		Nonaxial		Axial	
A_z	0.338	0.236	0.281	0.242	0.387	0.211	0.223	0.259
A_y	0.182	0.208	0.281	0.242	0.509	0.249	0.223	0.259
A_x	0.389	0.541	∞	∞	0.471	0.405	∞	∞

In these restricted cases the u 's and v 's may be taken to be real numbers. Since all physically interesting solutions for even-even nuclei have $T=0$, we shall present the relevant equations for the $T=0$ case only.

Having written a trial wave function for the number nonconserving part of the variational problem, we can correct the defect by projecting out that part of ψ which contains the proper number of nucleon pairs. We may express this formally as

$$\psi_{T=0} = C \oint d\xi \xi^{-n_0-1} \prod_{\nu>0;\tau} [\mathcal{U}_\nu + \xi(-1)^{1/2-\tau} v_\nu C_{\nu\tau}^\dagger C_{\nu-\tau}^\dagger] |0\rangle, \quad (35)$$

where C is the normalization constant and is given by

$$|C|^2 = -1/(4\pi^2 R_0^0), \quad (36)$$

n_0 is the number of neutron proton pairs, and the

$$R_n^N(\nu_1, \dots, \nu_N) = (2\pi i)^{-1} \oint dz z^{-(n_0-n)-1} \times \prod_{\nu \neq \nu_1, \dots, \nu_N} (\mathcal{U}_\nu^2 + z\nu_\nu^2)(\mathcal{U}_\nu^2 + z\nu_\nu^2), \quad (37)$$

and are called residuum integrals. Taking the expectation value of (1) in (35), we find the energy is given by

$$E = \sum_\nu \bar{\epsilon}_\nu v_\nu^2 R_1^1(\nu)/R_0^0 + \sum_{\nu\nu'} H_{\nu\nu'} v_\nu^2 v_{\nu'}^2 R_2^2(\nu\nu')/R_0^0 + \sum_{\nu\nu'} P_{\nu\nu'} \mathcal{U}_\nu v_\nu \mathcal{U}_{\nu'} v_{\nu'} R_1^2(\nu\nu')/R_0^0, \quad (38)$$

where

$$\bar{\epsilon}_\nu = 4\langle \nu | t | \nu \rangle + \langle \nu\bar{\nu} | V_a | \nu\bar{\nu} \rangle_{T=0}, \quad (39)$$

$$H_{\nu\nu'} = 3[\langle \nu\nu' | V_a | \nu\nu' \rangle_{T=1} + \langle \nu\bar{\nu}' | V_a | \nu\bar{\nu}' \rangle_{T=1}],$$

$$+ [\langle \nu\nu' | V_a | \nu\nu' \rangle_{T=0} + (-1)^{\delta_{\nu\nu'}} \langle \nu\bar{\nu}' | V_a | \nu\bar{\nu}' \rangle_{T=0}], \quad (40)$$

and

$$P_{\nu\nu'} = 2\langle \nu\bar{\nu}' | V_a | \nu\bar{\nu}' \rangle_{T=0} (1 - \delta_{\nu\nu'}). \quad (41)$$

Variation of the energy with respect to the v 's gives the set of equations

$$(\bar{\epsilon}_\alpha + \Gamma_\alpha + \Lambda_\alpha) u_\alpha v_\alpha + \frac{1}{2} \Delta_\alpha (u_\alpha^2 - v_\alpha^2) = 0, \quad (42)$$

where

$$\bar{\epsilon}_\alpha = \frac{1}{2} \bar{\epsilon}_\alpha R_1^1(\alpha)/R_0^0, \quad (43)$$

$$\Gamma_\alpha = \sum_{\nu} H_{\alpha\nu} v_\nu^2 [R_2^2(\nu\alpha)/R_0^0], \quad (44)$$

$$\Delta_\alpha = \sum_{\nu} P_{\alpha\nu} \mathcal{U}_\nu v_\nu [R_1^2(\nu\alpha)/R_0^0], \quad (45)$$

$$\Lambda_\alpha = \frac{1}{4} \sum_{\nu} \sigma(\alpha\nu) \bar{\epsilon}_\nu v_\nu^2 \{ [R_2^2(\nu\alpha) - R_1^2(\nu\alpha)]/R_0^0 \} + \frac{1}{4} \sum_{\nu\nu'} \sigma(\alpha\nu\nu') H_{\nu\nu'} v_\nu^2 v_{\nu'}^2 \times \{ [R_3^3(\nu\nu'\alpha) - R_2^3(\nu\nu'\alpha)]/R_0^0 \} + \frac{1}{4} \sum_{\nu\nu'} \sigma(\alpha\nu\nu') P_{\nu\nu'} \mathcal{U}_\nu v_\nu \mathcal{U}_{\nu'} v_{\nu'} \times \{ [R_2^3(\nu\nu'\alpha) - R_1^3(\nu\nu'\alpha)]/R_0^0 \} - \frac{1}{2} E \{ [R_1^1(\alpha) - R_0^1(\alpha)]/R_0^0 \},$$

$$\sigma(\alpha\nu_1 \dots \nu_N) = 4, \quad \alpha \neq \{\nu_1 \dots \nu_N\}$$

$$= 2, \quad \alpha = \nu_i, \nu_i \subset \{\nu_1 \dots \nu_N\}$$

$$= 0, \quad \alpha = \nu_i = \nu_j, \nu_i, \nu_j \subset \{\nu_1 \dots \nu_N\}.$$

As in the BCS equations, the potentials in (42) depend on the solutions and so they must be obtained by an iterative procedure. The solutions to these equations will be discussed in more detail in a future publication. Therefore, only one numerical example is presented here.

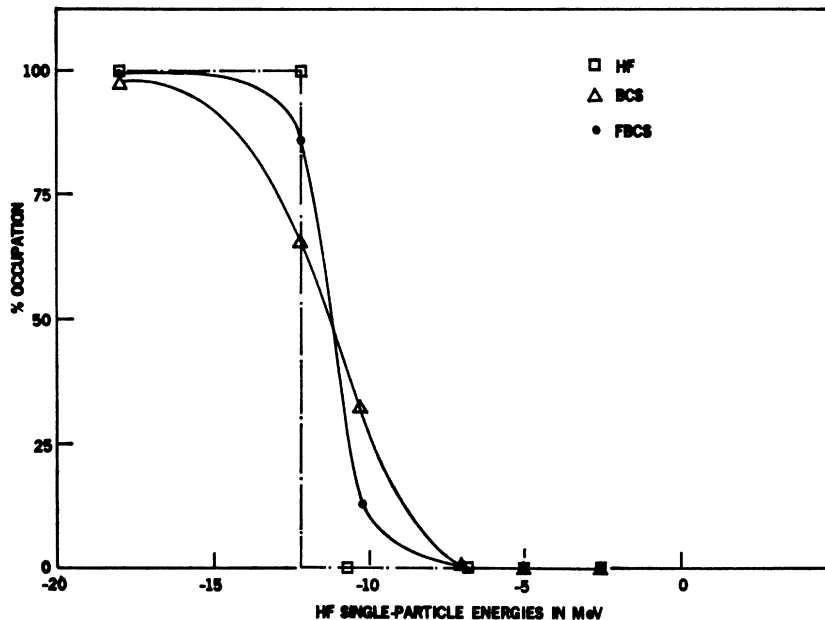
Previous investigations suggest that certain features are to be expected from such an approach:

(1) If we choose as the initial guess the solution to (15), then for the first iteration, (42) describes the BCS solution with the correct particle number projected out (PBCS). The solutions to (42) are always lower in energy than this solution (FBCS).

(2) No matter how large the HF gap or how weak the pairing interaction, there are nontrivial solutions to (42).

(3) In the limit, where BCS predicts uniform occupation (strong pairing), FBCS gives smaller dispersion while in the limit where BCS gives the trivial solution (weak pairing), the FBCS will always give finite dispersion.

FIG. 1. Occupation of the fourfold degenerate single-particle states of Mg^{24} for the HF and HFB (BCS) solutions, and for the projected eigenstate of the total number operator.



In order to illustrate the effects of number conservation, we will examine Mg^{24} , using the prolate HF solution (see Table I) for the single-particle basis, and the $T=0$ pairing solution as the initial guess for Eqs. (42). The HF energy is -74.605 MeV which is to be compared to -77.340 MeV for BCS, -76.430 MeV for PBCS, and -76.952 MeV for FBCS. In Fig. 1, we show the effect on the occupation of the six fourfold degenerate orbitals [see (7)].

Referring to this FBCS solution as a typical example for $N=Z$ even-even nuclei, we observe that the considerable gain in ground-state energy due to $T=0$ independent pairs is preserved in the good N scheme. This demonstrates that the HFB results are not seriously vitiated by the mixing of neighboring nuclei. It should be noted, however, that the dispersion is substantially reduced by number projection. For expectation values of operators sensitive to the occupation numbers (e.g., stripping spectroscopic factors), this result implies that projection is crucial. However, the number projection does *not* bring new dynamical correlations, hence the HFB solution is a good intrinsic state and reproduces ground-state properties.

F. Moment of Inertia

In this section, we shall discuss the effect of pairing correlations on the value of the moment of inertia given by the cranking model. The results of HF calculations (with $1\cdot s$ force strength of -2.8 MeV) give fair agreement with the experimental value for Ne^{20} and also for Mg^{24} when allowance is made for axial asymmetry.

It has been mentioned that with the two-body force used in this paper, pairing correlations do not build up

for Ne^{20} and Si^{28} . We shall therefore confine our discussion to Mg^{24} , S^{32} , and Ar^{36} . With the HFB wave function, the moment of inertia is given by

$$\mathfrak{J} = 2 \sum_{\alpha > 0; \text{all } \alpha} \frac{|\langle \alpha | j_x | \alpha' \rangle|^2}{E_\alpha + E_{\alpha'}} (u_\alpha | V_{\alpha'} | -u_{\alpha'} | V_\alpha |)^2.$$

HFB correlations on the axially symmetric HF basis already given in Secs. I and II for all Mg^{24} , S^{32} , and Ar^{36} tend to decrease the moment of inertia significantly. Table IV shows the effect of pairing on the moment-of-inertia parameter ($A = \hbar^2/2\mathfrak{J}$) for the axially symmetric state of Mg^{24} for different values of the $1\cdot s$ strength. The HF and the HFB moment-of-inertia parameters show opposite trends with regard to $\alpha_{1,s}$. For the value of $\alpha_{1,s}$ which corresponds to the $O^{17} 1\cdot s$ splitting, the ratio between the HFB and the HF values is more than 2 and, as expected, this ratio should drop to 1 when the increased $1\cdot s$ strength reproduces a HF gap large enough to suppress the pairing correlations. A comparison between the moment-of-inertia parameters of the unpaired axially asymmetric HF solutions and the corresponding axially symmetric HFB solution for Mg^{24} and S^{32} for the two choices of shell-model single-particle energies used in the present study is given in Table V. A comparison of these values with those presented in Fig. 2 for $\alpha_{1,s} = -2.8$ MeV reflects more stability for the HFB moments of inertia than for the HF asymmetric values.

The HFB results (including the limiting cases of zero pairing for Si^{28} and Ne^{20}) for the moment-of-inertia parameter are shown in Fig. 2 along with the experimental values. The experimental values of Ne^{20} , Mg^{24} , and Ar^{36} have been chosen as average values calculated

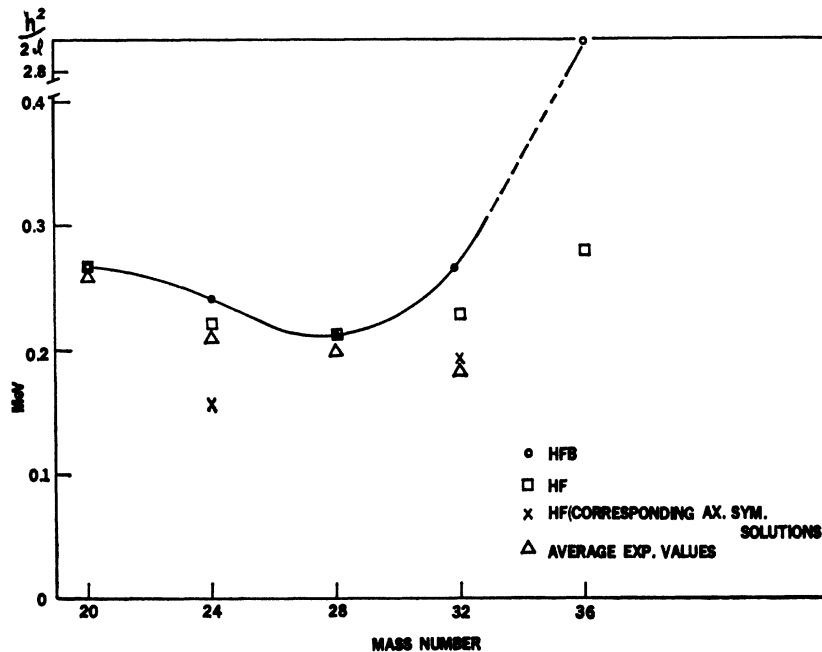


FIG. 2. Moment of inertia parameter $h^2/2J$ as function of the mass parameter for present HFB calculations. For comparison the HF results of Ref. 6 including the corresponding axially symmetric solutions of Mg^{24} and S^{32} and the average experimental values are shown.

from $0+ -2+$ and $2+ -4+$ spacing. The values for Si^{28} and S^{32} are extracted from the $2+ -4+$ spacing only. The $0+$ states of these two nuclei are lowered to their observed positions by their interaction with the first excited $0+$ states which correspond to spherical states observed at 4.97 and 3.78 MeV, respectively, in these two nuclei.²²⁻²⁴ The theoretical HFB values for the moment-of-inertia parameter are always overestimated, which is particularly desirable because of the expected reduction of the cranking estimate due to the Peierls correction,²⁵ which is not included here.

The preference of the HFB axially symmetric solution over the unpaired HF axially asymmetric solution for Mg^{24} suggested in the present study is supported by experimental data on stripping spectroscopic factors²⁶ and also the γ -branching ratio²⁷ of Mg^{25} . These experimental data in Mg^{25} favor an axially symmetric shape for the Mg^{24} even-even core. Also the HF asymmetric rotation of Mg^{24} underestimates the spacing between the ground-state $K=0$ rotational band and the first

$K=2$ excited band by at least 1 MeV. The HFB unperturbed $K=2$ band head, being related to the lowest $K=2$ two quasiparticle state, overestimates this spacing by about 1 MeV (see Table IV). This is favorable because of expected lowering by the residual interaction between the quasiparticles of the $K=2$ subspace.

In Ar^{36} the cranking value of the moment-of-inertia parameter is found to be 2.83 MeV for the paired prolate state. Such a high value implies that the excitation energy of the rotational states is much bigger than that of the vibrational states of the almost spherical Ar^{36} . Experimentally, the Ar^{36} spectrum resembles a pure vibrational spectrum. However a close check of experimental $BE2$ ratios reveals a large amount of anharmonicity, which is characteristic of a transitional nucleus.

Apart from the pairing-energy gain already mentioned, the significant increase of the HFB moment-of-inertia parameter brings another considerable energy gain caused by large rotational energy. The energy of the $J=0$ band head is given as $E(J=0) = \langle H \rangle - A \langle J^2 \rangle$ (the value of $\langle J^2 \rangle$ does not change appreciably). Thus the rotational energy gain [$\sim (A_{HFB} - A_{HF}) \langle J^2 \rangle$], with a proper choice of $I \cdot s$ strength, could be considerable and thus bring the axially symmetric paired solution and the unpaired axially asymmetric solution closer.

IV. SUMMARY AND CONCLUSIONS

We have considered the effect of generalized pairing correlations in the $N=Z$ even-even nuclei of the $s-d$ shell by approximate solution of the HFB equations.

²² J. Bar-Touv and A. Goswami, Phys. Letters **28**, B391 (1968).

²³ The reference to S^{32} as being deformed in the ground state may not be apparent from the energy spectrum alone. However, the large similarity of the angular correlation pattern of the pp' reaction (Ref. 24) in S^{32} and in Si^{28} (whose ground-state deformation is apparent from the clear rotational nature of its low-lying spectrum) suggests that S^{32} can also be considered deformed. However, there is a particularly big component of the spherical state in the S^{32} ground state.

²⁴ G. Crawley and G. Garvey, Phys. Rev. **160**, 981 (1967).

²⁵ R. Peierls and J. Yoccoz, Proc. Phys. Soc. (London) **A70**, 381 (1957).

²⁶ B. Cujec, Phys. Rev. **136**, B1305 (1964).

²⁷ G. J. McCallum and B. D. Sowerby, Phys. Letters **25**, B109 (1967).

It is well known that the HF equations give several solutions. The usual way of choosing one of these solutions (take the lowest value of $\langle H \rangle$) is not adequate because they differ often only slightly (about 1% of the first-order potential energy), whereas the second-order HF potential energy is $\sim 17\%$ of the first-order potential energy. Moreover, the energy fluctuation $\langle H^2 \rangle - \langle H \rangle^2$ in the lowest HF solution as well as the higher one is large except for the Ne^{20} axially symmetric state.²⁸ This shows that even the lowest HF solutions are not good approximations to the actual ground state of the system. In view of this, we assert that the HF solutions should be regarded only as bases for further calculations, for example those which include pairing correlations. Only when the higher correlations have been taken into account and the energy calculated to all significant orders can one make a reasonable choice of the proper solution. Alternatively one can try to make a selection on the basis of experimental data.

In this paper, we attempt to study the broad features of the HFB field with the usual choice of truncated s - d shell space and phenomenological effective two-body interaction. The HFB solutions thus derived have been compared with the HF solutions and also with the experimental data. More detailed considerations are under investigation and will be presented in a future publication.

The solutions of the HFB equations are obtained by constraining the pairing matrix Δ to be diagonal in the HF basis (only in the space-spin variables). We have restricted ourselves to $N=Z$ even-even nuclei where the further constraint $\langle \mathbf{T} \rangle = 0$ has been imposed. Further, for the $N=Z$ even-even nuclei, only $T=0$ pairing solutions are discussed on physical grounds. The major results of the work are as follows: (1) Pairing favors axially symmetric solutions in Mg^{24} (prolate) and S^{32} (oblate). The inclusion of pairing correlations restores the energy gap for the axially symmetric solution, which is essential for the stability of any single-particle basis. Further the pairing energy along with the gain in the rotational energy due to the decrease of the moment of inertia make the ground-state energies ($E_{J=0}$) of the axially symmetric state comparable to that of the axially asymmetric state, even in the first order. In view of the somewhat smaller energy gap the axially symmetric solution may also be

²⁸ M. K. Banerjee (private communication).

expected to gain more second-order potential energy. (2) With the inclusion of pairing for Mg^{24} and S^{32} , the over-all picture for the cranking moment of inertia seems to be in better agreement with experiment. The overestimate of the moment-of-inertia parameter ($A = \hbar^2/2\mathcal{I}$) found in all the cases is encouraging in view of Peierls correction to cranking. (3) For Ar^{36} we have shown that the pairing correlations favors the prolate state. Moreover, deformation of the prolate state is decreased considerably by the pairing correlations. Thus the moment of inertia decreases to the extent that the energy of the $2+$ rotational state becomes higher than the expected energy of the $2+$ vibrational state. Ar^{36} , therefore, seems to belong to the group of transitional nuclei. Experimentally Ar^{36} shows a vibrational spectrum with a large anharmonicity, which is characteristic of a transitional nucleus. The oblate state which corresponds to a $\Delta=0$ solution of the HFB equation does not agree with experimental data.

Many questions, however, remain unanswered. The role of realistic forces and an extended basis has to be examined. In particular, it is well known that the tensor forces play an important role in determining the strength of the effective $T=0$ central force which is important for the isospin pairing field. In this extended scheme one should calculate the binding energy to at least the second order for a choice between the various HFB solutions.

A detailed study of the one and two quasiparticle spectra, including the rotation particle coupling, will be important. Also it will be interesting to see how the $T=1$ and higher- T excited states are to be described, i.e., are they two or more quasiparticle states or does one have to generate them by constraining the isospin to take on prescribed values when solving the HFB equations. Some of these questions are expected to be answered in the near future.

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