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On the Application of the Hartree-Fock-Bogolyubov-Equations to a Microscopic Theory of Nuclear Rotations

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The Hartree-Fock-Bogolyubov-Equations of the cranking model are used to give a description of nuclear rotations in a general single particle model. Numerical results for some rare earth nuclei are presented.

I. Introduction

Since Baranger formulated the HFB-Theory for nuclei[1] several authors have used the HFB-Equations* in order to study the problem of nuclear equilibrium deformations[2]. In this paper we plan to go one step further and calculate excitation energies of rotational bands within the framework of the cranking model[3] and HFB-Theory.

In Section II we give a brief derivation of the HFB-Equations and the stability conditions for even and odd mass nuclei. Section III provides a discussion of symmetries of the HFB-Equations and their solutions[4] In Section IV the cranking model is discussed[5]. Finally Section V contains a description of the methods actually used to solve the HFB-Equations and results which have been obtained.

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* Throughout this paper we shall use HFB as an abbreviation for Hartree-Fock-Bogolyubov.

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

2 Baranger, M., Kumar, K.: Nucl. Phys. **62**, 113 (1965). — Dietrich, K., Mang, H. J., Pradal, J.: Z. Physik **190**, 357 (1966). — Faessler, A.: Proceedings of the Yugoslave Summer School Herceg Novi, 1967.

3 Inglis, D. R.: Phys. Rev. **96**, 1059 (1954). — Thouless, D. J., Valatin, I. G.: Nucl. Phys. **31**, 211 (1962). — Marshalek, E. R.: Phys. Rev. **139** B, 770 (1965).

4 Herbut, F., Vujicii, M.: Phys. Rev. **172**, 1031 (1968).

5 Kamlah, A.: Z. Physik **216**, 52 (1968). — Rogerson, N.: PHD-Thesis MIT (1967) (unpublished). — Meyer, J.: PHD-Thesis TH München (1969) (unpublished). — Beck, R., Mang, H. J., Ring, P.: Z. Physik **231**, 26 (1970).

II. Derivation of the HFB-Equations

The following derivation of the HFB-Equations is not the conventional one. It will, however, turn out to be most convenient for a discussion of the stability of the HFB-Solution and for generalization to the case of an odd particle number.

The Hamiltonian is:

$$H=\sum_n \varepsilon_n c_n^+ c_n+\tfrac{1}{4}\sum_{n_1\ldots n_4} v_{n_1 n_2 n_3 n_4} c_{n_1}^+ c_{n_2}^+ c_{n_4} c_{n_3} \tag{1}$$

where $\{c_n\}$ is a set of Fermi operators and the $v_{n_1 n_2 n_3 n_4}$ are matrix elements of an effective interaction.

We introduce the general Bogolyubov-Transformation

$$\gamma_\mu^+=\sum_n A_{n\mu} c_n^+ + B_{n\mu} c_n \tag{2}$$

where the γ's are again Fermi-Operators.

The wave function $|\Phi\{\gamma\}\rangle$ of the ground state of the system is

$$|\Phi\{\gamma\}\rangle=\prod_\mu \gamma_\mu |0\rangle \tag{3}$$

and fulfills $\gamma_K|\Phi\{\gamma\}\rangle=0$.

The set of operators $\{\gamma\}$ is determined from

$$\delta\frac{\langle\Phi\{\gamma\}|H-\lambda N|\Phi\{\gamma\}\rangle}{\langle\Phi\{\gamma\}|\Phi\{\gamma\}\rangle}=0. \tag{4}$$

The solution will be denoted by $\{\beta_\mu\}$.

To obtain the equations which determine this solution we first note that any function $|\Phi\{\gamma\}\rangle$, which is not orthogonal to $|\Phi\{\beta\}\rangle$, can be constructed in the following way:

$$|\Phi\{\gamma\}\rangle=C\cdot\exp\{\tfrac{1}{2}\sum_{\mu\nu} c_{\mu\nu}\beta_\mu^+\beta_\nu^+\}|\Phi\{\beta\}\rangle; \tag{5}$$

where C is a normalization constant.

The solution of the variational Eq. (4) is determined as follows: In an expansion of the expectation value of H' ($H'=H-\lambda N$) in powers of the coefficients $c_{\mu\nu}$ the linear terms must vanish because then the equation

$$\frac{\partial}{\partial c_{\mu\nu}}\frac{\langle\Phi|H'|\Phi\rangle}{\langle\Phi|\Phi\rangle}\Bigg|_{c_{\mu\nu}=0}=0 \tag{6}$$

holds for all values of μ and ν. The expansion up to quadratic terms is given by:

$$\begin{aligned}\frac{\langle\Phi\{\gamma\}|\,H'\,|\Phi\{\gamma\}\rangle}{\langle\Phi\{\gamma\}\,|\,\Phi\{\gamma\}\rangle} &= E_0' \\ &+\tfrac{1}{2}\sum_{\mu\nu}\left(c_{\mu\nu}\langle\Phi\{\beta\}|\,[H',\beta_\mu^+\,\beta_\nu^+]\,|\Phi\{\beta\}\rangle+\text{c.c.}\right) \\ &+\tfrac{1}{8}\sum_{\mu\nu\mu'\nu'}\left(c_{\mu\nu}c_{\mu'\nu'}\langle\Phi\{\beta\}|\,[H',\beta_\mu^+\,\beta_\nu^+\,\beta_{\mu'}^+\,\beta_{\nu'}^+]\,|\Phi\{\beta\}\rangle+\text{c.c.}\right) \\ &+\tfrac{1}{4}\sum_{\mu\nu\mu'\nu'}c_{\mu\nu}^*c_{\mu'\nu'}\cdot\left(\langle\Phi\{\beta\}|\,\beta_\nu\beta_\mu H'\,\beta_{\mu'}^+\beta_{\nu'}^+\,|\Phi\{\beta\}\rangle-2\cdot E_0'\,\delta_{\mu\mu'}\delta_{\nu\nu'}\right) \\ &+\cdots.\end{aligned} \tag{7}$$

The commutators are most easily evaluated, when H' is transformed to quasiparticle operators β:

$$H'=H_0'+H_{11}'+H_{20}'+H_{31}+H_{22}+H_{40}. \tag{8}$$

The explicit expressions for these operators are given in the Appendix. The necessary and sufficient condition for the linear terms to vanish is

$$H_{20}'=0. \tag{9}$$

This equation, however, does not determine the set of operators $\{\beta\}$ uniquely. Any linear transformation of the β's leaves the wave function (3) and Eq. (9) unchanged. Therefore we may further require that H_{11}' be diagonal.

$$H_{11}'=\sum_\mu E_\mu'\,\beta_\mu^+\,\beta_\mu. \tag{10}$$

Of course any other operator of the type

$$Q=\sum_{\mu\nu}Q_{\mu\nu}\beta_\mu^+\,\beta_\nu \tag{11}$$

might have been chosen instead of H_{11}'.

Eqs. (9) and (10) lead to the HFB-Equations for the coefficients $A_{n\mu}$, $B_{n\mu}$:

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}\begin{pmatrix} A_\mu \\ B_\mu \end{pmatrix}=E_\mu\begin{pmatrix} A_\mu \\ B_\mu \end{pmatrix}. \tag{12}$$

The matrices h, Δ, Γ are defined as:

$$\begin{aligned} h&=\varepsilon-\lambda+\Gamma \\ \Gamma_{lm}&=\sum_{rs}v_{lrms}\rho_{sr}; \qquad \Delta_{lm}=\tfrac{1}{2}\sum_{rs}v_{lmrs}\kappa_{rs} \\ \rho_{lm}&=\langle\Phi\{\beta\}|\,c_m^+\,c_l\,|\Phi\{\beta\}\rangle=(B^*\,B^T)_{lm} \\ \kappa_{lm}&=\langle\Phi\{\beta\}|\,c_m\,c_l\,|\Phi\{\beta\}\rangle=(B^*\,A^T)_{lm}. \end{aligned} \tag{13}$$

The system of Eqs. (12), (13) is a nonlinear eigenvalue problem which can be solved by iteration.

In order to have a minimum of the energy $E=\langle\Phi|H'|\Phi\rangle$ the matrix

$$\begin{pmatrix} K & W \\ W^* & K^* \end{pmatrix} \tag{14}$$

must be positive definite. K and W are:

$$\begin{aligned} K_{\mu\nu\mu'\nu'} &= \langle\Phi\{\beta\}|\beta_\nu\beta_\mu H'\beta^+_{\mu'}\beta^+_{\nu'}|\Phi\{\beta\}\rangle - H'_0(\delta_{\mu\mu'}\delta_{\nu\nu'}-\delta_{\mu\nu'}\delta_{\nu\mu'}) \\ W_{\mu\nu\mu'\nu'} &= \langle\Phi\{\beta\}|[H',\beta^+_\mu\beta^+_\nu\beta^+_{\mu'}\beta^+_{\nu'}]|\Phi\{\beta\}\rangle . \end{aligned} \tag{15}$$

If on the other hand this matrix is positive definite, then vibrations around the HFB-Solutions have real frequencies[6].

For a description of nuclei with an odd particle number we proceed analogously. The wave function is a one quasiparticle state $|\Phi_K\rangle = \gamma^+_K|\Phi\{\gamma\}\rangle$. The set of operators $\{\beta\}$ is again determined by:

$$\delta\frac{\langle\Phi_K|H'|\Phi_K\rangle}{\langle\Phi_K|\Phi_K\rangle}=0. \tag{16}$$

The expansion of the expectation value of H' yields instead of Eq. (9):

$$\begin{aligned} H^{11'}_{K\mu}&=0 \quad \text{for } K\neq\mu \\ H^{20}_{\mu\nu}+3\cdot H^{31}_{\mu\nu KK}&=0 \quad \text{for } \mu,\nu\neq K. \end{aligned} \tag{17}$$

We introduce the antisymmetric matrix $\tilde{H}^{20'}$ and the hermitian Matrix $\tilde{H}^{11'}$:

$$\begin{aligned} \tilde{H}^{20'}_{\mu\nu} = H^{20'}_{\mu\nu}+3\cdot H^{31}_{\mu\nu KK} &= \langle\Phi_K|H'\beta^+_\mu\beta^+_\nu|\Phi_K\rangle \quad \text{for } \mu,\nu\neq K \\ &= \langle\Phi|H'\beta^+_\mu\beta^+_K|\Phi\rangle \quad \text{for } \mu\neq K, \nu=K \\ \tilde{H}^{11'}_{\mu\nu} = H^{11'}_{\mu\nu}+4\cdot H^{22}_{\mu K\nu K} &= \langle\Phi_K|\beta_\mu(H'-E'_0-E'_K)\beta^+_\nu|\Phi_K\rangle \quad \text{for } \mu,\nu\neq K \\ &= \langle\Phi_K|(H'-E'_0-E'_K)\beta^+_\nu|\Phi\rangle \quad \text{for } \mu=K. \end{aligned} \tag{18}$$

The set of Eqs. (17) is fulfilled provided $\tilde{H}^{20'}$ is zero and $\tilde{H}^{11'}$ is diagonal.

This leads to a set of HFB-Equations for odd particle number, which was first given by Sugawara[7]:

$$\begin{pmatrix} \tilde{h} & \tilde{\Delta} \\ -\tilde{\Delta}^* & -\tilde{h}^* \end{pmatrix}\begin{pmatrix} A_\mu \\ B_\mu \end{pmatrix} = E_\mu\begin{pmatrix} A_\mu \\ B_\mu \end{pmatrix}. \tag{19}$$

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6 Mang, H. J., Weidenmüller, H. A.: Ann. Rev. Nucl. Sci. **18**, 1 (1968).
7 Sugawara, K.: Progr. Theoret. Phys. (Kyoto) **35**, 41 (1966).

The potentials $\tilde{h}$, $\tilde{\Gamma}$, $\tilde{\Delta}$ are constructed as in Eq. (13) from the density matrix $\tilde{\rho}$ and the pairing matrix $\tilde{\kappa}$:

$$\begin{aligned}\tilde{\rho}_{l\,m}&=\langle\Phi_K|\,c_m^+\,c_l\,|\Phi_K\rangle=\rho_{l\,m}-(B_{l\,K}^*\cdot B_{m\,K}-A_{l\,K}\cdot A_{m\,K}^*)\\ \tilde{\kappa}_{l\,m}&=\langle\Phi_K|\,c_m\,c_l\,|\Phi_K\rangle=\kappa_{l\,m}-(B_{l\,K}^*\cdot A_{m\,K}-B_{m\,K}^*\cdot A_{l\,K})\,.\end{aligned}\tag{20}$$

They depend on the quasi particle state $|\Phi_K\rangle$ and therefore Eq. (19) must be solved separately for each quasiparticle state $|\Phi_K\rangle$. The wave function $|\Phi_{K_0}\rangle$, which yields the lowest energy, describes the ground state of the nucleus. The remaining states $|\Phi_K\rangle$ are single particle excitations.

The Eqs. (19) are a straightforward generalization of the "blocking"-method of the BCS-Model. They correspond exactly to the usual HFB-Equations (12) in the case of even particle number. The ground state is now the one quasi particle state $|\Phi_K\rangle$ instead of the vacuum $|\Phi\rangle$. It is constructed so that in first order perturbation theory transitions to states of the type $\beta_\mu^+\,\beta_\nu^+\,|\Phi_K\rangle$ and $\beta_\mu^+\,|\Phi\rangle$ $(\mu\neq K)$ do not exist:

$$\begin{aligned}&\langle\Phi_K|\,H'\,\beta_\mu^+\,\beta_\nu^+\,|\Phi_K\rangle=0\\ &\langle\Phi_K|\,H'\,\beta_\mu^+\,|\Phi\rangle=0\quad\text{for }\mu\neq K\,.\end{aligned}\tag{21}$$

As in the case of even particle number the quasiparticle operators β_μ^+ are not uniquely determined by this equations. Any unitary transformation of the states $\beta_\mu^+\,|\Phi_K\rangle$ $(\mu\neq K)$ and $|\Phi\rangle$ leaves Eq. (21) invariant. This freedom is used to diagonalize the Hamiltonian H' within the subspace of these states. There is however an important difference between problems with even and odd particle number: For an even particle number the exact ground state does not contain contributions of two-quasiparticle-states in first order perturbation theory because of $H^{20'}=0$. The analogous matrix elements in the odd case, which connect the state $|\Phi_K\rangle$ with three-quasiparticle-states are not zero:

$$\langle\Phi_K|\,H'\,|3\,Q\,P\rangle\neq 0$$

unless the three quasiparticles contain β_K^+. Therefore three-quasiparticle-states are admixed into the ground state even in first order.

Therefore in order to obtain a wave function of the odd system which is of the same quality as the one obtained from the HFB-Equations for the even system, the coupling of one and three quasiparticle states must be taken into account. A natural way to do this would be to include states of the type: one quasiparticle plus one phonon in the treatment.

In this paper, however, the calculations will be restricted to the HFB-Model.

Even then an exact solution of the "blocked" HFB-Equations (19) creates some problems.

1. The iteration has to be carried out separately for every quasiparticle state.

2. The wave functions $|\Phi_K\rangle$ thus obtained are in general not orthogonal.

After the remarks just made it seems to be questionable whether such an effort is justified. We propose therefore the following approximation: The term H^{31} in Eq. (17) is neglected. Then Eq. (17) coincides with Eq. (9) of the even problem. In this approximation $\tilde{\rho}$ and $\tilde{\kappa}$ are replaced by ρ and κ, which do not depend on K. The only state $|\Phi\rangle$ must be determined from the normal HFB-Equations (12) with the subsidiary condition

$$\langle N\rangle = \mathrm{tr}\,\rho = \text{odd number} \tag{22}$$

and the states $|\Phi_K\rangle$ are obtained as one quasiparticle states

$$|\Phi_K\rangle = \beta_K^+ |\Phi\rangle . \tag{23}$$

Two shortcomings of this simple method must be mentioned:

1. The blocking effect is neglected. The coefficients $A_{n\mu}$ and $B_{n\mu}$ are not calculated by minimalization of $\langle\Phi_K|H'|\Phi_K\rangle$ but are simply taken from the even nucleus. Nilsson and Prior[8] have shown that the main effect of blocking is a reduction of the gap parameter Δ. Calculations within particle number conserving theories[9], however, have demonstrated that Δ is reduced too much.

2. The state $|\Phi_K\rangle$ do not have the correct expectation value of the particle number. And this is the most important shortcoming of the description of an odd nucleus by one-quasiparticle-states built on the ground state of a neighbouring even nucleus. Therefore in Section IV the chemical potential λ is determined separately for each state in such a way that $|\Phi_K\rangle$ has the correct expectation value of the particle number.

III. Symmetry Operations and HFB-Equations

The HFB-Equations define a nonlinear eigenvalue problem. In such a case symmetries of the Hamiltonian will not necessaryly lead to the usual consequences for the wave function as known from linear eigenvalue problems. Whereas the exact solution of the Schrödinger equation is an eigenstate of a complete set of operators which commute with the Hamiltonian, this must not be true for the HFB-Approximation.

8 Nilsson, S. G., Prior, O.: Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **32**, Nr. 16 (1961). — Soloviev, V. G.: Kgl. Danske Vedenskab. Selskab, Mat.-fys. Medd. **1**, Nr. 11 (1961).

9 Mang, H. J., Rasmussen, I. O., Rho, M.: Phys. Rev. **141**, 941 (1966).

The HFB-Groundstate is uniquely characterized by the density matrix ρ and the pairing matrix κ ($\tilde{\rho}$ and $\tilde{\kappa}$ in the odd case). The transformation properties of the wave functions are therefore determined by the transformation properties of these matrices. In the following we consider linear, or antilinear, unitary operations S which transform the single particle Hilbert space with basis $|n\rangle = c_n^+ |0\rangle$ into itself. Under such transformations ρ behaves as an operator:

$$\rho' = S^+ \rho S. \tag{24}$$

In the case of an antilinear $S = S_M \cdot K$ is a product of the matrix S_M and the operation of complex conjugation. The behavior of the pairing matrix κ on the other hand is that of the matrix part of an antilinear operation:

$$\kappa' = S^+ \kappa S^*. \tag{25}$$

Now the HFB-Groundstate is invariant under S, if ρ and κ fulfill the relations

$$\rho = S^+ \rho S, \quad \kappa = S^+ \kappa S^*. \tag{26}$$

Since the HFB-Equations are solved by iteration the symmetry relations of the solution depend on the initial values ρ_0 and κ_0. The following theorem holds:

Theorem. If S is a symmetry operator of the Hamilton and if S leaves the initial values ρ_0 and κ_0 invariant, then the iterative solutions of the HFB-Equations ρ and κ are also invariant. It is therefore necessary to choose initial values without any symmetry in order to obtain the most general solution. On the other hand if one knows from physical arguments that the solution must have a certain symmetry, then it is possible to use this fact to reduce the dimension of the HFB-Equations by means of (26).

IV. The HFB-Equations of the Cranking Model

It has already been said that the solutions of the HFB-Equations will in general not be eigenstates of the angular momentum operators J^2 and J_3. The proper procedure to correct for this shortcoming of HFB-theory would be to project from wave functions of the HFB-type eigenstates of angular momentum and solve the variational equations with these projected HFB-wave functions[10].

10 Zeh, H. D.: Z. Physik **188**, 361 (1965). — Villars, F., Cooper, G.: Ann. of Phys. (to be published). — Kamlah, A.: Z. Physik **216**, 52 (1968). — Rogerson, N.: PHD-Thesis MIT (1967) (unpublished). — Onishi, N.: Progr. Theoret. Phys. (Kyoto) **40**, 84 (1968).

The resulting equations are very complex and cannot be solved without approximations. Most attempts to handle these "projected" HFB-Equations yield as a first approximation the equations of the cranking model[11]:

$$\delta\langle\Phi|H'-\omega\cdot J_1|\Phi\rangle=0. \tag{27}$$

The cranking frequency is determined by

$$\langle\Phi|J_1|\Phi\rangle=\sqrt{J\cdot(J+1)}. \tag{28}$$

Therefore it is necessary to solve the HFB-Equations in the rotating frame:

$$\begin{pmatrix}\varepsilon-\lambda-\omega\cdot J_1 & \Delta\\ -\Delta^* & -\varepsilon+\lambda+\omega J_1^*\end{pmatrix}\begin{pmatrix}A_K\\ B_K\end{pmatrix}=E_K\begin{pmatrix}A_K\\ B_K\end{pmatrix}. \tag{29}$$

Within this approximation the HFB-Vacuum $|\Phi_{\omega(J)}\rangle$ describes a rotational state of angular momentum J. Eqs. (27), (28) apply to an even nucleus. They can be generalized to odd mass nuclei, i.e. to one quasi particle states. Only the subsidiary condition relating the expectation value of J_1 to the total angular momentum J is changed in the following way:

$$\langle\Phi_K|J_1|\Phi_K\rangle=\sqrt{J\cdot(J+1)-K^2} \tag{30}$$

where K is the projection of the angular momentum on the symmetry-axis. Further $|\Phi_K\rangle$ has to fulfill also the relation

$$e^{i\pi J_1}|\Phi_K\rangle\sim|\Phi_K\rangle. \tag{31}$$

Otherwise the approximate angular momentum projection will not lead to the subsidiary condition. It is instructive to treat the equations in lowest order in the cranking frequency ω. In the even case this leads to

$$\begin{aligned}&\langle\Phi|J_1|\Phi\rangle=\omega\,\Theta\\ &\langle\Phi|H|\Phi\rangle=E_0+\frac{\Theta}{2}\omega^2\end{aligned} \tag{32}$$

and

$$\langle\Phi|H|\Phi\rangle_J=E_0+\frac{1}{2\Theta}J(J+1). \tag{33}$$

In the odd case one has to take into account the symmetrization of the wave function

$$|\Phi_K\rangle=\frac{1}{\sqrt{2}}\cdot\{|\tilde{\Phi}_K\rangle+|\tilde{\Phi}_{-K}\rangle\} \tag{34}$$

11 Kamlah, A.: Z. Physik **216**, 52 (1968).

where $|\tilde{\Phi}_K\rangle$ and $|\tilde{\Phi}_{-K}\rangle$ are the one quasiparticle states with $\langle J_3\rangle$ equal to K and $-K$ respectively. Therefore

$$\langle\Phi_K|J_1|\Phi_K\rangle=\langle\tilde{\Phi}_K|J_1|\tilde{\Phi}_K\rangle+\langle\tilde{\Phi}_K|J_1|\tilde{\Phi}_{-K}\rangle. \tag{35}$$

The first term $\langle\tilde{\Phi}_K|J_1|\tilde{\Phi}_K\rangle$ allows the expansion

$$\langle\tilde{\Phi}_K|J_1|\tilde{\Phi}_K\rangle=\omega\cdot\Theta \tag{36}$$

whereas the second one is very small unless $K=\frac{1}{2}$. Then it leads to the socalled decoupling factor a [12] and the formula for the energy is:

$$E=E_0+\frac{1}{2\Theta}\cdot\left(J\cdot(J+1)+(-)^{J+\frac{1}{2}}\cdot a\cdot(J+\tfrac{1}{2})\cdot\delta_{K\frac{1}{2}}\right). \tag{37}$$

V. Numerical Solution of the HFB-Equations and Results

The dimension of the HFB-Equations (12) is twice the dimension of the configuration space. Some symmetries of the equations allow, however, a considerable reduction of the dimension. First we note that together with A, B and E also B^*, A^* and $-E$ is a solution of the HFB-Equations. If now h, Δ, A and B are real quantities the dimension of the matrix to be diagonalized can be reduced to half the original dimension in the following way. One defines:

$$\begin{aligned} X&=A+B; \quad & A&=\tfrac{1}{2}\cdot(X+Y)\\ Y&=A-B; \quad & B&=\tfrac{1}{2}\cdot(X-Y). \end{aligned} \tag{38}$$

The equations for X and Y read

$$\begin{aligned} (h-\Delta)\cdot X&=E\cdot Y\\ (h+\Delta)\cdot Y&=E\cdot X. \end{aligned} \tag{39}$$

Hence

$$(h+\Delta)\cdot(h-\Delta)\cdot X=E^2\cdot X, \tag{40}$$

$$Y=\frac{1}{E}\cdot(h-\Delta)X. \tag{41}$$

The unphysical solutions of the HFB-Equations with negativ eigenvalues are automatically excluded, if in Eq. (41) the positive squareroot of the eigenvalue E^2 of (40) is chosen.

In the calculations described here this simplification is possible. The single particle basis can be chosen in such a way that all matrix elements of the residual interaction $v_{\alpha\beta\gamma\delta}$ and of ωJ_1 are real. Further the sym-

12 Bohr, A., Mottelson, B. R.: Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **27**, Nr. 19 (1953).

metry operation $T*P*e^{i\pi J_2}$, which consist of a rotation of π around the 2-axis, the parity transformation and the time inversion, commutes with the hamiltonian $H'=H-\omega\cdot J_1$. It corresponds to complex conjugation in our basis which means it is antilinear and has the unity matrix as matrix part. It is plausible from physical arguments to require that the solution of the HFB-Equations be invariant under this operation. Eq. (26) leads immediately to

$$\rho^*=\rho\,, \qquad \kappa^*=\kappa\,. \tag{42}$$

Therefore the potentials Γ and Δ are real.

Conservation of charge (3-component of isospin) and parity offers a further possibility to reduce the dimension of the HFB-Equations.

The numerical calculations were carried out in the "quadrupole plus pairing force"-model, which is described extensively by Baranger and Kumar[13]. Since the HFB-Equations are solved exactly it is not necessary to neglect neither the contributions of the pairing force to the selfconsistent potential Γ, nor the contributions of the quadrupole force to the pairing potential Δ, nor the exchange term in the Hartree-Fock-potential Γ, as is usually done.

Hence we use the following Hamiltonian:

$$\begin{aligned} H=&\sum_n \varepsilon_n c_n^+ c_n+\tfrac{1}{2}\cdot Q\cdot \sum_{\substack{\mu=-2\\ m\,n\,r\,s}}^{2} Y_{rs}^{2\mu}\, Y_{mn}^{2\mu}\, c_s^+ c_m^+ c_n c_r \\ &+\tfrac{1}{4}\cdot G\cdot \sum_{m,n>0} c_m^+ c_{\bar m}^+ c_{\bar n} c_n\,. \end{aligned} \tag{43}$$

The single particle energies are chosen in such a way that they coincide for deformation zero with the energies of Nilsson[14] and the BCS phase convention is adopted[8]. The quadrupole matrix elements are given by

$$Y_{mn}^{2\mu}=\langle m\,|\,r^2\cdot Y_2^{\mu}(\vartheta,\varphi)\,|\,n\rangle\,. \tag{44}$$

In the calculation we include the most important shells above the magic numbers 50 (protons) and 82 (neutrons). There are 32 proton states: $4g^{7/2}$, $4d^{5/2}$, $4d^{3/2}$, $4s^{1/2}$, $5h^{11/2}$ and 32 neutron states: $5h^{9/2}$, $5f^{7/2}$ and $6i^{13/2}$.

The coupling constants Q and G of the quadrupole and the pairing force are not chosen so as to reproduce exactly some specific experimental data. We require only:

13 Baranger, M., Kumar, K.: Nucl. Phys. **62**, 113 (1965).

14 Nilsson, G. S.: Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **29**, Nr. 16 (1955). — Mottelson, B. R., Nilsson, S. G.: Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **1**, Nr. 8 (1959).

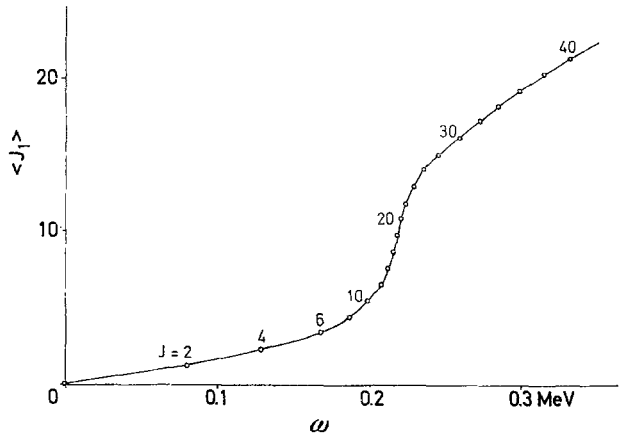

Fig. 1. Dependence of the expectation value $\langle \Phi | J_1 | \Phi \rangle$ an the cranking frequency ω. The values of the angular momentum J are given in the adjusted scale

1. The pairing correlations should be strong enough to produce an energy gap Δ of approximately 1 MeV.

2. The nucleus should be strongly deformed.

The equations are then solved by iteration. We obtain the initial values ρ_0 and κ_0 to start the iteration by a diagonalising a single particle hamiltonian with a deformed harmonic oscillator well, followed by a simple BCS calculation.

We have obtained numerical results for even and odd mass nuclei. In the even case we choose the particle number $N_p = N_n = 18$ which corresponds to Er^{168}.

Obviously all calculated quantities depend on the cranking frequency ω. With the help of the subsidiary condition

$$\langle \Phi | J_1 | \Phi \rangle = \sqrt{J \cdot (J+1)}$$

this dependence can be converted into a dependence on the angular momentum J (Fig. 1). The energy $E(J)$ then gives the position of the rotational levels (Fig. 2). For small cranking frequencies ω the energy depends quadratically and $\langle \Phi | J_1 | \Phi \rangle$ linearly on ω as predicted by perturbation theory. In this case the energies of the rotational levels are given by:

$$E = \frac{1}{2\Theta} \cdot J(J+1). \tag{45}$$

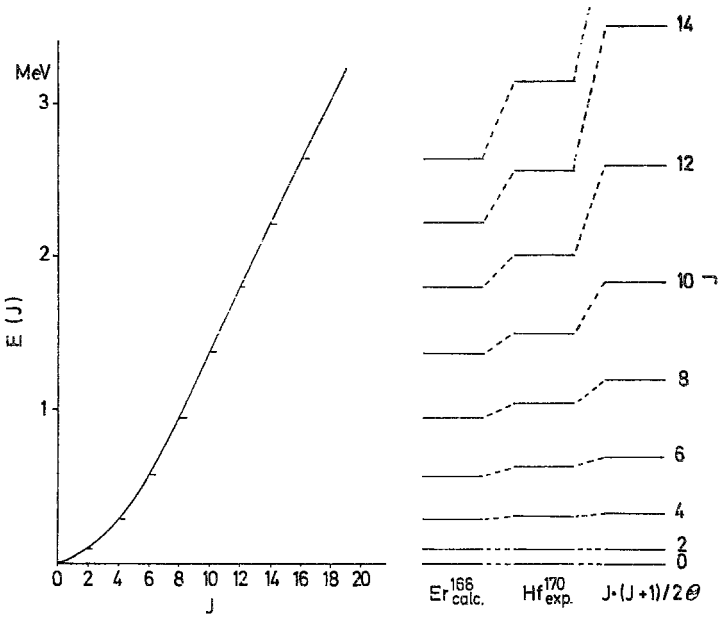

Fig. 2. Comparison of the calculated energies $E(J)$ with the spectrum of a typical rotational nucleus Hf^{170} and with a spectrum of the $J(J+1)$-Type. The $J=2$-levels are adjusted

Θ is the selfconsistent moment of inertia of Thouless and Valatin[15]. The numerical value in our case is $\Theta=15.40\ [\mathrm{MeV}^{-1}]$. This value is very close to the value calculated from the "Inglis Formula"

$$\Theta_{\mathrm{ing}}=\sum_{\mu\nu}\frac{|(A^{+}J_1B^{*}-B^{+}J_1A^{*})_{\mu\nu}|^2}{E_\mu+E_\nu} \tag{46}$$

which yields $\Theta_{\mathrm{ing}}=15.57\ [\mathrm{MeV}^{-1}]$.

It is a good approximation in this model to neglect the selfconsistency for small values of the cranking frequency. For higher frequencies ω the expectation value of J_1 (Fig. 1) as well as the energy increase more rapidly than predicted by perturbation theory. This leads to deviations from the $J\cdot(J+1)$-law for the energies of the rotational band.

When we compare the calculated energy spectrum with an experimental one we first note that the calculated moment of inertia is only half the experimental moment of inertia. The reason is mainly the relatively small configuration space which was used in the calculation.

15 Thouless, D. J., Valatin, I. G.: Nucl. Phys. **31**, 211 (1962).

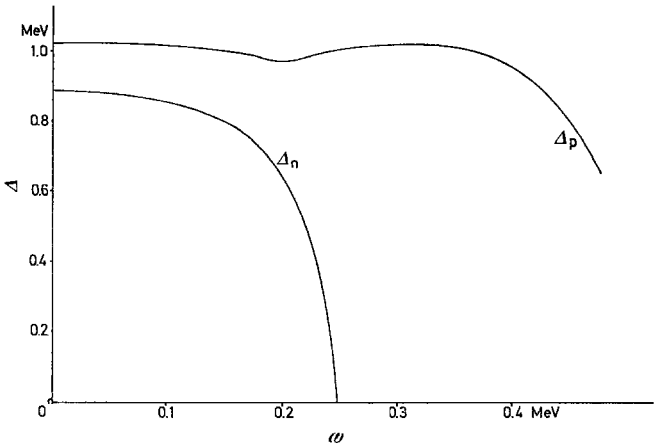

Fig. 3. The gap parameter Δ

We are, however, more interested in the behavior of the energy as a function of the angular momentum J than in a calculation of the absolute value of the moment of inertia. Therefore we adjust the energy scale and the angular momentum scale in such a way that for the 2^+ level calculated and experimental energy agree. We wish to point out that it is not enough to adjust the energy alone because of the relation

$$\frac{\partial}{\partial\omega}E(\omega)=\omega\frac{\partial}{\partial\omega}\langle\Phi|J_1|\Phi\rangle \tag{47}$$

which is rigorously valid provided we have performed a selfconsistent calculation. In Fig. 2 we compare calculated and experimental energies of a typical rotational nucleus. The calculated values are somewhat lower than the experimental ones, which means that in the expansion

$$E_J=\frac{1}{2\Theta}J(J+1)+B\cdot J^2(J+1)^2. \tag{48}$$

B has the correct negative sign, but its absolute value is too large. The reason for the deviation from the $J(J+1)$-law is the increasing influence of the rotation on the internal structure of the nucleus. There are two important effects: Antipairing and stretching.

Fig. 3 shows the decrease of the gap parameter Δ for increasing angular momentum J. In spite of the small difference of the proton and neutron gap for $J=0$ the neutron gap decreases much more rapidly with J. The critical angular momentum for the vanishing of the neutron gap is $J=28$. In this region the energy and the expectation value of J_1

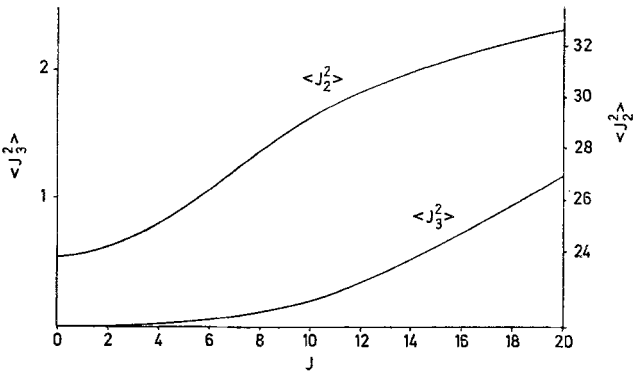

Fig. 4. The expectation values $\langle J_2 \rangle$ and $\langle J_3 \rangle$

increase rapidly with ω. Beyond the transition point the neutrons are in the normal phase ($\Delta_n = 0$). For even higher values of the angular momentum the proton gap goes to zero too. The antipairing effect increases the moment of inertia and therefore lowers the energies compared to the energies given by Eq. (45).

The stretching effect manifests itself in the change of the internal quadrupole moments $\langle r^2 Y_2^\mu \rangle$ or the expectation values of J_3^2 and J_2^2 (Fig. 4). For $J=0$ the nucleus is strongly deformed ($J_2^2 = 23.4$) and axially symmetric ($J_3^2 = 0$). With increasing J the deformation in the 3-direction increases somewhat. But this is not a very large effect. Furthermore the nucleus develops some asymmetry, i.e. $\langle r^2 Y_2^2 \rangle$ and $\langle J_3^2 \rangle$ are no longer zero. There are admixtures of $K \neq 0$ in the wave function.

As an example of an odd mass nucleus we have chosen a neighbouring nucleus to Er^{168} with odd proton number Ho^{167}. The Table gives the energies of the single particle excitations and the inertial parameters Θ and B of the rotational bands built on them. Each band

Table. *Ho^{167}: Energies of the single particle excitations and the inertial parameters Θ and B of the rotational bands built on them*

$K = \langle J_3 \rangle_{\omega=0}$	7/2	1/2	5/2	5/2	3/2	7/2	5/2
Parity	−	+	+	−	+	+	+
$E_{J=K}$ [MeV]	0	0.22	1.02	1.12	1.21	1.82	1.95
Θ [MeV^{-1}]	37.1	55.5	36.8	37.0	34.3	43.5	37.2
B [eV]	−35	−	−126	−121	+30	+190	+79

is characterized by the quantum numbers K and π. π is the parity and K the eigenvalue of J_3 at $\omega=0$. With increasing cranking frequency K is no longer a good quantum number but the expectation value of J_3 is not very different from K. Thus a classification according to this quantum number is possible. The different single particle states have very different inertial parameters. It is, however, possible to reproduce the following experimental facts: For $K\neq\frac{1}{2}$ the energy levels are given by

$$E_J=E_0+\frac{1}{2\Theta}\cdot\left(J(J+1)-K^2\right)+B\cdot\left(J(J+1)-K^2\right)^2+\cdots. \quad (49)$$

The moments of inertia Θ are generally larger than the correspondent values of the neighbouring even nucleus[14]. The B-coefficients are always larger than the B coefficient of the neighbouring even nucleus. For $K=\frac{1}{2}$ the spectrum is characterized by the decoupling parameter a. For the lowest $K=\frac{1}{2}+$band a has the value -0.57. (The experimental value for Ho^{165} is $a=-0.77$.)

VI. Conclusions

We may conclude that HFB-Theory allows a satisfactory treatment of nuclear rotations on the basis of a general single particle model. All physical quantities which we have calculated behave as expected. It is not surprising that only qualitative agreement with measured quantities can be obtained, because of the crude model we have used. The main defect of the model is the smallness of the single particle configuration space. The computational difficulties which arise when the single particle basis is enlarged could, however, be circumvented by using not a larger but a more appropriate basis. For instance instead of n eigenfunctions of a spherical harmonic oscillator one should use n eigenfunctions of a more realistic deformed single particle potential.Thus one would no longer be able to find out whether a nucleus is deformed or not – a question which can be answered with the help of a calcalculation in a spherical basis as described in this paper – but the properties of a deformed nucleus could be calculated much more satisfactorily. Finally we must admit that we have used a very simple effective interaction. We do not yet know, however, neither how a more realistic interaction would change our results, nor how to construct a sufficiently simple but realistic effective interaction to be used in HFB-Theory. Certainly any refinement of the interaction would only be meaningful if the single particle basis is chosen in such a way that any discrepancy between theory and experiment can only be attributed either to the interaction or to HFB-Theory itself. Therefore the two

problems of the single particle basis and the effective interaction should be attacked in this order. We hope to be able to present some results on the first problem in the near future.

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Appendix

The Hamiltonian in the Quasiparticle Representation

$$H = H^0 + \sum_{\mu\nu} H^{11}_{\mu\nu}\beta^+_\mu\beta_\nu + \sum_{\mu\nu}(H^{20}_{\mu\nu}\beta^+_\mu\beta^+_\nu + \text{h.c.}) + \sum_{\mu\nu\rho\sigma}(H^{40}_{\mu\nu\rho\sigma}\beta^+_\mu\beta^+_\nu\beta^+_\rho\beta^+_\sigma + \text{h.c.}) + \sum_{\mu\nu\rho\sigma}(H^{31}_{\mu\nu\rho\sigma}\beta^+_\mu\beta^+_\nu\beta^+_\rho\beta_\sigma + \text{h.c.}) + \sum_{\mu\nu\rho\sigma} H^{22}_{\mu\nu\rho\sigma}\beta^+_\mu\beta^+_\nu\beta_\sigma\beta_\rho .$$

With the definitions of Eq. (13) follows:

$$H^0 = \operatorname{tr}\{(\varepsilon + \tfrac{1}{2}\Gamma)\cdot\rho - \tfrac{1}{2}\Delta\cdot\kappa^*\}$$

$$H^{11} = A^+ h A - B^+ h^{\mathrm{T}} B + A^+ \Delta B - B^+ \Delta^* A$$

$$H^{20} = \tfrac{1}{2}(A^+ h B^* - B^+ h^{\mathrm{T}} A^* + A^+ \Delta A^* - B^+ \Delta^* B^*)$$

$$H^{40}_{\alpha\beta\gamma\delta} = \tfrac{1}{4}\sum_{nmrs} v_{nmrs} A^*_{n\alpha}\cdot A^*_{m\beta}\cdot B^*_{s\gamma}\cdot B^*_{r\delta}$$

$$H^{31}_{\alpha\beta\gamma\delta} = \tfrac{1}{4}\sum_{nmrs} v_{nmrs}\cdot\{A^*_{n\alpha}\cdot B^*_{s\beta}\cdot B^*_{r\gamma}\cdot B_{m\delta} - A^*_{n\alpha}\cdot A^*_{m\beta}\cdot B^*_{r\gamma}\cdot A_{s\delta}\}$$

$$H^{22}_{\alpha\beta\gamma\delta} = \tfrac{1}{4}\sum_{nmrs} v_{nmrs}\cdot\{A^*_{n\alpha}\cdot A^*_{m\beta}\cdot A_{r\gamma}\cdot A_{s\delta} + B^*_{r\alpha}\cdot B^*_{s\beta}\cdot B_{n\gamma}\cdot B_{m\delta} + 4\cdot A^*_{n\alpha}\cdot B^*_{s\beta}\cdot B_{m\gamma}\cdot A_{r\delta}\} .$$

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