1.D.2 Nuclear Physics A230 (1974) 466–476; 

# SELF-CONSISTENT SYMMETRIES OF THE HARTREE-FOCK-BOGOLIUBOV EQUATIONS IN A ROTATING FRAME†

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Received 1 April 1974

**Abstract:** The self-consistent symmetries $\sigma_x$ (reflection through the $yz$ plane) and $TR_z(\pi)$ and their eigenfunctions are employed to reduce the dimension of the Hartree-Fock-Bogoliubov equations in a rotating frame by a factor of two. In the canonical or BCS representation, $\sigma_x$ maps each single-particle orbital into itself.

## 1. Introduction

Several rare earth nuclei exhibit energy spectra at high angular momenta which deviate from the usual variable moment of inertia model [1]). These deviations are most dramatically presented in graphs of the moment of inertia as a function of the square of the angular frequency, sometimes producing the "backbending" phenomenon [2]).

The Hartree-Fock-Bogoliubov (HFB) theory [3,4]) coupled with the cranking model [5,6]) provides a good method for detailed investigations of this high spin behavior. The deformation of the nucleus, the Coriolis antipairing effect [7]), and the re-alignment mechanism [8]) all compete in a self-consistent fashion.

Banerjee, Mang and Ring [9]) have solved the HFB equations with cranking for several rare earth nuclei using a pairing plus quadrupole force. They obtain qualitative agreement with experiment. Bhargava and Thouless [10,11]) find that higher components of the particle-particle channel coupled angular momentum of the nucleon-nucleon potential must be included to obtain better agreement with experiment. The latter HFB calculation is restricted to the $1h_{\frac{11}{2}}$ level.

It is a formidable task to solve the HFB cranking equations with an interaction more realistic than the pairing plus quadrupole force in a model space which is not unduly truncated. Such a realistic calculation is difficult because the cranking term, $-\omega J_x$, does not commute with many of the symmetries of the nucleon-nucleon interaction. This loss of symmetry increases the dimension of the HFB equations. The purpose of this article is to find the self-consistent symmetries of the HFB cranking Hamiltonian, and to use these symmetries to reduce the dimension of the eigenvalue problem. Consequently, a realistic calculation would become more feasible.

† Supported in part by the National Science Foundation.

In a non-rotating frame the paired single-particle orbitals of a doubly even nucleus are degenerate in energy and related by time reversal. The cranking term removes all degeneracy in quasi-particle and HF single-particle energies, thereby eliminating any obvious identification of the paired single-particle orbitals. The nature of the paired orbitals in a rotating frame is investigated.

## 2. Theory

### 2.1. REVIEW OF HFB THEORY

The Hamiltonian is

$$H = \sum_{ij} \langle i|T|j\rangle C_i^\dagger C_j + \tfrac{1}{4}\sum_{ijkl} \langle ij|v_a|kl\rangle C_i^\dagger C_j^\dagger C_l C_k, \tag{1}$$

where $T$ is the kinetic energy and $v$ is an effective nucleon-nucleon interaction. The cranking model for number non-conserving wave functions replaces $H$ by

$$H' = H - \lambda N - \omega J_x, \tag{2}$$

where the angular frequency $\omega$ is adjusted so that

$$\langle J_x\rangle = \sqrt{J(J+1)}, \tag{3}$$

and the chemical potential $\lambda$ is adjusted so that the number operator $N$ has the correct expectation value.

The quasi-particle transformations

$$a_i^\dagger = \sum_j (U_{ij} C_j^\dagger + V_{ij} C_j), \tag{4}$$

are chosen so that $H'$ is approximately described by an independent quasi-particle Hamiltonian. That is,

$$H' = E_0' + \sum_i E_i a_i^\dagger a_i + H_{\text{int}}, \tag{5}$$

where $E_i$ are the quasi-particle energies and $H_{\text{int}}$ is the neglected quasi-particle interaction. Equating (2) and (5) results in the HFB equations appropriate for a rotating frame

$$\begin{pmatrix} (\mathscr{H} - \omega J_x) & \Delta \\ -\Delta^* & -(\mathscr{H} - \omega J_x)^* \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ V \end{pmatrix}. \tag{6}$$

This energy matrix is referred to as the HFB Hamiltonian. The HF Hamiltonian, the HF potential, and the pair potential are defined by

$$\mathscr{H}_{ij} = (T - \lambda + \Gamma)_{ij}, \tag{7}$$

$$\Gamma_{ij} = \sum_{kl} \langle ik|v_a|jl\rangle \rho_{lk}, \tag{8}$$

$$\Delta_{ij} = \tfrac{1}{2}\sum_{kl} \langle ij|v_a|kl\rangle t_{kl}. \tag{9}$$

The density matrix and the pairing tensor are

$$\rho_{ij} = \langle \Phi_0 | C_j^\dagger C_i | \Phi_0 \rangle = (V^\dagger V)_{ij}, \tag{10}$$

$$t_{ij} = \langle \Phi_0 | C_j C_i | \Phi_0 \rangle = (V^\dagger U)_{ij}, \tag{11}$$

where $|\Phi_0\rangle$ is the quasi-particle vacuum.

### 2.2. SYMMETRY IN A ROTATING FRAME

An operator $S$ is defined to be a self-consistent symmetry (SCS) if $S$ commutes with the HFB Hamiltonian [see (6)]. Let $S$ be a unitary or antilinear unitary operator which maps the single-particle space into itself. Sufficient conditions for $S$ to be a SCS are that:

(i) The Hamiltonian (2) is invariant with respect to the symmetry operation

$$[H', S] = 0. \tag{12}$$

(ii) The quasi-particle vacuum is invariant up to a phase under the symmetry operation

$$S|\Phi_0\rangle = e^{i\phi}|\Phi_0\rangle. \tag{13}$$

The HFB equations achieve self-consistency by an iterative process. If the trial wave function employed at the first iteration contains a SCS, then that symmetry will propagate through to the final self-consistent wave function. Consequently, introduction of a SCS does restrict the generality of the wave function. However, dynamical arguments may suggest that, for reasonable forces, the HFB absolute minimum will contain a particular SCS. That is, even though the trial wave function has no SCS, certain symmetries may be recovered when the iteration process is completed.

The symmetry properties of the HF density of doubly even $N = Z$ nuclei in a non-rotating frame have been investigated by Banerjee, Levinson and Stephenson [12]. They find that two features of effective shell-model interactions, *viz*, the general exchange nature and the short range, suggest that $\rho$ contains the following SCS:

(a) time-reversal, $T$;

(b) reflection through a plane, e.g., the $yz$ plane; $\sigma_x = P\,e^{-i\pi J_x}$;

(c) rotation by $\pi$ about an axis in the plane of reflection symmetry, e.g., the $z$-axis; $R_z(\pi) = e^{-i\pi J_z}$;

and by implication,

(d) parity, $P$.

The HF density is defined to have triaxial symmetry if it is invariant with respect to rotation by $\pi$ about the $x$-, $y$- and $z$-axes and reflection through the $xy$, $yz$ and $xz$ planes. The symmetries $\sigma_x$, $R_z(\pi)$, and $P$ are sufficient conditions for triaxial symmetry. For $N \neq Z$ doubly even nuclei it is reasonable to assume that the HF density in a non-rotating frame will also be triaxial and time-reversal invariant.

The Hamiltonian in a rotating frame contains inertial forces, that is, the Coriolis and centrifugal forces. The cranking term $-\omega J_x$ describes these two forces [2]. The operator $J_x$ violates many of the symmetries of $H$ (eq. (1)). For instance,

$$R_y(\pi) J_x R_y^{-1}(\pi) = -J_x, \qquad R_z(\pi) J_x R_z^{-1}(\pi) = -J_x, \tag{14}$$

$$\sigma_y J_x \sigma_y^{-1} = -J_x, \qquad \sigma_z J_x \sigma_z^{-1} = -J_x, \tag{15}$$

$$T J_x T^{-1} = -J_x. \tag{16}$$

Therefore, densities calculated from the cranking Hamiltonian (2) are neither time-reversal invariant nor triaxially symmetric.

The symmetries preserved by $J_x$ are

$$[J_x, R_x(\pi)] = [J_x, \sigma_x] = [J_x, P] = 0. \tag{17}$$

Since $\sigma_x = PR_x(\pi)$, only two of these three symmetries are independent. Because $T$ and $R_z(\pi)$ each anti-commute with $J_x$, the product $TR_z(\pi)$ commutes with $J_x$,

$$[J_x, TR_z(\pi)] = 0. \tag{18}$$

The operators $\sigma_x$ and $TR_z(\pi)$ differ only in that $\sigma_x$ is linear while $TR_z(\pi)$ is antilinear. The first sufficient condition (12) for a SCS is satisfied by

$$[H', \sigma_x] = [H', TR_z(\pi)] = [H', P] = 0. \tag{19}$$

Parity is a SCS in the rotating frame. The HFB Hamiltonian is block diagonalized by $P$. The details are identical with the non-rotating case and will not be repeated here.

Let $|k\rangle$ denote the spherical single-particle basis $|nljm\tau\rangle$, where $m$ is the projection of $j$ on the $z$-axis. The operator $J_x$ is not block diagonal with respect to $m$. Therefore, even if $\sigma_x$ or $TR_z(\pi)$ is employed as a symmetry, the HFB Hamiltonian will not be block diagonal if it is expressed in the basis $|k\rangle$. No reduction in the dimension of the eigenvalue equation occurs.

A new basis must be defined to take advantage of these symmetries. Restrict $|k\rangle$ to states where $m-\frac{1}{2}$ is an even integer. Let $|\bar{k}\rangle \equiv T|k\rangle$. The phase convention is $T|nljm\tau\rangle = (-1)^{j-m+l}|nlj{-m}\tau\rangle$. Define the single-particle basis $|K\bar{K}\rangle$ by

$$\begin{pmatrix} C_K^\dagger \\ C_{\bar{K}}^\dagger \end{pmatrix} = \sqrt{\tfrac{1}{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} C_k^\dagger \\ C_{\bar{k}}^\dagger \end{pmatrix}. \tag{20}$$

Note that $|\bar{K}\rangle = T|K\rangle$. The operator $\sigma_x$ maps the basis $|K\bar{K}\rangle$ into itself,

$$\sigma_x \begin{pmatrix} C_K^\dagger \\ C_{\bar{K}}^\dagger \end{pmatrix} \sigma_x^{-1} = i \begin{pmatrix} -C_K^\dagger \\ +C_{\bar{K}}^\dagger \end{pmatrix}. \tag{21}$$

The states $|K\rangle$ and $|\bar{K}\rangle$ are eigenvectors of $\sigma_x$ with eigenvalues, respectively, of $-i$ and $i$. Since $J_x$ and $\sigma_x$ commute (17), all matrix elements of their commutator are zero. In particular

$$\langle K|[J_x, \sigma_x]|\bar{K}'\rangle = \langle K|J_x|\bar{K}'\rangle\langle\bar{K}'|\sigma_x|\bar{K}'\rangle - \langle K|\sigma_x|K\rangle\langle K|J_x|\bar{K}'\rangle = 2i\langle K|J_x|\bar{K}'\rangle, \tag{22}$$

so that

$$\langle K|J_x|\bar{K}'\rangle = 0. \tag{23}$$

This result is an example of the general theorem that if two normal operators $A$ and $B$ commute, then there are no matrix elements of $B$ between eigenstates of $A$ belonging to different eigenvalues of $A$. Recalling that $|k\rangle$ has $m-\frac{1}{2}$ equal to an even integer, and using (16) and (20), eq. (23) may be directly verified. The non-zero matrix elements of $J_x$ are

$$\langle K|J_x|K'\rangle = -\langle\bar{K}|J_x|\bar{K}'\rangle = \langle k|J_x|\bar{k}'\rangle. \tag{24}$$

In this representation $J_x$ is block diagonal:

$$J_x = \begin{pmatrix} j_x & 0 \\ 0 & -j_x \end{pmatrix}, \tag{25}$$

where $(j_x)_{KK'} \equiv (J_x)_{KK'}$.

The quasi-particle transformation (4) is restricted by the symmetry invariance of the wave function (13). Eq. (21) indicates that $C_K^\dagger$ and $C_{\bar{K}}$ transform similarly with respect to $\sigma_x$. The quasi-particle operators can therefore be chosen as

$$\begin{aligned} a_i^\dagger &= \sum_K (U_{iK} C_K^\dagger + V_{iK} C_{\bar{K}}), \\ a_{\bar{i}}^\dagger &= \sum_K (\hat{U}_{iK} C_{\bar{K}}^\dagger + \hat{V}_{iK} C_K), \end{aligned} \tag{26}$$

where $\hat{U}$, $\hat{V}$ are not simply related to $U$, $V$, except at $\omega = 0$. The quasi-particle operators (26) transform as

$$\sigma_x \begin{pmatrix} a_i^\dagger \\ a_{\bar{i}}^\dagger \end{pmatrix} \sigma_x^{-1} = i \begin{pmatrix} -a_i^\dagger \\ +a_{\bar{i}}^\dagger \end{pmatrix}. \tag{27}$$

The quasi-particle vacuum for an even nucleus may be expressed as

$$|\Phi_0\rangle = c \prod_i a_i a_{\bar{i}} |0\rangle, \tag{28}$$

where $c$ is a normalization constant. A particular $a_i$ is excluded from the product if $V_{iK} = 0$ for all $K$, and similarly for $a_{\bar{i}}$. From (27) and (28) it follows that $|\Phi_0\rangle$ is invariant with respect to $\sigma_x$,

$$\sigma_x|\Phi_0\rangle = i^N|\Phi_0\rangle, \tag{29}$$

where $N$ is the number of $a_{\bar{i}}$ excluded from (28) minus the number of $a_i$ excluded. The symmetry $\sigma_x$ therefore satisfies the sufficient conditions for being a SCS in a rotating frame.

These arguments may be repeated for the symmetry $TR_z(\pi)$. The single-particle states transform as

$$TR_z(\pi)\begin{pmatrix} C_K^\dagger \\ C_{\bar{K}}^\dagger \end{pmatrix} R_z^{-1}(\pi)T^{-1} = i\begin{pmatrix} -C_K^\dagger \\ +C_{\bar{K}}^\dagger \end{pmatrix}. \tag{30}$$

The quasi-particle operators (26) transform as

$$TR_z(\pi)\begin{pmatrix} a_i^\dagger \\ a_{\bar{i}}^\dagger \end{pmatrix} R_z^{-1}(\pi)T^{-1} = i\begin{pmatrix} -a_i^\dagger \\ +a_{\bar{i}}^\dagger \end{pmatrix}, \tag{31}$$

if and only if the quasi-particle coefficients $U$, $V$, $\hat{U}$, $\hat{V}$, are restricted to be real. Consequently, $|\Phi_0\rangle$ is invariant with respect to $TR_z(\pi)$,

$$TR_z(\pi)|\Phi_0\rangle = i^N|\Phi_0\rangle, \tag{32}$$

only if these coefficients are real. The symmetry $TR_z(\pi)$ is a SCS in a rotating frame if the quasi-particle transformation (26) is real.

In a non-rotating frame dynamical arguments suggest that the density is invariant with respect to the SCS $\sigma_x$ and $TR_z(\pi)$ [ref. [12])]. These symmetries remain SCS in a rotating frame. It therefore seems likely that the HFB cranking absolute minimum will retain the symmetries $\sigma_x$ and $TR_z(\pi)$.

It remains to be determined whether these SCS and the basis $|K\bar{K}\rangle$ reduce the HFB Hamiltonian to block diagonal form. The density matrix (10) and the pairing tensor (11) are represented in the $|K\bar{K}\rangle$ basis by

$$\rho = \begin{pmatrix} \hat{V}^\dagger\hat{V} & 0 \\ 0 & V^\dagger V \end{pmatrix} \equiv \begin{pmatrix} \rho_1 & 0 \\ 0 & \rho_2 \end{pmatrix}, \tag{33}$$

$$t = \begin{pmatrix} 0 & \hat{V}^\dagger\hat{U} \\ V^\dagger U & 0 \end{pmatrix} \equiv \begin{pmatrix} 0 & t_1 \\ t_2 & 0 \end{pmatrix}. \tag{34}$$

Since $t$ is antisymmetric by definition, it follows that $t_2 = -\tilde{t}_1$, where the tilde signifies transpose. If $\omega \neq 0$, then $\rho_1 \neq \rho_2$ and $t_1 \neq -t_2$.

Consider the $K_1\bar{K}_2$ component of the HF potential (8)

$$\Gamma_{K_1\bar{K}_2} = \sum_{K_3K_4}[\langle K_1K_3|v_a|\bar{K}_2K_4\rangle\rho_{K_4K_3} + \langle K_1\bar{K}_3|v_a|\bar{K}_2\bar{K}_4\rangle\rho_{\bar{K}_4\bar{K}_3}]. \tag{35}$$

Each nucleon-nucleon matrix element may be re-expressed by using (20),

$$\langle K_1K_3|v_a|\bar{K}_2K_4\rangle = \tfrac{1}{4}\langle(k_1+\bar{k}_1)(k_3+\bar{k}_3)|v_a|(-k_2+\bar{k}_2)(k_4+\bar{k}_4)\rangle, \tag{36}$$

and expanded into sixteen matrix elements. Noting that $|k\rangle$ is restricted to states with $m-\frac{1}{2}$ equal to an even integer, eight of these sixteen matrix elements are identically zero by conservation of angular momentum projection. Using the time-reversal invariance of the nucleon-nucleon interaction, it may be shown that the remaining eight matrix elements cancel pairwise. Consequently $\langle K_1K_3|v_a|\bar{K}_2K_4\rangle$ vanishes. Similarly, $\langle K_1\bar{K}_3|v_a|\bar{K}_2\bar{K}_4\rangle$ is zero. Therefore, $\Gamma_{K_1\bar{K}_2} = 0$. Also $T_{K_1\bar{K}_2} = 0$. Consequently, the HF Hamiltonian (7) does not connect $|K_1\rangle$ and $|\bar{K}_2\rangle$. $\mathscr{H}$ is therefore block diagonal in the $|K\bar{K}\rangle$ basis:

$$\mathscr{H} = \begin{pmatrix} \mathscr{H}_1 & 0 \\ 0 & \mathscr{H}_2 \end{pmatrix}. \tag{37}$$

Consider the $K_1 K_2$ components of the pair potential (9)

$$\Delta_{K_1 K_2} = \sum_{K_3 K_4} \langle K_1 K_2 | v_a | K_3 \bar{K}_4 \rangle t_{K_3 \bar{K}_4}. \tag{38}$$

By arguments similar to those above, the matrix element $\langle K_1 K_2 | v_a | K_3 \bar{K}_4 \rangle$ is identically zero, so that $\Delta_{K_1 K_2} = 0$. Similarly $\Delta_{\bar{K}_1 \bar{K}_2} = 0$. The pair potential is therefore skew block diagonal in the $|K\bar{K}\rangle$ basis

$$\Delta = \begin{pmatrix} 0 & \Delta_1 \\ \Delta_2 & 0 \end{pmatrix}. \tag{39}$$

Since $\Delta$ is antisymmetric, it follows that $\Delta_2 = -\tilde{\Delta}_1$.

The HFB equations are given by (6). Substitute (25), (37) and (39) into (6). The HFB Hamiltonian is block diagonal. The resulting equations are

$$\begin{pmatrix} (\mathscr{H}_1 - \omega j_x) & \Delta_1 \\ \Delta_1^\dagger & -(\mathscr{H}_2 + \omega j_x)^* \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ V \end{pmatrix}, \tag{40}$$

$$\begin{pmatrix} (\mathscr{H}_2 + \omega j_x)^* & \Delta_1^\dagger \\ \Delta_1 & -(\mathscr{H}_1 - \omega j_x) \end{pmatrix} \begin{pmatrix} \hat{U}^* \\ -\hat{V}^* \end{pmatrix} = \hat{E} \begin{pmatrix} \hat{U}^* \\ -\hat{V}^* \end{pmatrix}. \tag{41}$$

If $\omega \neq 0$, then $U \neq \hat{U}^*$, $V \neq -\hat{V}^*$ and $E \neq \hat{E}$. There is no quasi-particle degeneracy in a rotating frame.

The energy matrices in (40) and (41) each have a dimension equal to half the dimension of the original energy matrix (6). By using the SCS $\sigma_x$ and the basis $|K\bar{K}\rangle$, the dimension of the HFB equations in a rotating frame has been reduced by a factor of two.

The preceding arguments may be repeated for the SCS $TR_z(\pi)$. The only alteration is that the quasi-particle transformation coefficients and all matrices are required to be real.

### 2.3. PAIRED ORBITALS IN A ROTATING FRAME

The Bloch-Messiah theorem [13]) states that any HFB quasi-particle vacuum may be expressed in BCS form, where each paired orbital is paired with only one other orbital. That is, there exists a single-particle basis such that $\rho$ is diagonal and $t$ has non-zero components only between paired orbitals. This is the canonical representation.

In a non-rotating frame the single-particle orbitals of a doubly even nucleus occur in degenerate time-reversed pairs. These pairs are obvious candidates for the correlated orbitals in a BCS wave function. Since $J_x$ is not time-reversal invariant, in a rotating frame there are no time-reversed pairs of orbitals. It is therefore of interest to determine the nature of the correlated orbitals in a rotating frame.

Consider the HFB unitarity constraint

$$R^2 = R, \tag{42}$$

where $R$ is the generalized density matrix [4])

$$R = \begin{pmatrix} \rho & t \\ t^\dagger & 1-\tilde{\rho} \end{pmatrix}. \tag{43}$$

From (42) it follows that

$$\rho - \rho^2 = tt^\dagger \equiv \theta, \tag{44}$$

$$\rho t = t\tilde{\rho}. \tag{45}$$

Assume that the quasi-particle vacuum is invariant with respect to $\sigma_x$ (29), and substitute (33) and (34) into (44)

$$\rho_1 - \rho_1^2 = t_1 t_1^\dagger \equiv \theta_1, \tag{46}$$

$$\rho_2 - \rho_2^2 = (t_1^\dagger t_1)^* \equiv \theta_2. \tag{47}$$

Note that $\theta_1$ and $\theta_2$ are hermitian. From (46) it follows that $\rho_1$ and $\theta_1$ commute. Consequently, they can be diagonalized by the same unitary transformation. The eigenvectors of $\rho_1$ and $\theta_1$ are

$$C_\alpha^\dagger = \sum_K D_{\alpha K} C_K^\dagger. \tag{48}$$

Similarly the eigenvectors of $\rho_2$ and $\theta_2$ are

$$C_{\hat{\alpha}}^\dagger = \sum_K \hat{D}_{\alpha K} C_{\bar{K}}^\dagger. \tag{49}$$

If $\omega \neq 0$, then $\hat{D} \neq D^*$, that is $|\hat{\alpha}\rangle \neq T|\alpha\rangle$. These single-particle orbitals transform under $\sigma_x$ as

$$\sigma_x \begin{pmatrix} C_\alpha^\dagger \\ C_{\hat{\alpha}}^\dagger \end{pmatrix} \sigma_x^{-1} = i \begin{pmatrix} -C_\alpha^\dagger \\ +C_{\hat{\alpha}}^\dagger \end{pmatrix}. \tag{50}$$

The operator $\sigma_x$ maps each orbital into itself.

If $A$ and $B$ are square matrices, then $AB$ and $BA$ have the same eigenvalues [14]). The hermitian matrices $\theta_1$ (46) and $\theta_2$ (47) therefore have real identical eigenvalues. Consequently, if $\rho_1$ has an eigenvalue $\rho_\alpha$, then (46) and (47) imply that $\rho_2$ has an eigenvalue $\rho_{\hat{\alpha}}$ such that

$$\theta_\alpha = \rho_\alpha - \rho_\alpha^2 = \rho_{\hat{\alpha}} - \rho_{\hat{\alpha}}^2. \tag{51}$$

It therefore follows that

$$\rho_{\hat{\alpha}} = \rho_\alpha, \tag{52a}$$

or

$$\rho_{\hat{\alpha}} = 1 - \rho_\alpha. \tag{52b}$$

Eq. (52a) states that even though $|\hat{\alpha}\rangle$ is not simply related to $|\alpha\rangle$, both orbitals have the same occupation probability.

Inserting (33) and (34) into the constraint (45) determines that

$$\rho_1 t_1 = t_1 \rho_2^* . \tag{53}$$

Expressed in the $|\alpha\hat{\alpha}\rangle$ basis eq. (53) is

$$t_{\alpha\hat{\alpha}'}(\rho_\alpha - \rho_{\hat{\alpha}'}) = 0. \tag{54}$$

The pairing tensor has non-zero components only between states $|\alpha\rangle$ and $|\hat{\alpha}'\rangle$ having the same occupation probability.

Conditions (52) and (54) may be satisfied in the following manner:

(i) $\theta_\alpha = 0$. Then eq. (51) implies $\rho_\alpha = 0$ or 1 and $\rho_{\hat{\alpha}} = 0$ or 1. The state $|\alpha\rangle$ is fully occupied or empty, and similarly for $|\hat{\alpha}\rangle$. An even nucleus must have an even number of completely occupied orbitals.

(ii) $\theta_\alpha \neq 0$. (a) $\theta_1$ and $\theta_2$ are non-degenerate. Then (51) indicates that $\rho_1$ and $\rho_2$ are non-degenerate. Therefore, the only non-vanishing components of the pairing tensor are $t_{\alpha\hat{\alpha}}$. The orbitals $|\alpha\rangle$ and $|\hat{\alpha}\rangle$ are correlated and have equal occupation probability $\rho_\alpha$. (b) $\theta_1$ and $\theta_2$ are degenerate. The pairing tensor connects the subspace of states $|\alpha\rangle$ associated with the eigenvalue $\theta_\alpha$ to the subspace of states $|\hat{\alpha}\rangle$ associated with the same eigenvalue. It is demonstrated in the appendix that the matrix $t_1$ may be reduced to diagonal form with elements $t_{\alpha\hat{\alpha}}$, where $\rho_{\hat{\alpha}} = \rho_\alpha$. The resultant orbitals remain eigenfunctions of $\sigma_x$.

Consequently, the HFB quasi-particle vacuum can be expressed as

$$|\Phi_0\rangle = \prod_{\alpha_1} C^\dagger_{\alpha_1} \prod_{\alpha_2} C^\dagger_{\hat{\alpha}_2} \prod_{\alpha \neq \alpha_1, \alpha_2} (u_\alpha + v_\alpha C^\dagger_\alpha C^\dagger_{\hat{\alpha}})|0\rangle, \tag{55}$$

where the single-particle orbitals are defined by (48) and (49). The orbitals $|\alpha_1\rangle$ and $|\hat{\alpha}_2\rangle$ are fully occupied and uncorrelated, while the states $|\alpha\rangle$ and $|\hat{\alpha}\rangle$ are partially occupied and correlated. That is, $\rho_{\alpha_1} = \rho_{\hat{\alpha}_2} = 1$, $\rho_\alpha = |v_\alpha|^2$, and $t_{\alpha\hat{\alpha}} = u_\alpha v_\alpha$. Eq. (50) indicates that $|\Phi_0\rangle$ is invariant up to a phase with respect to $\sigma_x$.

These arguments may be repeated for the SCS $TR_z(\pi)$ with the following alterations: The density matrix is real, so that $D$ (48) and $\hat{D}$ (49) are real. The pairing tensor is real, so that $u_\alpha$ and $v_\alpha$ are real. In eq. (50) $\sigma_x$ is replaced by $TR_z(\pi)$.

## 3. Conclusion

A microscopic description of energy spectra at high angular momenta and the "backbending" phenomenon may be obtained with the HFB cranking equations. The symmetries $\sigma_x$ and $TR_z(\pi)$ are SCS in a rotating frame. To take advantage of these symmetries, their eigenfunctions should be used as the single-particle basis states. The dimension of the HFB cranking equations is then reduced by a factor of two. Consequently, it becomes more feasible to obtain solutions for heavy nuclei with realistic forces.

The HFB wave function is reduced to BCS form. In this canonical representation, $\sigma_x$ maps each single-particle orbital into itself. The paired orbitals are not related by any obvious symmetry.

The author is indebted to R. Sorensen for many informative discussions and for suggesting improvements in the manuscript. We also thank P. Ring for an illuminating conversation.

## Appendix

### REDUCTION TO CANONICAL FORM

It must be demonstrated that there exists a single-particle basis such that $\rho$ is diagonal and $t$ connects only paired states with equal occupation probability. It is shown that $\sigma_x$ maps each of these states into itself.

Let $\theta = tt^\dagger$ (44). Since $\tilde{t} = -t$ (11), then $\theta t = t\tilde{\theta}$. If $t$ is given by (34), then

$$\theta_1 t_1 = t_1 \theta_2^*, \tag{A.1}$$

where $\theta_1$ and $\theta_2$ are defined in (46) and (47). The basis $|\alpha\rangle$ (48) simultaneously diagonalizes $\rho_1$ and $\theta_1$. The basis $|\hat{\alpha}\rangle$ (49) diagonalizes $\rho_2$ and $\theta_2$. In this representation (A.1) is

$$t_{\alpha\hat{\alpha}'}(\theta_\alpha - \theta_{\hat{\alpha}'}) = 0, \tag{A.2}$$

where $\theta_\alpha$ is an eigenvalue of $\theta_1$ and $\theta_{\hat{\alpha}}$ is an eigenvalue of $\theta_2$. It has been demonstrated (51) that if $\theta_1$ has an eigenvalue $\theta_\alpha$, then $\theta_2$ has the same eigenvalue. Let $E_1(\alpha)$ be the subspace of eigenvectors of $\theta_1$ corresponding to the eigenvalue $\theta_\alpha$. Let $E_1(\alpha)$ have dimension $d_1$. Similarly $E_2(\alpha)$ and $d_2$ are associated with the eigenvalue $\theta_\alpha$ of $\theta_2$. Then (A.2) states that $t$ connects $E_1(\alpha)$ to $E_2(\alpha)$. This subspace of $t$ is the matrix $t_1(\alpha)$, which has dimension $d_1 \times d_2$. Let $\theta_1(\alpha)$ be the subspace of $\theta_1$ associated with $E_1(\alpha)$, so that $\theta_1(\alpha) = \theta_\alpha I = t_1(\alpha)t_1^\dagger(\alpha)$. Similarly, $\theta_2(\alpha) = \theta_\alpha I = t_1^\dagger(\alpha)t_1(\alpha)$. Take the trace of these two equations

$$\theta_\alpha d_1 = \sum_{ij} |(t_1(\alpha))_{ij}|^2 = \theta_\alpha d_2. \tag{A.3}$$

*Case 1.* $\theta_\alpha = 0$: Eq. (51) has the solutions $\rho_\alpha = 0$ or 1 and $\rho_{\hat{\alpha}} = 0$ or 1. From (A.3) it follows that $t_1(\alpha) = 0$. The states $|\alpha\rangle$ and $|\hat{\alpha}\rangle$ are full or empty and are not pair correlated. They are eigenfunctions of $\sigma_x$ (50).

*Case 2.* $\theta_\alpha \neq 0$: From (A.3) it follows that $d_1 = d_2 = d$. Let $\rho_1(\alpha)$ be the subspace of $\rho_1$ associated with $E_1(\alpha)$. Define $\rho_2(\alpha)$ similarly. Eqs. (51) and (52) state that the diagonal matrices $\rho_1(\alpha)$ and $\rho_2(\alpha)$ have elements $\rho_\alpha$ and $1-\rho_\alpha$. Let $\rho_1(\alpha)$ contain $M_1$ elements of $\rho_\alpha$ followed by $N_1$ elements of $1-\rho_\alpha$, and similarly define $M_2$ and $N_2$ for $\rho_2(\alpha)$, where $M_1+N_1 = M_2+N_2 = d$. Since $t$ only connects states of equal density (54), then

$$t_1(\alpha) = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix},$$

where $A$ and $B$ have dimensions, respectively, of $M_1 \times M_2$ and $N_1 \times N_2$. Consequently,

$$\theta_1(\alpha) = \begin{pmatrix} AA^\dagger & 0 \\ 0 & BB^\dagger \end{pmatrix}, \qquad \theta_2(\alpha) = \begin{pmatrix} A^\dagger A & 0 \\ 0 & B^\dagger B \end{pmatrix}.$$

Since $AA^\dagger$ and $A^\dagger A$ have dimensions, respectively, of $M_1 \times M_1$ and $M_2 \times M_2$, then $\mathrm{Tr}[AA^\dagger] = \theta_\alpha M_1$ and $\mathrm{Tr}[A^\dagger A] = \theta_\alpha M_2$. Since $\mathrm{Tr}[AA^\dagger] = \mathrm{Tr}[A^\dagger A]$ and $\theta_\alpha \neq 0$, then $M_1 = M_2$. Therefore, $N_1 = N_2$. Since $\theta_1(\alpha) = \theta_\alpha I = \theta_2(\alpha)$, then $AA^\dagger = A^\dagger A$. Therefore $A$ is normal. Since $A^\dagger A = \theta_\alpha I$, then $\theta_\alpha^{-\frac{1}{2}} A$ is unitary. Therefore $A$ can be diagonalized by a unitary transformation. This is to be understood in the following sense: The states in $E_1(\alpha)$ with density $\rho_\alpha$ transform as $C_\alpha^\dagger \to \sum_\alpha U_{\beta\alpha} C_\alpha^\dagger$. The states in $E_2(\alpha)$ with density $\rho_\alpha$ transform as $C_{\hat{\alpha}}^\dagger \to \sum_\alpha U_{\beta\alpha}^* C_{\hat{\alpha}}^\dagger$. Therefore the components of $t_1(\alpha)$ transform as $C_{\hat{\alpha}} C_{\alpha'} \to \sum_{\alpha\alpha'} U_{\beta\alpha} C_{\hat{\alpha}} C_{\alpha'} U_{\beta'\alpha'}^*$, so that $t_1(\alpha) \to U t_1(\alpha) U^\dagger$. That is, $t_1(\alpha)$ transforms as an operator. Similarly, $B$ can be diagonalized, mixing states with density $1-\rho_\alpha$. The matrix $t_1(\alpha)$ is then diagonal. All rotated states remain eigenvectors of $\sigma_x$. Consequently, a single-particle basis $|\alpha\hat{\alpha}\rangle$ has been found which diagonalizes $\rho$ and for which the only non-zero components of $t$ (34) are $t_{\alpha\hat{\alpha}}$. The states $|\alpha\rangle$ and $|\hat{\alpha}\rangle$ have equal density. The operator $\sigma_x$ maps each orbital into itself.

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