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THE SELF-CONSISTENT SINGLE-PARTICLE MODEL IN NUCLEAR PHYSICS

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Contents:

Abstract:

The nuclear many body problem is treated in the single particle approximation, i.e. on the basis of the Hartree–Fock–Bogolyubov approximation. Results of various applications are presented and discussed with emphasis on properties of rotational states of deformed nuclei.

THE SELF-CONSISTENT SINGLE-PARTICLE MODEL IN NUCLEAR PHYSICS

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1. Introduction: The shell-model

Starting from the very first picture nuclear physicists have made themselves of a nucleus, namely the liquid drop model, one may easily arrive at what has been called the other extreme, the nuclear shell model [1]. The constant rather low density and the short range of the forces (short relative to the dimensions of the nucleus and comparable to the distance between two nucleons) provide an average potential which follows in its space dependence rather closely the matter-density distribution. It is a relatively simple example of elementary quantum mechanics to show that such a potential, given the nuclear parameters like nucleon mass, nuclear radius, binding energy of the last nucleon etc., will lead to shell structure with all its consequences known from atomic physics. The argument, that the strong nucleon–nucleon interaction will destroy the single particle picture by scattering nucleons out of their undisturbed orbits, is simply false in this generality, because it neglects the stablizing effect of the Pauli principle. Scattering is only allowed into energetically higher lying unoccupied states [1,2].

If one has unfilled shells however these energy differences are small. But this affects only a small number of states (and hence nucleons) and moreover one is able to show that a large part of this scattering around the Fermi surface can be taken into account by the introduction of the "pairing potential", i.e., nuclear BCS-theory [3].

The main problem, however, which remains, is the construction of a single particle potential which accounts for the known experimental effects as magic numbers, spins and moments of odd mass nuclei, isomerism in certain regions of the periodic table. The most important information obtained from these data was the need for a strong spin orbit potential [1].

Another important achievement was the introduction of a deformed shell model potential by Nilsson in 1955 [4]. Thus many nuclei which did not fit into the shell model picture before could now be satisfactorily described within this generalized shell model [5].

2. Effective interactions

It is obvious that the success of the phenomenological single particle model requires an explanation on the basis of Schrödinger's equation

$$H|\Psi\rangle = E|\Psi\rangle\,. \tag{2.1}$$

The straightforward approach is the use of the Hartree–Fock method in order to obtain an approximate solution of eq. (2.1). However, one encounters several difficulties and finally realizes that such a direct approach is bound to fail. The first problem is to write down the Hamiltonian. While in atomic physics

$$H = \sum_{lm} t_{lm}\, C_l^+ C_m + \sum_{lmrs} \mathcal{V}_{lmrs} C_l^+ C_m^+ C_r C_s\,, \tag{2.2}$$

is an extremely good approximation, one is by no means sure that the nucleon–nucleon interaction can be approximated by a potential $\mathcal{V}$ acting between pairs of nucleons. But even if one asserts the validity of eq. (2.2) for the nuclear Hamiltonian one has to determine the interaction from scattering experiments. It then turns out that all the potentials $\mathcal{V}$ which give good fits to phase shifts up

to 300 MeV are sufficiently repulsive at short distances so as to invalidate the Hartree–Fock approximation. A first suggestion how to circumvent such difficulties was made by Brueckner in 1954 [2, 6]. He treats the interaction between two particles exactly, in the sense that he solves a two-particle Schrödinger equation like

$$(T_1 + V_1 + T_2 + V_2 + \mathcal{V}_{12})\Psi_{\rho\sigma}(1,2) = E_{\rho\sigma}\Psi_{\rho\sigma}(1,2)\,, \tag{2.3}$$

with the subsidary condition that $\Psi_{\rho\sigma}(1,2)$ tends towards $\mathcal{A}(\varphi_\rho\varphi_\sigma)$ for $r_{12}\to\infty$ and is orthogonal to all occupied states i.e.

$$\langle\varphi_\nu\varphi_\mu|\Psi_{\rho\sigma}\rangle = C(\delta_{\nu\rho}\delta_{\mu\sigma} - \delta_{\nu\sigma}\delta_{\mu\rho})\,, \tag{2.4}$$

if one of the states ν, μ is occupied. V is the single particle potential.

Weiskopf has coined the term "independent pair model" [7] for this model, in analogy to the single particle model. The interaction of the pair of nucleons is fully taken into account (eq. (2.3)) while the rest of the nucleons enters into eq. (2.3) only through the Pauli principle (eq. (2.4)) and the single particle potential V. Of course, the calculation of V requires knowledge of Ψ. Therefore one has two sets of coupled equations, the HF equations

$$(T + V)\varphi_\rho = \epsilon_\rho\varphi_\rho\,,$$

with

$$\langle\varphi_\mu|V|\varphi_\sigma\rangle = \sum_\rho \langle\varphi_\mu\varphi_\rho|\mathcal{V}|\Psi_{\rho\sigma}\rangle\,, \tag{2.5}$$

and the two-particle equations (2.3) which have to be solved selfconsistently.

Moreover three-particle correlations must be taken into account as has been shown by Bethe and Rajaraman [8]. The problem is hence quite complex. Nevertheless, Negele [9] has succeeded in performing such a calculation at least in a reasonably good approximation. This work and a quite large number of papers which followed have clearly demonstrated the possibility of calculating *closed shell nuclei* from first principles. A representative sample of them is quoted in [10]. All the calculations are, however, very time consuming and a little bit of phenomenology has to be put in anyway. It is therefore not surprising that attempts have been made to use a phenomenological effective interaction in nuclear Hartree–Fock calculations. The most successful effective interaction until now is the Skyrme interaction [11]. In coordinate space this interaction reads

$$\mathcal{V} = [t_0(1+P_\sigma) - \tfrac{1}{2}t_2(\Delta+\Delta') - t_1\nabla\cdot\nabla' - \mathrm{i}W\sigma[\nabla\times\nabla']]\,\delta(\boldsymbol{r}-\boldsymbol{r}') + t_3\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(\boldsymbol{r}-\boldsymbol{r}'')\,\delta(\boldsymbol{r}'-\boldsymbol{r}'') \tag{2.6}$$

where t_0, t_1, t_2, W and t_3 are constants.

The last term is a three-body contact interaction which in a Hartree–Fock calculation is equivalent to a density dependent two-body interaction

$$\mathcal{V}_3 = t_3\rho(\boldsymbol{r})\delta(\boldsymbol{r}-\boldsymbol{r}')\,. \tag{2.7}$$

As a matter of fact, however, one should always start from (2.6) in order to avoid any trouble with the use of a variation principle.

As already mentioned the Skyrme force has been very successful in explaining many data on binding energies, root mean square radii etc. as will be discussed in section 5.

An even more widely used, but also more phenomenological, effective interaction is the "pairing plus quadrupole–quadrupole force"

$$\mathcal{V} = G \sum_{KK'} C_K^+ C_{\bar{K}}^+ C_{\bar{K}'} C_{K'} + \frac{\chi}{2} \sum_{K_1K_2K_3K_4} (Y_2^{\mu *})_{K_1K_3} (Y_2^{\mu})_{K_2K_4} C_{K_1}^+ C_{K_2}^+ C_{K_4} C_{K_3} \tag{2.8}$$

where $|K\rangle$ and $|\bar{K}\rangle$ are conjugate states $|\bar{K}\rangle = T|K\rangle$ and where T means time reversal.

The use of this interaction was first suggested by Bohr and Mottelson and extensive calculations have been made by Kisslinger and Sørensen [12] and particularly by Kumar and Baranger [13]. The pairing plus quadrupole–quadrupole interaction is thought to be used in a truncated configuration space and the strength constants G and χ depend strongly on the dimension of this configuration space. It accounts for two important phenomena in nuclei; namely, pairing correlations (the existence of Cooper pairs) and nuclear deformations. They arise quite naturally in a selfconsistent single particle model and will be discussed in sections 3 and 4. Of course, the pairing plus quadrupole–quadrupole interaction is a nonsaturating force and cannot be used to calculate absolute values of binding energies. Applications will be discussed in section 5.

3. Hartree–Fock–Bogolyubov theory

In this chapter the Hartree–Fock–Bogolyubov theory [14,15] will be discussed. It allows the treatment of the selfconsistent field and of pair correlations on the same footing. Since this theory is the corner stone, in one way or another, of all applications of the single particle model in nuclear physics, a thorough discussion is necessary. This discussion is presented in two sections, the first on the general Bogolyubov Transformation and the second on the Hartree–Fock–Bogolyubov equations (HFB) itself.

The principal issue of the discussion is to show how flexible the method is and that it is capable of accounting for a sizeable fraction of the correlations present in nuclei.

3.1. The Bogolyubov transformation

The Bogolyubov transformation transforms a set of Fermion operators C_k^+ (the particle operators) into a new set of Fermion operators a_ν^+ (the quasi-particle operators)

$$\begin{aligned} \alpha_\nu^+ &= \sum_k (A_{k\nu} C_k^+ + B_{k\nu} C_k) , \qquad \alpha_\nu = \sum_k (A_{k\nu}^* C_k + B_{k\nu}^* C_k) , \\ C_k^+ &= \sum_\nu (A_{k\nu}^* \alpha_\nu^+ + B_{k\nu} \alpha_\nu) , \qquad C_k = \sum_\nu (A_{k\nu} \alpha_\nu + B_{k\nu}^* \alpha_\nu^+) . \end{aligned} \tag{3.1}$$

The coefficients $A_{k\nu}$ and $B_{k\nu}$ are not completely arbitrary, but are restricted by the relations

$$A^+A + B^+B = AA^+ + B^*B^{\mathrm{T}} = 1 , \qquad A^{\mathrm{T}}B + B^{\mathrm{T}}A = AB^+ + B^*A^{\mathrm{T}} = 0 , \tag{3.2}$$

which are consequences of the communication relations

$$\begin{aligned} &\{\alpha_\nu^+, \alpha_\mu\} = \delta_{\mu\nu}, \quad \{C_k^+, C_l\} = \delta_{kl} \\ &\{\alpha_\nu^+, \alpha_\nu^+\} = 0, \qquad \{C_k^+, C_l^+\} = 0 . \end{aligned} \tag{3.3}$$

The quasi-vacuum and quasi-particle states. To both sets of operators $C_k^+ C_k$ and $\alpha_\nu^+ \alpha_\nu$ belong

"vacuum states" which are defined by ☆

$$C_k|0\rangle = 0\,, \tag{3.4a}$$

and

$$\alpha_\nu|\Phi\rangle = 0\,, \tag{3.4b}$$

$|\Phi\rangle$ is usually called quasi-vacuum.

As is well known, one can construct a complete set of N-particle wavefunctions with the help of the creation operators C_k^+

$$|k_1 k_2 \ldots k_N\rangle = \prod_{i=1}^{N} C_{k_i}^+|0\rangle\,, \tag{3.5}$$

provided the one-particle wavefunctions

$$|k\rangle = C_k^+|0\rangle\,, \tag{3.6}$$

are complete.

In an analogous manner, N quasi-particle states can be constructed:

$$|\nu_1 \ldots \nu_N\rangle = \prod_{\mu=1}^{N} \alpha_{\nu_\mu}^+|\Phi\rangle\,. \tag{3.7}$$

As long as eqs. (3.2) are valid, these quasi-particle states form another (equivalent) basis of the Hilbert-space spanned by the N-particle wavefunctions ☆☆ ($N = 0, 1, 2, \ldots$) of eq. (3.5). From this follows a very simple proof that, if the quasivacuum $|\Phi\rangle$ exists, it must be unique.

Be $|\Phi_1\rangle$ and $|\Phi_2\rangle$ two states which fulfill

$$\alpha_\nu|\Phi_1\rangle = 0, \quad \alpha_\nu|\Phi_2\rangle = 0, \quad \langle\Phi_1|\Phi_1\rangle = \langle\Phi_2|\Phi_2\rangle = 1, \quad \langle\Phi_1|\Phi_2\rangle = 0. \tag{3.8}$$

In case the last condition is not fulfilled, one can redefine $|\Phi_1\rangle$ and $|\Phi_2\rangle$ so that it is valid. $|\Phi_2\rangle$ can now be expanded in terms of the N quasi-particle states with respect to $|\Phi_1\rangle$:

$$|\Phi_2\rangle = \sum_{N=1} \sum_{\{\nu_1 \ldots \nu_N\}} a_{\nu_1 \ldots \nu_N}|\nu_1 \ldots \nu_N\rangle\,, \tag{3.9}$$

with

$$a_{\nu_1 \ldots \nu_N} = \langle\nu_1 \ldots \nu_N|\Phi_2\rangle\,.$$

Because of

$$a_{\nu_1 \ldots \nu_N} = \langle\Phi_1|\alpha_{\nu_N} \ldots \alpha_{\nu_1}|\Phi_2\rangle = 0, \tag{3.10}$$

one finds

$$|\Phi_2\rangle = 0 \quad \text{or} \quad |\Phi_1\rangle = 0. \tag{3.11}$$

One therefore concludes that either $|\Phi_1\rangle$ or $|\Phi_2\rangle$ must be identically zero.

☆ Such vacuum states will also be called Bogolyubov wavefunctions.

☆☆ In all practical calculations in nuclear physics sums are finite and the statement made above is trivially correct.

As a simple application it is now possible to convince oneself that the vacuum state $|\Phi\rangle$ is invariant (up to an irrelevant phase factor) under a transformation of the type

$$a_\nu^+ = \sum_\mu C_{\mu\nu}\gamma_\mu^+, \quad C^+C = CC^+ = 1. \tag{3.12}$$

This is so because the vacuum to γ_μ is also vacuum to α_ν and vice versa. Therefore the two vacua must be the same.

Density matrix and pairing tensor. I shall now discuss some further important properties of the Bogolyubov transformation and the quasi-vacuum $|\Phi\rangle$. Two quantities, the density matrix ρ and the pairing tensor κ, play a central role. They are defined as follows:

$$\rho_{kl} = \langle\Phi|C_l^+C_k|\Phi\rangle, \quad \kappa_{kl} = \langle\Phi|C_lC_k|\Phi\rangle\ , \tag{3.13}$$

or in matrix notation

$$\rho = B^*B^{\mathrm{T}}, \quad \kappa = B^*A^{\mathrm{T}}.$$

For everything that follows it will be useful to know the transformation properties of ρ and κ.

Under a transformation D of the basic operators C^+, C into new operators d^+, d

$$d_k^+ = \sum_l d_{lk}C_l^+$$

or (3.14)

$$d^+ = D^{\mathrm{T}}C^+, \quad d = D^+C$$

ρ and κ transform into ρ', κ' in the following way:

$$\rho' = D^+\rho D, \quad \kappa' = D^+\kappa D^*\ . \tag{3.15a}$$

According to eqs. (3.15a), ρ transforms like an operator, whereas κ transforms like an antisymmetric tensor.

The coefficients of the Bogolyubov transformation A and B transforms as follows:

$$A' = D^+A, \quad A = DA', \quad B' = D^{\mathrm{T}}B, \quad B = D^*B'\ . \tag{3.15b}$$

An important equation which relates ρ and κ follows from eqs. (3.13) and (3.1). It is

$$\rho - \rho^2 = \kappa\kappa^+\ . \tag{3.16}$$

This relation plays a decisive role in the proof of a famous theorem by Bloch and Messiah [16].

The theorem of Bloch and Messiah. The theorem states that any Bogolyubov transformation can be decomposed into three subsequent transformations.

(1) A transformation to a new set of particle operators $d_l d_l^+$

$$d_l^+ = \sum_k d_{kl}C_k^+\ . \tag{3.17}$$

This transformation diagonalizes ρ and puts κ into canonical form, as will be shown.

(2) A special Bogolyubov–Valatin transformation given by

$$\gamma_l^+ = U_l d_l^+ + V_{\bar{l}}^* d_{\bar{l}}\ , \qquad \gamma_{\bar{l}}^+ = U_{\bar{l}} d_{\bar{l}}^+ + V_l^* d_l\ , \tag{3.18}$$

where $U_{\bar{l}}$ and U_l can be taken as real without loss of generality with

$$|U_l|^2 + |V_{\bar{l}}|^2 = 1, \quad |U_{\bar{l}}|^2 + |V_l|^2 = 1, \quad U_l V_l^* + U_{\bar{l}} V_{\bar{l}}^* = 0. \tag{3.19}$$

Eqs. (3.19) are a consequence of the commutation relations (3.3).
(3) A transformation to the final quasi-particle operators

$$\alpha_\nu^+ = \sum_l S_{l\nu} \gamma_l^+, \tag{3.20}$$

with $SS^+ = S^+S = 1$.
Clearly the operators α_ν and γ_l have the same vacuum state $|\Phi\rangle$ (see eq. (3.12)). The proof of the theorem will now be given in an abbreviated form.

A transformation d, which diagonalizes ρ and hence ρ^2, also diagonalizes $\kappa\kappa^+$. Denote $\kappa\kappa^+$ by Θ. From the definition it follows that Θ is hermitian and positive semidefinite. Because of

$$\kappa = -\kappa^{\mathrm{T}}, \tag{3.21}$$

and using the basis in which Θ and ρ are diagonal, one can directly write down the relations

$$\Theta = \kappa\kappa^+ = \Theta^* = \kappa^*\kappa^{\mathrm{T}} = \kappa^+\kappa. \tag{3.22}$$

Eq. (3.22) implies

$$\kappa \cdot \Theta = \Theta \cdot \kappa, \tag{3.23a}$$

or written out explicitly

$$\kappa_{ki}(\Theta_k - \Theta_i) = 0. \tag{3.23b}$$

If, as in the simplest case, the eigenvalues of ρ and hence of Θ are not degenerate, eq. (3.23b) has only the solution

$$\kappa = 0, \tag{3.24}$$

and because of

$$\rho_i^2 - \rho_i = 0, \quad \rho_i = 1 \quad \text{or} \quad \rho_i = 0.$$

The next simple case is that ρ is twofold degenerate. Then one defines $|k\rangle$ and its conjugate state $|\bar{k}\rangle$ by

$$\rho_k = \rho_{\bar{k}} = |V_k|^2, \quad \Theta_k = \Theta_{\bar{k}} = |V_k|^2 - |V_k|^4, \tag{3.25}$$

and finds with the help of eqs. (3.19)

$$\kappa_{ki} = \delta_{i\bar{k}} U_{\bar{k}} V_k, \quad \kappa_{\bar{k}k} = -\kappa_{k\bar{k}}, \tag{3.26}$$
$$|U_k|^2 = 1 - |V_k|^2, \quad V_{\bar{k}} = -V_k, \quad U_{\bar{k}} = U_k.$$

Any higher degeneracy of ρ can be reduced to a combination of these two cases. For a discussion of this general case the reader is referred to ref. [16].

Summing up, one knows that ρ and κ can be put simultaneously into the following form, provided all eigenvalues of ρ are at least twofold degenerate[☆]:

[☆] In order not to complicate things unduely U_k and V_k have been taken as real quantities.

$$\begin{array}{|cc|cc|cc|}
\hline
V_1^2 & 0 & 0 & 0 & & \\
0 & V_1^2 & & & & \\
\hline
 & & V_2^2 & 0 & 0 & \\
0 & & 0 & V_2^2 & & \\
\hline
 & & & & V_3^2 & 0 \\
0 & & 0 & & 0 & V_3^2 \\
\hline
\end{array} = \rho$$

$$\begin{array}{|cc|cc|cc|}
\hline
0 & U_1V_1 & & & & \\
-U_1V_1 & 0 & & & & \\
\hline
 & & 0 & U_2V_2 & & \\
 & & -U_2V_2 & 0 & & \\
\hline
 & & & & 0 & U_3V_3 \\
 & & & & -U_3V_3 & 0 \\
\hline
\end{array} = \kappa.$$

It is now obvious that the vacuum $|\Phi\rangle$ of the operators γ defined in eq. (3.16) has a density matrix ρ and a pairing tensor κ of the form just described. Such a state will be called completely paired. It is furthermore clear that the third transformation will change neither $|\Phi\rangle$ nor ρ and κ.

In case of non-degenerate eigenvalues (unpaired states) of ρ one finds

$$\gamma_l^+ = d_l, \quad \gamma_{\bar{l}}^+ = d_{\bar{l}}^+ , \tag{3.27a}$$

or with l and $\bar{l}$ exchanged

$$\gamma_l^+ = d_l^+, \quad \gamma_{\bar{l}}^+ = d_l. \tag{3.27b}$$

Obviously there can be an arbitrary number of unpaired states for which (3.27) is valid*.

It follows that

$$\rho_{ll} = \langle\Phi|d_l^+ d_l|\Phi\rangle = \langle\Phi|\gamma_l\gamma_l^+|\Phi\rangle = 1, \qquad \rho_{\bar{l}\bar{l}} = \langle\Phi|\gamma_{\bar{l}}^+\gamma_{\bar{l}}|\Phi\rangle = 0, \tag{3.28}$$

and

$$\kappa_{l\bar{l}} = \langle\Phi|d_{\bar{l}}\, d_l|\Phi\rangle = \langle\Phi|\gamma_{\bar{l}}\gamma_l^+|\Phi\rangle = 0. \tag{3.29}$$

(The other case with l and $\bar{l}$ exchanged is analogous.)

* Eqs. (3.27) are distinctively different from (3.18) with either $V_l = -V_{\bar{l}} = 1$ or $U_l = U_{\bar{l}} = 1$.

In the unpaired case, quasi-particles are essentially equivalent to particles except for a possible exchange of hole and particle operators as $\gamma_l^+ = d_l$.

The explicit form of the wavefunction of the vacuum state. In many cases it is quite useful to have an explicit form of the quasi-vacuum $|\Phi\rangle$. Obviously any wavefunction of the type

$$|\Phi\rangle = \prod_\nu \alpha_\nu |\chi\rangle \,, \tag{3.30}$$

has the property

$$\alpha_\nu |\Phi\rangle = 0,$$

because of

$$\alpha_\nu^2 = 0.$$

But one must be sure that $|\chi\rangle$ is chosen in such a way that $|\Phi\rangle$ does not vanish identically (see eq. (3.12) and the discussion following it).

The case of a completely paired wavefunction will be discussed first. In this case one may take the particle vacuum $|0\rangle$ as $|\chi\rangle$. Since the third transformation may always be disregarded, $|\Phi\rangle$ can be written as*

$$|\Phi\rangle = \prod_\nu \alpha_\nu |0\rangle = \prod_{l>0} \gamma_l \gamma_{\bar{l}} |0\rangle = \prod_{l>0} V_l \prod_{k>0} (U_k + V_k d_k^+ d_{\bar{k}}^+)|0\rangle \,. \tag{3.31}$$

The normalized quasi-vacuum $|\Phi\rangle$ is given by

$$|\Phi\rangle = \prod_{k>0} (U_k + V_k d_k^+ d_{\bar{k}}^+)|0\rangle \,, \tag{3.32}$$

and one concludes that $|\Phi\rangle$ does not vanish. This result is well known from BCS theory.

In the case of one unpaired state 1, $\bar{1}$, one shows immediately

$$\gamma_1 \gamma_{\bar{1}} |0\rangle = d_1^+ d_{\bar{1}} |0\rangle = 0. \tag{3.33}$$

Hence the quasi-vacuum $|\Phi\rangle$ constructed with $|\chi\rangle$ vanishes identically. But after normalization, $|\chi\rangle = d_{\bar{1}}^+ |0\rangle$ gives

$$|\Phi_1\rangle = d_1^+ \prod_{k>1} (U_k + V_k d_k^+ d_{\bar{k}}^+)|0\rangle \,. \tag{3.34}$$

This wavefunction does not vanish and is well known as a one-quasi-particle wavefunction or "blocked BCS wavefunction" [17]. It can also be written in the form $|\Phi_1\rangle = \gamma_1'^+ |\Phi\rangle$ with $|\Phi\rangle$ given by eq. (3.32) and $\gamma_1'^+$ by eq. (3.18).**

Number parity. In any dynamic theory going from a quasi-vacuum to one quasi-particle states is very important. It is therefore necessary to discuss the difference between such states in terms of the general Bogolyubov Transformation of eq. (3.1).

First of all one notices that, while a completely paired wavefunction consists only of components with even-particle number, a one quasi-particle wavefunction consists of components with

* $l>0$ in eq. (3.31) means that the product runs only over $N/2$ states l and not over the other $N/2$ states denoted by $\bar{l}$.

** It is important to realise that $\gamma_1'^+$ is a paired quasi-particle operator.

odd particle numbers only. To indicate this difference, the term *number parity* will be used. If only components of even-particle number are present in the wavefunction, it has even-number parity, whereas it has odd-number parity if only odd numbers are present.

It is clear that the third transformation (eq. (3.20)) cannot change the number parity. Therefore the classification according to number parity is general. Moreover, if one starts with a completely paired wavefunction $|\Phi\rangle$ with even-number parity, it is possible to construct wavefunctions of odd-number parity by applying an odd number of quasi-particle creation operators α_ν^+ and wavefunctions of even-number parity by applying an even number of creation operators α_ν^+ to the quasi-vacuum $|\Phi\rangle$. Of course, any of the multi quasi-particle states thus obtained is itself vacuum to another set of quasi-particle operators. To make this point absolutely clear, these sets of operators will be explicitly constructed for some simple cases.

Let $|\Phi\rangle$ be a completely paired vacuum $|\Phi\rangle = \Pi_\nu \alpha_\nu |0\rangle$ to $\{\alpha_1, \alpha_2 \ldots \alpha_N\}$. It is obvious that

$$|\Phi_1\rangle = \alpha_1^+ |\Phi\rangle , \tag{3.35}$$

is a one quasi-particle state (odd-number parity) and that it is vacuum to $\{\alpha_1^+, \alpha_2 \ldots \alpha_N\}$.[☆] (N.B. The state $|\Phi_1'\rangle = \alpha_1^+ \Pi_{\nu \pm 1} \alpha_\nu |0\rangle$ is identically zero because the vacuum is uniquely defined as has been shown and $|\Phi_1'\rangle$ vanishes because of different number parity.) A two quasi-particle state

$$|\Phi_{1,2}\rangle = \alpha_1^+ \alpha_2^+ |\Phi\rangle , \tag{3.36}$$

is vacuum to $\{\alpha_1^+ \alpha_2^+ \alpha_3 \ldots \alpha_N\}$. This procedure can be continued.

Finally one notices that going to the one quasi-particle state $\alpha_1^+ |\Phi\rangle$ simply means that in the Bogolyubov transformation (3.1) the following replacements take place:

$$\begin{aligned} &A_{k1} \text{ is replaced by } B_{k1}^* \\ &\text{and} \\ &B_{k1} \text{ is replaced by } A_{k1}^* \end{aligned} \tag{3.37}$$

Such replacements change ρ and κ by

$$\Delta\rho_{kl} = A_{k1} A_{l1}^* - B_{k1}^* B_{l1} , \quad \Delta\kappa_{kl} = A_{k1} B_{l1}^* - B_{k1}^* A_{l1} . \tag{3.38}$$

For two or more quasi-particle states, analogous replacements have to be made for the other quasi-particle operators.

Summing up, one concludes that any multi quasi-particle state which is defined with respect to a certain quasi-particle vacuum may itself be considered as the vacuum of another set of quasi-particle operators. All these vacua may be classified according to their number parity, and states of different number parity are orthogonal.

The theorem of Thouless. Another important theorem on Bogolyubov wavefunctions is due to Thouless [19]. He proved it for the Hartree–Fock case, but the generalization to the Bogolyubov case is straightforward. The theorem concerns the connection between two vacuum states $|\Phi\rangle$ and $|\Psi\rangle$ which belong to different sets of operators, $\{\alpha_\nu, \alpha_\nu^+\}$ and $\{\gamma_\nu \gamma_\nu^+\}$. Set

[☆] Of course one can select any other quasi-particle operator α_μ^+ and obtain a one quasi-particle wavefunction.

$$\langle\Psi|\Phi\rangle \neq 0\,,^{\star} \quad \alpha_\nu|\Phi\rangle = 0, \quad \gamma_\nu|\Phi\rangle = 0\,. \tag{3.39}$$

Then $|\Psi\rangle$ can be written

$$|\Psi\rangle = C_0 \exp\left(\tfrac{1}{2}\sum_{\nu\mu}\alpha_\nu^+\alpha_\mu^+ C_{\nu\mu}\right)|\Phi\rangle, \quad \gamma_\mu = \sum_\rho Q_{\rho\mu}\left(\alpha_\rho + \sum_\nu C_{\nu\rho}\alpha_\nu^+\right) \tag{3.40}$$

with $C_{\mu\nu} = -C_{\nu\mu}$, C_0 = normalization constant. (N.B. The transformation Q does not affect the vacuum, but guarantees the commutation relations in the form (3.3).) On the other hand, if γ_μ is given in terms of α_ν, α_ν^+

$$\gamma_\mu = \sum_\rho (P_{\rho\mu}\alpha_\rho + R_{\rho\mu}\alpha_\rho^+) \tag{3.41}$$

then $C_{\mu\nu}$ can be calculated from

$$C_{\mu\nu} = (RP^{-1})_{\mu\nu}\,, \tag{3.42}$$

where P^{-1} exists unless $\langle\Psi|\Phi\rangle$ vanishes. The proof goes as follows:

$$\left(\alpha_\rho + \sum_{\nu'} C_{\nu'\rho}\alpha_{\nu'}^+\right)\exp\left(\tfrac{1}{2}\sum_{\nu\mu} C_{\nu\mu}\alpha_\nu^+\alpha_\mu^+\right)|\Phi\rangle$$

$$= \left[\alpha_\rho \exp\left(\tfrac{1}{2}\sum_{\nu\mu} C_{\nu\mu}\alpha_\nu^+\alpha_\mu^+\right) + \exp\left(\tfrac{1}{2}\sum_{\nu\mu} C_{\nu\mu}\alpha_\nu^+\alpha_\mu^+\right)\sum_{\nu'} C_{\nu'\rho}\alpha_\rho^+\right]|\Phi\rangle \tag{3.43}$$

$$\alpha_\rho \exp\left(\tfrac{1}{2}\sum_{\nu\mu} C_{\nu\mu}\alpha_\nu^+\alpha_\mu^+\right) = \exp\left(\tfrac{1}{2}\sum_{\nu\mu} C_{\nu\mu}\alpha_\nu^+\alpha_\mu^+\right)\left(\alpha_\rho + \left[\alpha_\rho, \tfrac{1}{2}\sum_{\nu\mu} C_{\nu\mu}\alpha_\nu^+\alpha_\mu^+\right]\right)$$

$$= \exp\left(\tfrac{1}{2}\sum_{\nu\mu} C_{\nu\mu}\alpha_\nu^+\alpha_\mu^+\right)\left[\alpha_\rho - \sum_\mu C_{\mu\rho}\alpha_\mu^+\right]. \tag{3.44}$$

Upon introducing this result into (3.43), one obtains

$$\left(\alpha_\rho + \sum_{\nu'} C_{\nu'\rho}\alpha_{\nu'}^+\right)|\Psi\rangle = 0\,. \tag{3.45}$$

In order to prove eq. (3.42), one must show that a singular matrix P has necessarily $\langle\Psi|\Phi\rangle = 0$ as a consequence.

Assume $\det P = 0$; then the first row of P is a linear combination of all the others and one can perform a linear transformation of the operators γ_μ to operators γ'_ν so that γ'_1 has the form

$$\gamma'_1 = \sum_\rho R'_{\rho 1}\alpha_\rho^+\,, \tag{3.46}$$

whereas all other relations for $\gamma'_2\gamma'_3\ldots$ remain formally the same as eq. (3.41). From eq. (3.46) follows that $|\Psi\rangle$ is vacuum to a quasi-particle creation operator $\alpha_1'^+$

$$\alpha_1'^+ = \gamma'_1\,. \tag{3.47}$$

Therefore $|\Psi\rangle$ can be written as

[☆] Because of this relation $|\Psi\rangle$ cannot be a multi quasi-particle state with respect to $|\Phi\rangle$.

$$|\Psi\rangle = \alpha_1'^{+}|\chi\rangle\,, \tag{3.48}$$

where $|\chi\rangle$ is vacuum to $\alpha_1' = \gamma_1^+$. One obtains for $\langle\Phi|\Psi\rangle$

$$\langle\Phi|\Psi\rangle = \langle\Phi|\alpha_1'^{+}|\chi\rangle = 0, \tag{3.49}$$

because of

$$\alpha_1'|\Phi\rangle = 0.$$

If more than one operator γ' can be brought into the form (3.46), the argument given is *valid a forteriori*. This completes the proof of the theorem.

3.2. The Hartree–Fock–Bogolyubov equations

Given a Hamiltonian

$$H = \sum_{kl} \mathcal{E}_{kl} C_k^+ C_l + \tfrac{1}{4} \sum_{klmn} \mathcal{V}_{klmn} C_k^+ C_l^+ C_n C_m \tag{3.50}$$

one may ask which of the vacuum states $|\Phi\rangle$ of the preceding section (or Bogolyubov wavefunctions, or HFB wavefunctions, as they will be called from now on) provides the best approximation to the solution of Schrödinger's equation

$$H|\Psi\rangle = E|\Psi\rangle\,, \tag{3.51}$$

with lowest energy E, i.e. to the groundstate of the system.

A very convenient way to answer the question is to use the equivalence of the Schrödinger equation and the variational principle

$$\frac{\delta}{\delta\Psi} \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = 0\,. \tag{3.52}$$

The variational equations. The theorem of Thouless provides a very suitable parametrization of an arbitrary variation around a stationary point within the space spanned by the HFB-wavefunctions. If $|\Phi\rangle$ is a HFB-wavefunction and $|\Phi\rangle + |\delta\Phi\rangle$ is a varied HFB-wavefunction, then $|\Phi\rangle + |\delta\Phi\rangle$ can be written as

$$|\Phi\rangle + |\delta\Phi\rangle = \exp\left(\tfrac{1}{2} \sum_{\nu\mu} C_{\nu\mu} \alpha_\nu^+ \alpha_\mu^+ |\Phi\rangle\right). \tag{3.53}$$

(N.B. $\alpha_\nu|\Phi\rangle = 0$ for all ν.) Before eq. (3.53) can be used to solve eq. (3.52), a few words must be said about particle number conservation, or more precisely, non-conversation in HFB theory.

Clearly, the Hamiltonian eq. (3.50) commutes with the number operator $\hat{N}$

$$\hat{N} = \sum_k C_k^+ C_k\,. \tag{3.54}$$

But the Bogolyubov transformation (3.1) mixes creation and annihilation operators and hence the corresponding HFB-wavefunction is in general not an eigenstate of the number operator (see also the discussion of number parity). The proper procedure would certainly be to project $|\Phi\rangle$ onto an

eigenstate of the number operator with eigenvalue N

$$P_N |\Phi\rangle = |\Psi_N\rangle , \tag{3.55}$$

and use the projected wavefunction $|\Psi_N\rangle$ to approximate the wavefunction of the groundstate.

Of course $|\Psi_N\rangle$ is not a HFB-wavefunction and much more complicated to handle. As will be shown later, a first approximation to the exact procedure is to restrict variations by

$$\langle\Phi|N|\Phi\rangle = \hat{N}. \tag{3.56}$$

Usually one takes care of this constraint by introducing a Lagrangian multiplier λ, the chemical potential, i.e. H is replaced by $H' = H - \lambda\hat{N}$. The condition for $|\Phi\rangle$ to be a solution of the variational equation is now

$$\frac{\delta}{\delta\Phi} \frac{\langle\Phi|H'|\Phi\rangle}{\langle\Phi|\Phi\rangle} = 0,$$

or

$$\frac{\partial}{\partial C_{\lambda\rho}} E(\{C_{\nu\mu}\})|_{\{C_{\nu\mu}=0\}} = 0 \text{ for all values of } \lambda, \rho \tag{3.57}$$

with

$$E(\{C_{\nu\mu}\}) = \frac{\langle\Phi|\exp(\frac{1}{2}\sum_{\nu\mu} C^*_{\nu\mu}\alpha_\mu\alpha_\nu) H' \exp(\frac{1}{2}\sum_{\nu\mu} C_{\nu\mu}\alpha^+_\nu\alpha^+_\mu)|\Phi\rangle}{\langle\Phi|\exp(\frac{1}{2}\sum_{\nu\mu} C^*_{\nu\mu}\alpha_\mu\alpha_\nu)\exp(\frac{1}{2}\sum_{\nu\mu} C_{\nu\mu}\alpha^+_\nu\alpha^+_\mu)|\Phi\rangle}.$$

Eqs. (3.57) are equivalent to

$$\langle\Phi|H'\alpha^+_\lambda\alpha^+_\rho|\Phi\rangle = (H_{20})_{\lambda\rho} = 0 \tag{3.58}$$

for all values of λ, ρ.

These equations involve only the operators $\alpha_\nu\alpha^+_\nu$ because $|\Phi\rangle$ is defined in terms of these operators. Therefore eqs. (3.58) are a set of equations for the transformation coefficients $A_{k\nu}, B_{k\nu}$. $(H_{20})_{\lambda\rho}$ is defined by eqs. (3.58). Of course this is only the condition for $|\Phi\rangle$ to be a stationary point of E. In order to have a minimum of E, one must be sure that the term which is quadratic in $C_{\nu\mu}$ is positive for all possible values of $C_{\nu\mu}$. By carrying the expansion in $C_{\nu\mu}$ to second order, one obtains

$$\tfrac{1}{2}(C^* C)\begin{pmatrix} P & R \\ R^* & P^* \end{pmatrix}\begin{pmatrix} C \\ C^* \end{pmatrix} > 0 \tag{3.59}$$

with

$$(C^* C) = (C^*_{12}, C^*_{13} \ldots, C_{12}, C_{13} \ldots)$$

$$P_{\nu\mu\rho\lambda} = \langle\Phi|\alpha_\mu\alpha_\nu (H' - E(0))\alpha^+_\rho\alpha^+_\lambda|\Phi\rangle$$

$$R_{\nu\mu\rho\lambda} = \langle\Phi|H'\alpha^+_\nu\alpha^+_\mu\alpha^+_\rho\alpha^+_\lambda|\Phi\rangle.$$

In all matrix multiplications sums are taken over pairs of indices $\{\nu, \mu\}$ with $\nu < \mu$.

The inequality (3.59) is simply the statement that the "stability matrix" $\begin{pmatrix} P & R \\ R^* & P^* \end{pmatrix}$ must be positive definite in order to guarantee a stable solution of the variational equation (3.57).

The Hamiltonian in quasi-particle representation. It is of great advantage to transform the Hamiltonian into the quasi-particle representation. The result is

$$H = H_0 + H_{11} + H_{20} + H_{22} + H_{31} + H_{40} \,, \tag{3.60}$$

with

$$H_0 = \mathrm{tr}(\rho\epsilon + \tfrac{1}{2}\rho\Gamma - \tfrac{1}{2}\kappa\Delta)$$

$$H_{11} = \sum_{\nu\mu} (H_{11})_{\nu\mu}\alpha^+_\nu\alpha_\mu$$

$$(H_{11})_{\nu\mu} = (A^+hA - B^+h^*B + A^+\Delta B - B^+\Delta^*A)_{\nu\mu}$$

$$H_{20} = \sum_{\nu\mu}(H_{20})_{\nu\mu}\alpha^+_\nu\alpha^+_\mu + (H_{20})^*_{\nu\mu}\alpha_\mu\alpha_\nu$$

$$(H_{20})_{\nu\mu} = (A^+hB^* - B^+h^*A^* + A\Delta A^* - B^+A^*B^*)_{\nu\mu}$$

$$\hat{h} = \hat{\epsilon} - \lambda\hat{N} + \hat{\Gamma}$$

$$\Gamma_{lm} = \sum_{r,s} \mathcal{V}_{lrms}\,\rho_{sr}, \quad \Delta_{lm} = \tfrac{1}{2}\sum_{r,s} \mathcal{V}_{lmrs}\kappa_{rs} \tag{3.61}$$

$$H_{22} = \sum_{\nu\mu\lambda\rho} (H_{22})_{\nu\mu\lambda\rho}\alpha^+_\nu\alpha^+_\mu\alpha_\rho\alpha_\lambda$$

$$H_{31} = \sum_{\nu\mu\lambda\rho} (H_{31})_{\nu\mu\lambda\rho}\,\alpha^+_\nu\alpha^+_\mu\alpha^+_\lambda\alpha_\rho + \mathrm{h.c}$$

$$H_{40} = \sum_{\nu\mu\lambda\rho} (H_{40})_{\nu\mu\lambda\rho}\alpha^+_\nu\alpha^+_\mu\alpha^+_\lambda\alpha^+_\rho + \mathrm{h.c.}$$

H_{20} defined in eqs. (3.60) and (3.61) is of course the same as H_{20} defined in eq. (3.58) through the matrix elements $(H_{20})_{\nu\mu}$. This equation (3.58) takes the form

$$(H_{20})_{\nu\mu} = (A^+hB^* - B^+h^*A^* + A^+\Delta A^* - B^+\Delta^*B^*)_{\nu\mu} = 0. \tag{3.62}$$

The HFB equations. The variational equations (3.58) or (3.62) are not affected by a transformation of the type $\gamma_\mu = \Sigma_\nu C_{\nu\mu}\alpha_\nu$ and are therefore not sufficient to determine the coefficients $A_{k\nu}$ and $B_{k\nu}$ of the Bogolyubov transformation uniquely. In other words, the requirement $H_{20} = 0$ determines only the first two of the Bloch–Messiah transformations. The third transformation remains arbitrary and can be used to diagonalize any Hermitian operator F of the type

$$\hat{F} = \sum_{\mu\nu} F_{\mu\nu}\alpha^+_\mu\alpha_\nu, \quad F_{\mu\nu} = F^*_{\nu\mu}. \tag{3.63}$$

It has become customary to take H_{11} as the operator to be diagonalized. This leads to the following set of equations:

$$\begin{aligned}(A^+hA - B^+h^*B + A^+\Delta B - B^+\Delta^*A)_{\nu\mu} &= \delta_{\nu\mu}E_\nu,\\ (A^+hB^* - B^+h^*A^* + A^+\Delta A^* - B^+\Delta^*B^*)_{\nu\mu} &= 0,\end{aligned} \tag{3.64}$$

or

$$A^+(hA + \Delta B) - B^+(h^*B + \Delta^*A) = 1 \cdot E$$

$$A^+(hB^* + \Delta A^*) - B^+(h^*A^* + \Delta^*B^*) = 0.$$

If one defines

$$hA + \Delta B = \eta E, \quad -\Delta^*A - h^*B = \varphi E\,, \tag{3.65}$$

where η and φ are matrices, then one has

$$A^+\eta E + B^+\varphi E = 1 \cdot E, \quad -A^*\varphi^*E - B^+\eta^*E = 0 = A^{\mathrm{T}}\varphi E + B^{\mathrm{T}}\eta E. \tag{3.66}$$

One easily finds a solution of this system of inhomogenous linear equations for η and φ by comparing eqs. (3.66) with eqs. (3.2). The solution is

$$\eta = A, \quad \varphi = B\,, \tag{3.67}$$

and it is the only solution because the solution of such a system of inhomogenous equations is unique.

Therefore

$$h \cdot A + \Delta B = A \cdot E, \quad -\Delta^*A - h^*B = B \cdot E\,, \tag{3.68}$$

provides a solution of (3.64). This equation can be rewritten as

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} A \\ B \end{pmatrix} E\,. \tag{3.69}$$

These are the HFB equations. They are a rather complicated non-linear set of equations for A and B. In any attempt to solve them, a knowledge about the symmetries of these equations will be of great value. Therefore symmetries of the HFB equations will be discussed now.

Symmetries of the HFB equations. Because of the nonlinearity of the HFB equations, the well-known relations between symmetries of the Hamiltonian and transformation properties of the wavefunctions are no longer valid. For instance, rotational invariance of the Hamiltonian does not guarantee that the HFB solution is an eigenfunction of the angular momentum operators J^2, J_z. The same is true for linear momentum, particle number, parity etc. One can, however, prove the following theorem [21]. Let U be a unitary or anti-unitary symmetry operation which leaves H invariant. If one starts the iterative solution of the HFB equations with initial values of the density matrix and the pairing tensor (ρ_0 and κ_0) which are also invariant under U, then one will obtain a solution whose density matrix ρ and pairing tensor κ are also invariant under the symmetry operation U, provided, of course, the iteration converges. One proves that every step of the iteration leads from invariant $\rho^{(n-1)}$ and $\kappa^{(n-1)}$ to invariant ρ^n and $\kappa^{(n)}$. In order to do this, one first proves that Γ and Δ computed from an invariant density matrix ρ and an invariant pairing tensor κ are also invariant.

One has (primes denote transformed quantities)

$$\Gamma_{ln} = \sum_{r,s} \mathcal{V}'_{lrns}\rho'_{sr}$$

$$= \sum_{\substack{r,s,p,v \\ k,t,m,q}} U^+_{lk} U^+_{rt} U^{\mathrm{T}}_{nm} U^{\mathrm{T}}_{sq} U^+_{sp} U_{vr} \rho_{pv} \mathcal{V}_{ktmq} \tag{3.70}$$

$$= \sum_{kmqt} U^+_{lk} \mathcal{V}_{ktmq} \rho_{qt} U_{mn} \,.$$

It is obvious that if $\mathcal{V}$ and ρ are invariant, Γ is also invariant. The proof for κ is analogous. Therefore

$$U^+ \Gamma U = \Gamma, \quad U^+ \Delta U^* = \Delta. \tag{3.71}$$

This implies that the HFB matrix $(\underline{}^{h}_{\Delta^*} \ \underline{}^{\Delta}_{h^*})$ = HFB is invariant. Keeping in mind that in every single step of an iteration the HFB equations are linear equations, one can deduce how the coefficients A and B transform. Define S in terms of U as

$$S = \begin{pmatrix} U & 0 \\ 0 & U^* \end{pmatrix}. \tag{3.72}$$

S is unitary $S^+S = SS^+ = 1$ and commutes with the HFB matrix, as was just shown,

$$S^+ \cdot \mathrm{HFB} \cdot S = \mathrm{HFB}.$$

Therefore (A, B) is eigenvector to HFB and S, S^+ simultaneously

$$S^+ \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} A \\ B \end{pmatrix} \varphi \,,$$

or (3.73)

$$U^+ A = A \cdot \varphi, \quad U^{\mathrm{T}} B = B \cdot \varphi \,,$$

with

$$\varphi = \begin{pmatrix} \varphi_1 & & \\ & \ddots & \\ & & \varphi_N \end{pmatrix}, \quad \varphi_\nu = \exp(\mathrm{i}\Psi_\nu) \,.$$

That this is the proper definition follows from eq. (3.15b).

One obtains for ρ and κ

$$\begin{aligned} U^+ \rho U &= U^+ B^* B^{\mathrm{T}} U = B^* \Phi^* \Phi B^{\mathrm{T}} = B^* B^{\mathrm{T}} = \rho \\ U^+ \kappa U^* &= U^+ B^* A^{\mathrm{T}} U^* = B^* \Phi^* \Phi A^{\mathrm{T}} = B^* A^{\mathrm{T}} = \kappa. \end{aligned} \tag{3.74}$$

If the symmetry operation is anti-unitary, the proof of the invariance properties is analogous. One concludes that starting the iteration with invariant ρ_0 and κ_0 will lead to invariant ρ and κ in every step of the iteration.

Another important symmetry is related to the special form of the HFB equations.

If one considers the equation

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} A \\ B \end{pmatrix} E \,, \tag{3.75}$$

for the moment as a linear equation, i.e. disregards that h and Δ contain A and B, one shows easily that if $\{A_\nu, B_\nu\}$ form an eigenvector of the eigenvalue problem (3.75) with eigenvalue E_ν, then $\{B_\nu^*, A_\nu^*\}$ also form an eigenvector with eigenvalue $-E_\nu$. One has to consider the equations in the following form:

$$hA_\nu + \Delta B_\nu = A_\nu E_\nu, \quad \Delta^* A_\nu + h^* B_\nu = -B_\nu E_\nu \,. \tag{3.76}$$

The complex conjugate equations are

$$hB_\nu^* + \Delta \overset{*}{A}_\nu = -\overset{*}{B}_\nu E_\nu, \quad \Delta^* B_\nu^* + h^* \overset{*}{A}_\nu = \overset{*}{A}_\nu E_\nu,$$

and with

$$A'_\nu = \overset{*}{B}_\nu, \quad B'_\nu = \overset{*}{A}_\nu, \quad E'_\nu = -E_\nu \,,$$

one obtains

$$hA'_\nu + \Delta B'_\nu = A'_\nu E'_\nu, \quad \Delta^* A'_\nu + h^* B'_\nu = -B'_\nu E'_\nu \,. \tag{3.77}$$

Eqs. (3.76) and (3.77) are formally identical. The transformation $\{A_\nu B_\nu\}$ to $\{A'_\nu B'_\nu\}$ is identical with the transformation (3.37) discussed in connection with number parity.

It must be noted in this context that the eigenvalue problem of eq. (3.75) has $2N$ eigenvalues $E_\nu, -E_\nu$ (ν=1, ... N) and $2N$ corresponding eigenvectors $\{A_\nu, B_\nu\}$, $\{B_\nu^*, A_\nu^*\}$ (ν=1, ... N). The number of quasi-particle operators in eq. (3.1), however, is only N. Therefore any choice of N eigenvectors and eigenvalues out of the N will give a set of quasi-particle operators which solve the linear eigenvalue problem. Usually, choosing the N positive eigenvalues one obtains a completely paired vacuum state and the exchange $\{A_\nu B_\nu\}_1 E_\nu \leftrightarrow \{B_\nu^* A_\nu^*\}_1 - E_\nu$ leads to a state with odd-number parity. This must not necessarily be so but may be just reversed [18].

This property of the HFB equations opens the possibility of computing one- and two-quasi-particle states selfconsistently* by treating them in each step of an iteration as vacuum states of a new set of operators as described before; and provided the iteration converges. One should keep in mind, however, that such states are not necessarily orthogonal to each other unless they differ in parity, number parity etc. or special precaution is taken. The reason is once more the non-linearity of the problem.

4. Effective operators

It has been pointed out in section 3 that the nonlinearity of the HFB equations leads in general to solutions which are not eigenstates of symmetry operators which commute with the Hamiltonian. It has also been mentioned that the proper procedure would be to reformulate the theory in terms of "projected HFB wavefunctions", i.e. write the variational equations as follows

$$|\Psi\rangle = P|\Phi\rangle \,, \tag{4.1}$$

* Of course, one could try to calculate N quasi-particle states in this way.

with $P^+ = P; P^2 = P$, and

$$\frac{\delta}{\delta\Phi} \frac{\langle\Phi|HP|\Phi\rangle}{\langle\Phi|P|\Phi\rangle} = 0 .$$

In full generality P would project onto eigenstates of given linear and angular momentum as well as particle number and parity. Obviously the variation could be performed with the help of Thouless' Theorem in exactly the same way as before. The resulting equations, however are extremely complicated [22] and there is little hope to handle them numerically exactly except in the case of particle number projection in the BCS-approximation [23]. Moreover, it will be shown that an appropriate approximate treatment of angular momentum projection, for instance, brings out the intuitive pictures physicists have of a rotating nucleus.

4.1. Projection of particle number

Because particle number projection is the simplest case possible it will be treated first. One has

$$P_N|\Phi\rangle = \frac{1}{2\pi} \int_0^{2\pi} \exp(-iN\varphi) \exp(i\hat{N}\varphi)|\Phi\rangle \, d\varphi . \tag{4.2}$$

The "projected energy" E_{proj} takes the form

$$E_{\text{proj}} = \frac{(1/2\pi)\int_0^{2\pi} \exp(-iN\varphi)\langle\Phi|H \exp(i\hat{N}\varphi)|\Phi\rangle \, d\varphi}{(1/2\pi)\int_0^{2\pi} \exp(-iN\varphi)\langle\Phi| \exp(i\hat{N}\varphi)|\Phi\rangle \, d\varphi} . \tag{4.3}$$

This can be brought into the form given by Bayman [24], if one uses for $|\Phi\rangle$ a BCS-wavefunction $|\Phi\rangle = \Pi_k (U_k + V_k a_k^+ a_{\bar{k}}^+)|0\rangle$ and performs a transformation of variables $z = \exp(i\varphi)$. This then yields the results given in ref. [23], provided the operators d_k^+, d_k are taken as fixed i.e. are not submitted to a variation in (4.1).

In order to obtain an approximate expression for E_{proj} we expand $\langle\Phi|H \exp(i\hat{N}\varphi)|\Phi\rangle$ as follows [25]:

$$\langle\Phi|H \exp(i\hat{N}\varphi)|\Phi\rangle = \sum_{n=0}^{\infty} a_n (\hat{p})^n \langle\Phi| \exp(i\hat{N}\varphi)|\Phi\rangle , \tag{4.4}$$

with

$$\hat{p} = \frac{1}{i} \frac{\partial}{\partial\varphi} - \langle\Phi|N|\Phi\rangle .$$

Before discussing how the coefficients a_n are determined one should demonstrate the usefulness of eq. (4.4) by introducing it into (4.3).

Because $\hat{p}$ is a hermitian operator with respect to the integration on φ between 0 and 2π, one obtains a very simple result for E_{proj}^N

$$E_{\text{proj}}^N = \sum_{n=0}^{\infty} a_n (N - \langle\Phi|\hat{N}|\Phi\rangle)^n . \tag{4.5}$$

This result simplifies even more if one realizes that E_{proj}^N is invariant under a transformation of $|\Phi\rangle$ like

$$|\Phi'\rangle = \exp(\lambda\hat{N})|\Phi\rangle, \quad \lambda \text{ arbitrary} \tag{4.6}$$

because $\exp(\lambda\hat{N})$ commutes with the projector P_N. On the other hand, $\langle\Phi|N|\Phi\rangle$ is not invariant and can be given any value greater than zero by a proper choice of λ. Obviously one will use this freedom to have

$$\langle\Phi|\hat{N}|\Phi\rangle = N\,, \tag{4.7}$$

which reduces eq. (4.5) to

$$E^N_{\text{proj}} = a_0\,. \tag{4.8}$$

The next step is, of course, to calculate a_0. One obtains a set of M equations for the first M coefficients $a_0, a_1 \ldots a_{M-1}$ by operating with $1, p, p^2 \ldots p^{M-1}$ on eq. (4.4) and setting φ equal to zero afterwards:

$$\langle\Phi|H(\Delta N)^m|\Phi\rangle = \sum_{n=0}^{M-1} a_n \langle\Phi|(\Delta\hat{N})^{n+m}|\Phi\rangle\,, \tag{4.9}$$

$m = 0, 1, 2, \ldots M-1$ with

$$\Delta\hat{N} = \hat{N} - \langle\Phi|\hat{N}|\Phi\rangle\,. \tag{4.10}$$

As an illustrative example the case $M = 2$ will be worked out explicitly.

$$\langle\Phi|H|\Phi\rangle = a_0\langle\Phi|\Phi\rangle + a_1\,\langle\Phi|\Delta\hat{N}|\Phi\rangle$$

$$\langle\Phi|H\Delta\hat{N}|\Phi\rangle = a_0\langle\Phi|\Delta\hat{N}|\Phi\rangle + a_1\langle\Phi|(\Delta\hat{N})^2|\Phi\rangle\,.$$

Because $\langle\Phi|\Delta N|\Phi\rangle$ equals zero per definition (compare eq. (4.10)) one finds

$$\begin{aligned} a_0 &= \langle\Phi|H|\Phi\rangle/\langle\Phi|\Phi\rangle \\ a_1 &= \langle\Phi|H\Delta\hat{N}|\Phi\rangle/\langle\Phi|\Delta\hat{N}^2|\Phi\rangle\,. \end{aligned} \tag{4.11}$$

Making use of eqs. (4.7) and (4.8), one obtains as first approximation to the variational equations (4.1)

$$\frac{\delta}{\delta\Phi}\,\frac{\langle\Phi|H|\Phi\rangle}{\langle\Phi|\Phi\rangle} = 0\,, \tag{4.12}$$

under the constraint

$$\langle\Phi|N|\Phi\rangle = N.$$

This is exactly the way number conservation is handled in ordinary HFB theory. It is interesting to note that a_1 turns out to be equal to the chemical potential λ provided $|\Phi\rangle$ is a solution of eqs. (4.12). To show this, one writes (4.12) in the form

$$\langle\Phi|H - \lambda N - E|\delta\Phi\rangle = 0$$

and takes as $|\delta\Phi\rangle$

$$|\delta\Phi\rangle = \Delta N|\Phi\rangle\,.$$

This is an admissible variation because $\Delta\hat{N}$ creates two quasi-particle excitations when applied to $|\Phi\rangle$. Upon introducing this $|\delta\Phi\rangle$ into the variational equation, one obtains

$$\langle\Phi|H\Delta\hat{N}|\Phi\rangle - \lambda\langle\Phi|N\Delta\hat{N}|\Phi\rangle = 0, \tag{4.13}$$

or

$$\lambda = \langle\Phi|H\Delta\hat{N}|\Phi\rangle/\langle\Phi|(\Delta\hat{N})^2|\Phi\rangle\,. \tag{4.13a}$$

In order to go beyond HFB theory which was treated in the preceeding section one must set $M = 3$. Here only the result for a_0 is given:

$$E^N_{\text{proj}} = a_0 = \langle\Phi|H|\Phi\rangle - \tfrac{1}{2}\frac{\langle\Phi|(H - \langle H\rangle)\,(\Delta N)^2|\Phi\rangle}{\langle\Phi|(\Delta N)^2|\Phi\rangle + 2}\,. \tag{4.14}$$

The second term gives the lowering of the energy due to projection of particle number. It vanishes if $\langle(\Delta N)^2\rangle$ goes to zero, i.e. if $|\Phi\rangle$ becomes an eigenstate of the number operator.

The variation of the projected energy given by eq. (4.14) can now be performed with the techniques developed in connection with usual HFB theory (theorem of Thouless) [19]. Of course, E^N_{proj} is a much more complicated functional of $|\Phi\rangle$ than before. Indeed we can interpret this situation as having transformed to an *effective Hamiltonian* which is a non-linear operator.

4.2. Projection of angular momentum

Turning now to angular momentum projection one realizes right away that the problem is appreciably more complicated, because in this case there are three operators $(\hat{J}_1\hat{J}_2\hat{J}_3)$ involved instead of one $(\hat{N})$ which moreover do not commute. This latter fact is particularly troublesome.

The most general projector* is given by

$$P^M_J|\Phi\rangle = \sqrt{\frac{2J+1}{8\pi^2}} \sum_{K=-J}^{J} \int \mathring{D}^J_{MK}(\Omega)\,\hat{R}(\Omega)|\Phi\rangle\,\mathrm{d}\Omega \tag{4.15}$$

with

$\Omega = \{\alpha, \beta, \gamma\}$ Euler angles

$$R(\Omega) = \exp(\mathrm{i}\alpha\hat{J}_3)\exp(\mathrm{i}\beta\hat{J}_2)\exp(\mathrm{i}\gamma\hat{J}_3). \tag{4.16}$$

The expression for the projected energy turns out to be (in complete analogy to the case of particle number projection):

$$E^J_{\text{proj}} = \frac{\sqrt{(2J+1)/8\pi^2}\sum_{KK'}\int \mathring{D}^J_{KK'}(\Omega)\langle\Phi|H\hat{R}(\Omega)|\Phi\rangle\,\mathrm{d}\Omega}{\sqrt{(2J+1)/8\pi^2}\sum_{KK'}\int \mathring{D}^J_{KK'}(\Omega)\langle\Phi|\hat{R}(\Omega)|\Phi\rangle\,\mathrm{d}\Omega}\,. \tag{4.17}$$

An approximate expression for E^J_{proj} can be obtained in close analogy to eq. (4.4). Of course there are now three operators $\hat{L}_1\hat{L}_2\hat{L}_3$ [25] to consider instead of the one operator p (the L_i are angular momentum operators in Euler angles)

* In case weight-factors g_K are introduced, P^M_J is no longer a projector, i.e. $P^2 \neq P$, and the g_K are additional parameters, hence one goes beyond a strict single-particle model.

$$\langle\Phi|H\hat{R}(\Omega)|\Phi\rangle = \sum_{n_1 n_2 n_3}^{\infty} a_{n_1 n_2 n_3} \hat{L}_1^{n_1} \hat{L}_2^{n_2} \hat{L}_3^{n_3} \langle\Phi|\hat{R}(\Omega)|\Phi\rangle \,. \tag{4.18}$$

Equations for the coefficient $a_{n_1 n_2 n_3}$ are obtained in the same way as in the case of particle number projection. But before this is explicitly done, a few remarks about symmetries of the wavefunction $|\Phi\rangle$ are in order. The first remark concerns the expectation value of the angular momentum operator J

$$I = \langle\Phi|\hat{J}|\Phi\rangle \,. \tag{4.19}$$

Because the Hamiltonian H is rotationally invariant, E^J_{proj} does not depend on the orientation of the coordinate system in which $|\Phi\rangle$ is explicitly calculated. This means that two wavefunctions which differ only by the orientation of I i.e. $|\Phi'\rangle = R(\Omega')|\Phi\rangle$ are equivalent as far as $E^J_{\text{proj.}}$ is concerned. One can therefore restrict oneself to wavefunctions for which the following relations hold

$$\langle\Phi|\hat{J}_1|\Phi\rangle = I, \quad \langle\Phi|\hat{J}_2|\Phi\rangle = 0, \quad \langle\Phi|\hat{J}_3|\Phi\rangle = 0. \tag{4.20}$$

An important property of the projector P^M_J is that it selects parts of the wavefunction $|\Phi\rangle$ with definite behaviour under the transformation $\exp(i\pi\hat{J}_1)$. For even systems (integer angular momentum) one has

$$P_J|\Phi\rangle = 0 \quad \text{if } J \text{ is odd and} \quad \exp(i\pi\hat{J}_1)|\Phi\rangle = |\Phi\rangle, \tag{4.21}$$

$$P^M_J|\Phi\rangle = 0 \quad \text{if } J \text{ is odd and} \quad \exp(i\pi\hat{J}_1)|\Phi\rangle = -|\Phi\rangle. \tag{4.22}$$

For odd systems (half integer angular momentum) one has

$$P^M_J|\Phi\rangle = 0 \quad \text{if } J-\tfrac{1}{2} \text{ is odd and} \quad \exp(i\pi\hat{J}_1)|\Phi\rangle = i|\Phi\rangle, \tag{4.23}$$

$$P^M_J|\Phi\rangle = 0 \quad \text{if } J-\tfrac{1}{2} \text{ is even and} \quad \exp(i\pi\hat{J}_1)|\Phi\rangle = -i|\Phi\rangle. \tag{4.24}$$

Naturally these statements depend on the adopted phase conventions. Here BCS phases [26] are used*. It should be noted at this point that one can generalize P^M_J by introducing phase factors $(-1)^{J-K}$ in the sum over K. Then the statements (4.21) to (4.24) are so to say reversed. Of course the projected energy (eq. (4.17)) then contains phase factors $(-1)^{K-K'}$ and is therefore changed. Such anomalous bands have been discussed for even nuclei by Volkov and Das Gupta [27]. Finally it is to be mentioned that the generalized P^M_J *does not fulfill* $(P^M_J)^2 = P^M_J$. Now an approximate expression for $E_{\text{proj.}}$ will be worked out. In doing this, it will be of great value that the symmetries of $|\Phi\rangle$ under $\exp(i\pi J_1)$ guarantee that any expectation value of angular momentum operators which contains J_2 and J_3 in odd numbers vanishes because of

$$\exp(-i\pi\hat{J}_1)\,\hat{J}_2\,\exp(i\pi\hat{J}_1) = -\hat{J}_2, \quad \exp(-i\pi\hat{J}_1)\,\hat{J}_3\,\exp(i\pi\hat{J}_1) = -\hat{J}_3. \tag{4.25}$$

Therefore the first approximation will be given by writing (instead of (4.18)):

$$\langle\Phi|HR(\Omega)|\Phi\rangle = (a_{000} + a_{100}L_1)\langle\Phi|R(\Omega)|\Phi\rangle \,. \tag{4.26}$$

Before going on, a few more words must be said about the operators L_i which are angular mo-

* These phases are related to the Condon–Shortley phase convention by $|lj-m\rangle_{\text{BCS}} = (-1)^{j-m+l}|lj-m\rangle_{\text{CS}}$.

mentum operators in terms of Euler angles [28]. As is well known, there are two sets of these operators, one referring to the laboratory frame and the other to the intrinsic frame of reference. Both must be used in a symmetric way. For instance

$$\hat{L}_1 = \tfrac{1}{2}(\hat{L}_1^{\text{intr}} + \hat{L}_1^{\text{lab}}). \tag{4.27}$$

It can be shown [25, 28] that the following useful relations hold

$$\begin{aligned} \hat{L}_k^{\text{lab}}\langle\Phi|R(\Omega)|\Phi\rangle &= \langle\Phi|J_k R(\Omega)|\Phi\rangle \\ \hat{L}_k^{\text{intr}}\langle\Phi|R(\Omega)|\Phi\rangle &= \langle\Phi|R(\Omega)J_k|\Phi\rangle. \end{aligned} \tag{4.28}$$

The proof is trivial for $k = 3$ because of

$$\hat{L}_3^{\text{lab}} = \frac{1}{\mathrm{i}}\frac{\partial}{\partial\alpha}, \quad \hat{L}_3^{\text{intr}} = \frac{1}{\mathrm{i}}\frac{\partial}{\partial\gamma}, \tag{4.29}$$

and somewhat more tedious but straightforward for $k = 1$ and 2.

Relations analogous to (4.28) hold if $R(\Omega)$ is replaced by $HR(\Omega)$ because H commutes with all angular momentum operators. Therefore (4.26) leads to two equations to determine a_{000} and a_{100}

$$\begin{aligned} \langle\Phi|H|\Phi\rangle &= a_{000} + a_{100}\langle\Phi|\hat{J}_1|\Phi\rangle \\ \langle\Phi|H\hat{J}_1|\Phi\rangle &= a_{000}\langle\Phi|J_1|\Phi\rangle + a_{100}\langle\Phi|\hat{J}_1^2|\Phi\rangle. \end{aligned} \tag{4.30}$$

The solution is

$$\begin{aligned} a_{000} &= \langle\Phi|H|\Phi\rangle - \frac{\langle\Phi|(H-\langle H\rangle)\hat{J}_1|\Phi\rangle}{\langle\Phi|(\Delta\hat{J}_1)^2|\Phi\rangle}\langle\Phi|\hat{J}_1|\Phi\rangle \\ a_{100} &= \frac{\langle\Phi|(H-\langle H\rangle)\hat{J}_1|\Phi\rangle}{\langle\Phi|(\Delta\hat{J}_1)^2|\Phi\rangle} \\ \Delta\hat{J}_1 &= \hat{J}_1 - \langle\Phi|\hat{J}_1|\Phi\rangle. \end{aligned} \tag{4.31}$$

Inserting this result into (4.17), one obtains for E^J_{proj}

$$\begin{aligned} E^J_{\text{proj}} &= a_{000} + a_{100}\frac{\frac{1}{2}\int\Sigma_{KK'}((\hat{L}_1^{\text{lab}} + \hat{L}_1^{\text{int}})D^J_{KK'})^*\langle\Phi|R|\Phi\rangle\,\mathrm{d}\Omega}{\int\sum_{KK'}D^{J*}_{KK'}\langle\Phi|R|\Phi\rangle\,\mathrm{d}\Omega} = a_{000} \\ &+ a_{100}\frac{\frac{1}{4}\sum_{KK'}[\sqrt{J(J+1)-K(K+1)} + \sqrt{J(J+1)-K(K-1)} + \sqrt{J(J+1)-K'(K'+1)} + \sqrt{J(J+1)-K'(K'-1)}]\,n^J_{KK'}}{\sum n^J_{KK'}} \\ &= a_{000} + a_{100}\langle\Phi|P_J\hat{J}_1|\Phi\rangle, \\ n^J_{KK'} &= \int D^{*J}_{KK'}(\Omega)\langle\Phi|R(\Omega)|\Phi\rangle\,\mathrm{d}\Omega \end{aligned} \tag{4.32}$$

where $\langle\Phi|P_J\hat{J}_1|\Phi\rangle$ is a shorthand notation for everything multiplying a_{100}. If a_{000} and a_{100} from (4.31) are introduced, one obtains

$$E^J_{\text{proj}} = \langle\Phi|H|\Phi\rangle + \frac{\langle\Phi|(H-\langle H\rangle)\hat{J}_1|\Phi\rangle}{\langle\Phi|(\Delta\hat{J}_1)^2|\Phi\rangle}\left(\langle\Phi|P_J\hat{J}_1|\Phi\rangle - \langle\Phi|\hat{J}_1|\Phi\rangle\right). \tag{4.33}$$

The term which causes trouble in a variation of E^J_{proj} is $\langle\Phi|P_J J_1|\Phi\rangle$. If one, however, compares (4.33) with the corresponding equation in the case of particle number projection (4.5), one realizes that there the analogous term is independent of $|\Phi\rangle$ and equal to N. A close inspection of (4.32) now shows that provided $|\Phi\rangle$ deviates not too much from axial symmetry one has to a very good approximation [25]

$$\langle\Phi|P\hat{J}_1|\Phi\rangle = \sqrt{J(J+1)}\,. \tag{4.34}$$

The main reasons are that for $J = 0$ the result is exact and that for small J only $K = 0, \pm 1$ are important and for most of these terms one has $\sqrt{J(J+1)}\,n^J_{KK'}$ as a contribution to the sum in (4.32). Moreover the properties of the coefficients $n^J_{KK'}$ work in favor of the relation (4.34).

Therefore the variation of E^J_{proj} in the form

$$E^J_{\text{proj}} = \langle\Phi|H|\Phi\rangle + \frac{\langle\Phi|(H-\langle H\rangle)\hat{J}_1|\Phi\rangle}{\langle\Phi|(\Delta\hat{J}_1)^2|\Phi\rangle}\left(\sqrt{J(J+1)} - \langle\Phi|\hat{J}_1|\Phi\rangle\right), \tag{4.35}$$

will not be performed. This will be done in two steps. First, E^J_{proj} will be varied with the constraint

$$\frac{\langle\Phi|(H-\langle H\rangle)\hat{J}_1|\Phi\rangle}{\langle\Phi|(\Delta\hat{J}_1)^2|\Phi\rangle} = \nu(\Phi) = \omega. \tag{4.36}$$

This yields the equation

$$\delta E^J_{\text{proj}} = \delta\langle\Phi|H|\Phi\rangle - \nu\delta\langle\Phi|\hat{J}_1|\Phi\rangle + \delta\nu(\sqrt{J(J+1)} - \langle\hat{J}_1\rangle - \mu) = 0, \tag{4.37}$$

where μ is the Lagrangian multiplier which ensures the validity of (4.36). In order to determine μ, one uses a particular variation $|\delta\Phi\rangle$:

$$|\delta\Phi\rangle = (\hat{J}_1 - \langle\hat{J}_1\rangle)|\Phi\rangle\,. \tag{4.38}$$

Upon inserting (4.38) in (4.37), one finds

$$\langle\Phi|H\Delta\hat{J}_1|\Phi\rangle - \nu\langle\Phi|(\Delta\hat{J}_1)^2|\Phi\rangle + \delta\nu(\sqrt{J(J+1)} - \langle\hat{J}_1\rangle - \mu) = 0$$

and using the constraint (4.36)

$$\delta\nu(\sqrt{J(J+1)} - \langle\Phi|\hat{J}_1|\Phi\rangle - \mu) = 0, \tag{4.39}$$

where $\delta\nu$ is now the *special* variation of ν induced by the special variation of $|\Phi\rangle$ given in eq. (4.38). Since this $\delta\nu$ will in general not vanish, one has

$$\sqrt{J(J+1)} - \langle\Phi|\hat{J}_1|\Phi\rangle - \mu = 0,$$

and the variational equation which automatically fulfills the constraint (4.36) is

$$\delta\langle\Phi|H - \omega\hat{J}_1|\Phi\rangle = 0. \tag{4.40}$$

The projected energy which follows from this equation is

$$E^J_{\text{proj}}(\omega) = \langle\Phi|H|\Phi\rangle + \omega(\sqrt{J(J+1)} - \langle\Phi|\hat{J}_1|\Phi\rangle)\,. \tag{4.41}$$

(N.B. It still depends on ω.)

Differentiation with respect to ω yields

$$\frac{\partial}{\partial\omega}\left[\langle\Phi|H-\omega\hat{J}_1|\Phi\rangle+\omega\sqrt{J(J+1)}\right]=-\langle\Phi|J_1|\Phi\rangle+\sqrt{J(J+1)}.$$

The condition $\partial E^J_{\mathrm{proj}}/\partial\omega=0$ gives

$$\langle\Phi|J_1|\Phi\rangle=\sqrt{J(J+1)}\,. \tag{4.42}$$

Eqs. (4.40) and (4.42) are nothing else but the well-known equation of the self-consistent cranking model [29]

$$\delta\langle\Phi|H-\omega J_1|\Phi\rangle=0,\quad \langle\Phi|J_1|\Phi\rangle=\sqrt{J(J+1)}.$$

It must be emphasized at this point that the only assumptions which enter into the derivation of the self-consistent cranking model are the validity of the truncated expansion (4.30) and the approximate evaluation of $\langle\Phi|P_J\hat{J}_1|\Phi\rangle$ (eq. (4.34)). Both have nothing to do with classical pictures of a rotating nucleus, but remain completely within the frame of a quantum mechanical treatment.

As in the case of particle-number projection, however, one must ask the question whether it is justified to stop the expansion (4.18) at linear terms in the operators $\hat{L}_k$ as was done in eq. (4.26). If the expansion is carried to second order one obtains for the projected energy of well deformed nuclei [29]:

$$\begin{aligned}E^J_{\mathrm{proj}}&=\langle\Phi|H|\Phi\rangle-\frac{1}{\Theta_\gamma}\langle\Phi|\Delta J_1^2+J_2^2|\Phi\rangle+\omega(\langle\Phi|P_JJ_1|\Phi\rangle-\langle\Phi|J_1|\Phi\rangle)+\\&+\frac{1}{2\Theta_\gamma}\left[J(J+1)-\langle\Phi|PJ_3^2|\Phi\rangle-2\langle\Phi|P_JJ_1|\Phi\rangle\langle\Phi|J_1|\Phi\rangle+\langle\Phi|J_1|\Phi\rangle^2\right]\end{aligned} \tag{4.43}$$

$$\omega=\frac{\langle\Phi|H\Delta J_1|\Phi\rangle}{\langle\Phi|\Delta J_1^2|\Phi\rangle},\quad \Theta_\gamma^{-1}=\frac{\langle\Phi|(H-\langle H\rangle)\,(\Delta J_1^2+J_2^2)|\Phi\rangle}{(\Delta J_1^2+J_2^2)^2}\,.$$

In the case of an even nucleus one may insert the crudest approximation

$$\langle\Phi|PJ_1|\Phi\rangle\approx\sqrt{J(J+1)},\quad \langle\Phi|PJ_3^2|\Phi\rangle\approx 0,$$

and obtains

$$\begin{aligned}E^J_{\mathrm{proj}}&=\langle\Phi|H|\Phi\rangle-\frac{1}{\Theta_\gamma}\langle\Phi|\Delta J_1^2+J_2^2|\Phi\rangle\\&+\omega(\sqrt{J(J+1)}-\langle\Phi|J_1|\Phi\rangle)+\frac{1}{2\Theta_\gamma}(\sqrt{J(J+1)}-\langle\Phi|J_1|\Phi\rangle)^2\,.\end{aligned} \tag{4.44}$$

The only difference to eq. (4.35) is now that an additional lowering of the energy occurs which is not explicitly dependent on the angular momentum and only very weakly dependent on ω. The last term in (4.44) introduces no change at all; its value and derivative are zero for $\langle\Phi|J_1|\Phi\rangle=\sqrt{J(J+1)}$. It remains to give the expression for E^J_{proj} in case of an odd mass nucleus. Here one has to consider the possibility of "band mixing", i.e. the possibility that the average potential deviates strongly from axial symmetry, in particular for some states close to the Fermi surface. One finds

$$E^J_{\mathrm{proj}} = \langle\Phi|H|\Phi\rangle - \frac{1}{\Theta_\gamma}\langle\Phi|\Delta J_1^2 + J_2^2|\Phi\rangle$$
$$+ \omega(\sqrt{J(J+1) - \langle\Phi|J_3^2|\Phi\rangle} - \langle\Phi|J_1|\Phi\rangle) + \frac{1}{2\Theta_\gamma}(\sqrt{J(J+1) - \langle\Phi|J_3^2|\Phi\rangle} - \langle\Phi|J_1|\Phi\rangle)^2 . \tag{4.45}$$

Performing the variation under the assumption that the second term on the right-hand side is practically constant*, one finds

$$\delta\langle\Phi|H - \omega J_1|\Phi\rangle = 0,$$
$$\langle\Phi|J_1|\Phi\rangle^2 + \langle\Phi|J_3^2|\Phi\rangle = J(J+1) . \tag{4.46}$$

This includes the variation of E^J_{proj} of eq. (4.44) if one takes into account that in all cases of even nuclei studied so far [29, 30] the ratio $\langle\Phi|J_3^2|\Phi\rangle/\langle\Phi|J_1|\Phi\rangle^2$ never exceeded 1.5%.

Again the problem has been reduced to the treatment of an effective Hamiltonian – a relatively simple one – within the framework of a general single-particle model as described in section 3.

4.3. Transition rates

To conclude this section, we shall outline how one can calculate transition rates using the techniques developed in the preceeding sub-section. The emphasis will be on angular momentum projection, the reason being that it has been demonstrated [31] that particle number projection will in general not significantly alter the results obtained with simple BCS theory. Moreover, we shall concentrate on electromagnetic transitions and moments. An electromagnetic transition operator of rank L will be denoted by T^M_L and the following matrix element will be calculated:

$$\langle JM|T^0_L|J'M\rangle = \langle\Phi|P^M_J\, T^0_L P^M_{J'}|\Phi'\rangle$$
$$= \frac{(\sqrt{(2J+1)(2J'+1)}/8\pi^2)\sum_{KK'}\int\int \mathrm{d}\Omega\mathrm{d}\Omega' D^J_{MK}(\Omega)\overset{*}{D}{}^{J'}_{MK'}(\Omega')\langle\Phi|R^+(\Omega)T^0_L R(\Omega')|\Phi'\rangle}{[\sum_{KK'}\int \overset{*}{D}{}^J_{KK'}(\Omega)\langle\Phi|R|\Phi\rangle\,\mathrm{d}\Omega\cdot\sum_{KK'}\int\overset{*}{D}{}^{J'}_{KK'}\langle\Phi'|R|\Phi'\rangle\,\mathrm{d}\Omega']^{1/2}} . \tag{4.47}$$

In the following only the numerator will be considered:

$$\sum_{KK'}\int\int \mathrm{d}\Omega\mathrm{d}\Omega' D^J_{MK}(\Omega)\overset{*}{D}{}^J_{MK}(\Omega')\langle\Phi|R^+(\Omega)T^0_L R(\Omega')|\Phi'\rangle =$$

$$= \sum_{KK'}\int\int \mathrm{d}\Omega\mathrm{d}\Omega' D^J_{MK}(\Omega)\overset{*}{D}{}^{J'}_{MK'}(\Omega')\tfrac{1}{2}[\langle\Phi|R^+(\Omega)R(\Omega')R^+(\Omega')T^0_L R(\Omega')|\Phi'\rangle$$
$$+ \langle\Phi|R^+(\Omega)T^0_L R(\Omega)R^+(\Omega)R(\Omega')|\Phi'\rangle]$$
$$= \sum_{KK'}\int\int \mathrm{d}\Omega\mathrm{d}\Omega' D^J_{MK}(\Omega)\overset{*}{D}{}^{J'}_{MK'}(\Omega')\tfrac{1}{2}[\Phi|R(\Omega'')R^+(\Omega')T^0_L R(\Omega')|\Phi'\rangle$$
$$+ \langle\Phi|R^+(\Omega)T^0_L R(\Omega)R(\Omega'')|\Phi'\rangle$$
$$= \sum_{KK'}\int\int \mathrm{d}\Omega\mathrm{d}\Omega' D^J_{MK}(\Omega)\overset{*}{D}{}^{J'}_{MK'}(\Omega')\tfrac{1}{2}\Big[\sum_m \overset{*}{D}{}^L_{0m}(\Omega')\langle\Phi|R(\Omega'')T^m_L|\Phi'\rangle + \sum_m \overset{*}{D}{}^L_{0m}(\Omega)\langle\Phi|T^m_L R(\Omega'')|\Phi'\rangle\Big]$$

* This assumption is only justified for strongly deformed nuclei.

$$
\begin{aligned}
&= \tfrac{1}{2} \sum_{KK'} \int d\Omega' d\Omega'' \sum_{M'} D^J_{MM'}(\Omega') \overset{*}{D}{}^J_{KM'}(\Omega'') \overset{*}{D}{}^{J'}_{MK'}(\Omega') \sum_m \overset{*}{D}{}^L_{0m}(\Omega') \langle \Phi | R(\Omega'') T^m_L | \Phi' \rangle \\
&\quad + \tfrac{1}{2} \sum_{KK'} \int d\Omega d\Omega'' D^J_{MK}(\Omega) \sum_{M'} \overset{*}{D}{}^{J'}_{MM'}(\Omega) \overset{*}{D}{}^{J'}_{M'K'}(\Omega'') \sum_m \overset{*}{D}{}^L_{0m}(\Omega) \langle \Phi | T^m_L R(\Omega'') | \Phi' \rangle \\
&= \frac{4\pi^2}{2J+1} \sum_{\substack{KK' \\ m}} \int d\Omega'' C(LJ'J; 0M) C(LJ'J; mK') \overset{*}{D}{}^J_{KK'+m}(\Omega'') \langle \Phi | R(\Omega'') T^m_L | \Phi' \rangle \\
&\quad + \frac{4\pi^2}{2J+1} \sum_{\substack{KK' \\ m}} \int d\Omega'' C(LJ'J; 0M)\, C(LJ'J; mK-m) \overset{*}{D}{}^{J'}_{K-m\,K'}(\Omega'') \langle \Phi | T^m_L R(\Omega'') | \Phi' \rangle \\
&= \frac{4\pi^2}{2J+1} C(LJ'J; 0M) \sum_{KK'm} \Big[C(LJ'J; mK') \int d\Omega'' \overset{*}{D}{}^J_{KK'+m}(\Omega'') \langle \Phi | R(\Omega'') T^m_L | \Phi' \rangle \\
&\quad + C(LJ'J; mK-m) \int d\Omega'' \overset{*}{D}{}^{J'}_{K-m\,K'}(\Omega'') \langle \Phi | T^m_L R(\Omega'') | \Phi' \rangle \Big].
\end{aligned}
$$

If one includes the normalisation $\sqrt{(2J+1)(2J'+1)}/8\pi^2$, the factor in front changes to $\frac{1}{2}\sqrt{(2J'+1)/(2J+1)}$. Finally the result can be brought into the completely symmetric form

$$
\begin{aligned}
&\langle JM | T^0_L | J'M \rangle = (-1)^{J-M-L} C(JJ'L; M-M) \langle J \| T_L \| J' \rangle \\
&\langle J \| T_L \| J' \rangle = N_J N_{J'} \frac{\sqrt{(2J+1)(2J'+1)}}{2(2L+1)} \sum_{KK'm} (-)^{J-K+L} \Big[C(JJ'L; K+m-K) \int d\Omega'' \overset{*}{D}{}^{J'}_{KK'} \langle \Phi | T^m_L R | \Phi' \rangle \\
&\quad + C(J'JL; K+m-K) \int d\Omega'' D^J_{KK'} \langle \Phi' | T^m_L R | \Phi \rangle^* \Big]
\end{aligned}
$$

$$
\text{with } N_J = \Big[\sum_{KK'} \int d\Omega \overset{*}{D}{}^J_{KK'} \langle \Phi | R | \Phi \rangle \Big]^{-1/2}. \tag{4.48}
$$

It is very important to have the result in an explicitly symmetric form if one wants to introduce approximations for the quantities $\langle \Phi | T^m_L R | \Phi' \rangle$ and $\langle \Phi' | T^m_L R | \Phi \rangle^*$.

Exactly this will be done now. As a first approximation one writes

$$
\langle \Phi' | T^m_L R | \Phi \rangle = \Big[a_m + \sum_{k=1}^{3} \hat{L}_k b_{km} \Big] \langle \Phi | R | \Phi \rangle. \tag{4.49}
$$

The resulting system of equations reads:

$$
\begin{aligned}
&\langle \Phi' | T^m_L | \Phi \rangle = a_m + \sum_{k=1}^{3} \langle \Phi | \hat{J}_k | \Phi \rangle b_{km} \\
&\langle \Phi' | T^m_L \hat{J}_l | \Phi \rangle = a_m \langle \Phi | \hat{J}_l | \Phi \rangle + \sum_{k=1}^{3} \langle \Phi | \hat{J}_k \hat{J}_l | \Phi \rangle b_{km} \\
&l = 1, 2, 3.
\end{aligned} \tag{4.50}
$$

Clearly $\langle \Phi | T^m_L R | \Phi' \rangle$ can be expanded in an analogous way. Because of the symmetry of $|\Phi\rangle$ and $|\Phi'\rangle$ under $\exp(i\pi J_x)$ many of the matrix elements in (4.50) vanish. Instead of using $\hat{L}_1 \hat{L}_2 \hat{L}_3$, one better uses $\hat{L}_{+1} \hat{L}_{-1} \hat{L}_0$ defined by:

$$\hat{L}_{+1}^{\text{lab}} = -\frac{1}{\sqrt{2}}(\hat{L}_1^{\text{lab}} + \mathrm{i}\hat{L}_2^{\text{lab}}), \qquad \hat{L}_{+1}^{\text{intr}} = -\frac{1}{\sqrt{2}}(\hat{L}_1^{\text{intr}} - \mathrm{i}\hat{L}_2^{\text{intr}})$$
$$\hat{L}_{-1}^{\text{lab}} = \frac{1}{\sqrt{2}}(\hat{L}_1^{\text{lab}} - \mathrm{i}\hat{L}_2^{\text{lab}}), \qquad \hat{L}_{-1}^{\text{intr}} = \frac{1}{\sqrt{2}}(\hat{L}_1^{\text{intr}} + \mathrm{i}\hat{L}_2^{\text{intr}}) \tag{4.51}$$
$$\hat{L}_0^{\text{lab}} = \hat{L}_3^{\text{lab}}, \qquad \hat{L}_0^{\text{intr}} = \hat{L}_3^{\text{intr}}.$$

For the quantities a_m^L and b_{km}^L one then obtains

$$a_m^L = \langle\Phi'|T_L^m|\Phi\rangle - \frac{\langle\Phi'|T_L^m \Delta\hat{J}_1|\Phi\rangle}{\langle\Phi|(\Delta J_1)^2|\Phi\rangle} \cdot \langle\Phi|\hat{J}_1|\Phi\rangle$$
$$b_{+1m}^L = \frac{\langle\Phi'|T_L^m \Delta\hat{J}_1|\Phi\rangle}{\langle\Phi|\Delta\hat{J}_1^2|\Phi\rangle} + \frac{\mathrm{i}\langle\Phi'|T_L^m \hat{J}_2|\Phi\rangle\langle\Phi|\hat{J}_3^2|\Phi\rangle - \frac{1}{2}\langle\Phi'|T_L^m \hat{J}_3|\Phi\rangle\langle\Phi|\hat{J}_1|\Phi\rangle}{\langle\Phi|\hat{J}_2^2|\Phi\rangle\langle\Phi|\hat{J}_3^2|\Phi\rangle - \frac{1}{4}\langle\Phi|\hat{J}_1|\Phi\rangle^2} \tag{4.52}$$
$$b_{-1m}^L = -\frac{\langle\Phi'|T_L^m \Delta\hat{J}_1|\Phi\rangle}{\langle\Phi|\Delta\hat{J}_1^2|\Phi\rangle} + \frac{\mathrm{i}\langle\Phi'|T_L^m \hat{J}_2|\Phi\rangle\langle\Phi|\hat{J}_3^2|\Phi\rangle - \frac{1}{2}\langle\Phi'|T_L^m \hat{J}_3|\Phi\rangle\langle\Phi|\hat{J}_1|\Phi\rangle}{\langle\Phi|\hat{J}_2^2|\Phi\rangle\langle\Phi|\hat{J}_3^2|\Phi\rangle - \frac{1}{4}\langle\Phi|\hat{J}_1|\Phi\rangle^2}$$
$$b_{0m}^L = \frac{\langle\Phi'|T_L^m \hat{J}_3|\Phi\rangle\langle\Phi|\hat{J}_2^2|\Phi\rangle + (1/2\mathrm{i})\langle\Phi'|T_L^m \hat{J}_2|\Phi\rangle\langle\Phi|\hat{J}_1|\Phi\rangle}{\langle\Phi|\hat{J}_2^2|\Phi\rangle\langle\Phi|\hat{J}_3^2|\Phi\rangle - \frac{1}{4}\langle\Phi|\hat{J}_1|\Phi\rangle^2}.$$

With the relations

$$\hat{L}_k^{\text{lab}} D_{KK'}^J = \sqrt{J(J+1)}\, C(J1J; Kk) D_{K+k\,K'}^J$$
$$\hat{L}_k^{\text{intr}} D_{KK'}^J = \sqrt{J(J+1)}\, C(J1J; Kk) D_{K\,K'+k}^J, \tag{4.53}$$

the final expression for the reduced matrix element reads

$$\langle J\|T_L\|J'\rangle = N_J N_{J'} \frac{\sqrt{(2J+1)(2J'+1)}}{2(2L+1)} (-1)^{J-L} \Bigg\{ \sum_{KK'mk} (-1)^K C(JJ'L; K+m-K)$$
$$\times [a_m^{*L}\delta_{k0} n_{KK'}^J + \tfrac{1}{2}\sqrt{J(J+1)}\, b_{km}^{*L} [C(J1J; Kk) n_{K+k,K'}^J + (-1)^k C(J1J; K'-k) n_{KK'-k}^J]]$$
$$+ (-1)^K C(J'JL; K+m-K)[a_m'^L \delta_{k0} n'^{*J'}_{KK'} + \tfrac{1}{2}\sqrt{J'(J'+1)}\, b_{km}^L [C(J'1J'; Kk) n'^{*J'}_{K+k\,K'}$$
$$+ (-1)^k C(J'1J'; K'-k) n'^{*J'}_{K\,K'-k}]]\Bigg\}.$$

Here $n_{KK'}^J$ is computed with $|\Phi\rangle$ and $n'^{J'}_{KK'}$ with $|\Phi'\rangle$. The same holds for a_m^L and a'^L_m as well as b_{km}^L and b'^L_{km}.

5. Applications

5.1. Hartree–Fock calculations with effective interactions

The most sophisticated Hartree–Fock calculations were done with effective interactions derived from nucleon–nucleon interactions which describe scattering data very well. Table 1 lists a sample

Table 1

Experimental and calculated root mean square radii and binding energies per nucleon [9, 32, 33, 34].

		Experiment	Negele [9]	Campi and Sprung [32]	Nemeth et al. [33]	Skyrme III [34]
^{16}O	E	−7.98	−6.75	−7.68	−7.98	−7.96
	r_c	2.73	2.80	2.75	2.77	2.69
^{40}Ca	E	−8.55	−7.49	−8.33	−8.47	−8.54
	r_c	3.49	3.49	3.49	3.40	3.48
^{48}Ca	E	−8.67	−7.48	−8.40	−8.55	−8.71
	r_c	3.48	3.52	3.51	3.44	3.53
^{90}Zr	E	−8.71	−7.85	−8.63	−8.70	−8.71
	r_c	4.23	4.25	4.27	4.13	4.32
^{208}Pb	E	−7.87	−7.53	−7,87	−7.87	−7.87
	r_c	5.50	5.44	5.45	5.22	5.57

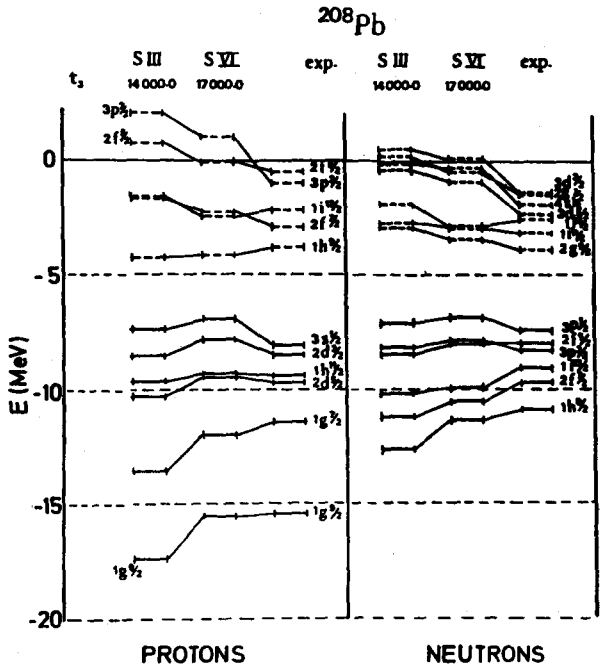

Fig. 1. Experimental and calculated single particle energies in the lead region. Calculated values were obtained with two different versions of the Skyrme-force [34].

of representative results [9, 10, 32, 33]. Also listed are results obtained with the Skyrme force [37], which show that this phenomenological force does as well in describing the existing data, as the more fundamental effective interactions. Most important is the fact that the Hartree–Fock energies give essentially the correct ordering of the single particle levels in nuclei like ^{209}Pb, ^{207}Pb, ^{209}Bi,

Table 2
Experimental and calculated quadrupole moments and binding energies for various rare earch nuclei [35].

Nucleus	$Q_{exp.}$	$Q_{calc.}$	$E_{exp.}$	$E_{calc.}$
^{152}Sm	590	600	1253.1	1243.1
^{158}Gd	736	722	1295,9	1284.5
^{162}Dy	720	752	1324.1	1312.1
^{166}Er	770	789	1351.6	1339.0
^{174}Yb	758	782	1406.6	1393.4
^{178}Hf	682	712	1432.9	1420.0
^{184}W	615	633	1473.0	1459.0
^{190}Os	511	472	1512.8	1498.0

^{207}Tl. This means nothing less than that the most important and decisive part of the nuclear interaction is taken into account. More evidence for this are the results for deformed nuclei given in table 2 [35]. In this context it must, however, be mentioned that in these calculations the effects of pair-correlations have been taken into account by adding to the Skyrme interaction a pairing force of such a strength that the experimental energy gap is reproduced. The question how to improve this, not completely satisfactory, procedure will be taken up in connection with HFB theory.

Summing up one may say that the theory is in good shape as far as the calculation of properties of nuclear groundstates is concerned. For details the reader is referred to ref. [34], where also many references to earlier work can be found.

5.2. HFB calculations

As has been mentioned in the preceeding section pairing-correlations were ad hoc put into the calculations with the Skyrme force. Of course, one should perform a full HFB calculation with the Skyrme force (or even a "better" effective force [36]). It is, however, unknown whether it is possible to find a set of parameters t_i (compare eq. (2.6)) which produce the required pairing properties. The reason why one would like to work with the Skyrme force is that in this case the energy gap $\Delta(x, x')$ is a local function $\Delta(x)\,\delta(x-x')$ as is the average potential, $\Gamma(x)\cdot\delta(x-x')$. This in turn implies that the HFB equations are just a set of coupled non-linear differential equations.

Nevertheless, important insight into nuclear structure has been gained by doing HFB calculations with much simpler effective forces like the quadrupole-quadrupole plus pairing force (compare eq. (2.8)).

I shall not dwell upon the classical papers by Baranger and Kumar on this subject [13] but try to discuss some of the more recent developments. They mostly deal with rotational states in deformed nuclei [37,38].

The basic assumptions are as follows: A core of nucleons is considered as inert and the interaction of this core with the "valence" nucleons is taken into account through single particle energies t_{nlj}. The Hamiltonian of the system is then

$$H = \sum_{nljm} t_{nlj} C^{+}_{nljm} C_{nljm} + G \sum_{\substack{n_1 l_1 j_1 m_1 \\ n_2 l_2 j_2 m_2}} C^{+}_{n_1 l_1 j_1 m_1} C^{+}{}_{n_1 l_1 j_1 - m_1} C_{n_2 l_2 j_2 - m_2} C_{n_2 l_2 j_2 m_2} \tag{5.1}$$

$$+ \frac{Q}{2} \sum_{\substack{n_1 l_1 j_1 m_1 ; n_3 l_3 j_3 m_3 ; \\ n_2 l_2 j_2 m_2 ; n_4 l_4 j_4 m_4}} (r^2 Y^{\mu}_2)_{n_1 l_1 j_1 m_1 ; n_3 l_3 j_3 m_3} (r^2 \overset{*}{Y}{}^{\mu}_2)_{n_2 l_2 j_2 m_2 ; n_4 l_4 j_4 m_4} C^{+}_{n_1 l_1 j_1 m_1} C^{+}_{n_2 l_2 j_2 m_2} C_{n_4 l_4 j_4 m_4} C_{n_3 l_3 j_3 m_3}.$$

For the calculations described in detail in ref. [37] the parameters t_{nlj} were taken from the work by Gustafson and Nilsson [39] with a slight shift of the energies of neutrons of positive parity. These energies are given in table 3 together with the force constants of the quadrupole quadrupole and the pairing force.

The HFB equations were solved by an iterative procedure for various nuclei and several suitably chosen cranking frequencies for each nucleus. The physical quantities which have been extracted from the solutions are listed below.

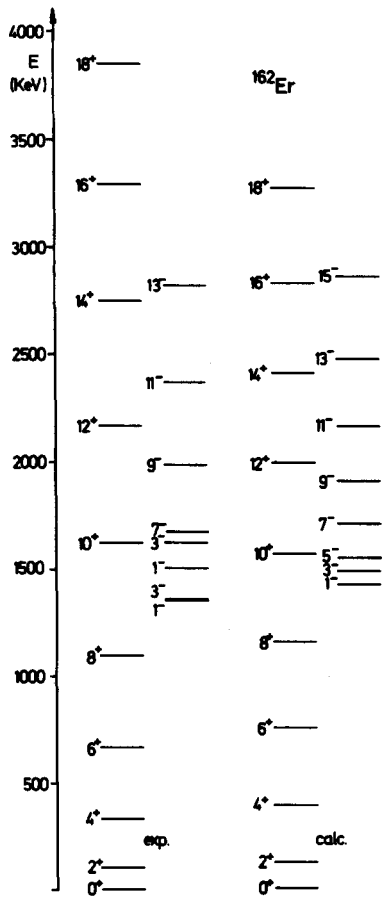

Fig. 2a. Experimental and calculated energy levels of ^{162}Er. Calculated values were obtained with the single particle energies and force constants given in table 3.

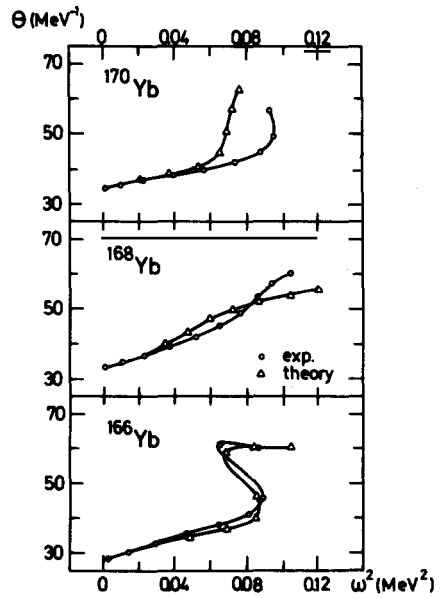

Fig. 2b. Moments of inertia of the Y-rast bands of ^{166}Yb, ^{168}Yb and ^{170}Yb versus the square of the angular frequency ω^2. After Faessler et al. [38].

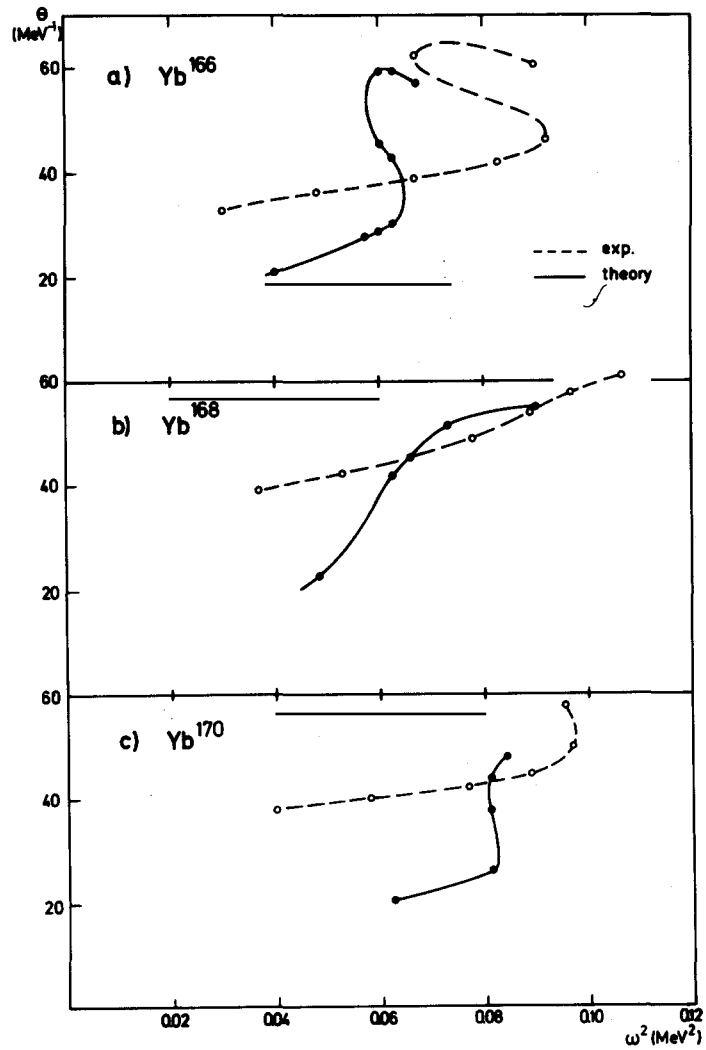

Fig. 2c. Moments of inertia of the Y-rast bands of ^{166}Yb, ^{168}Yb and ^{170}Yb versus the square of the angular frequency ω^2 [41].

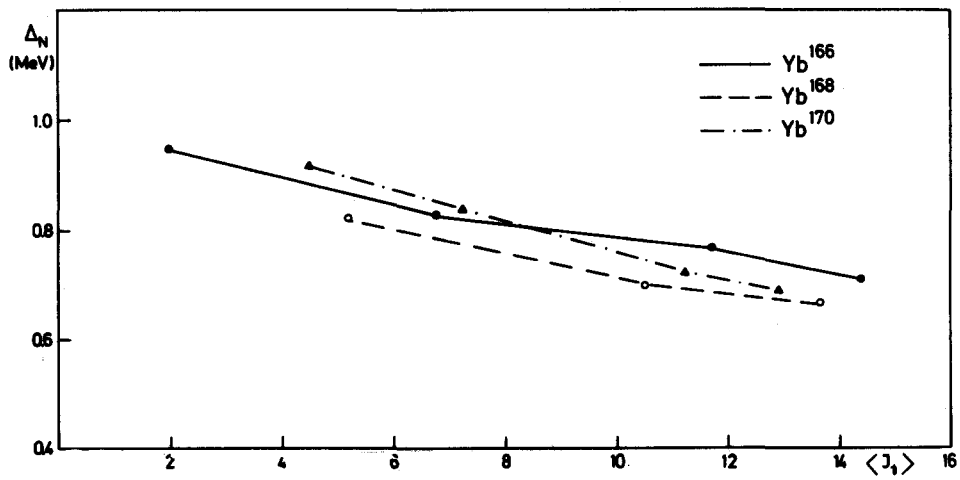

Fig. 2d. Energy gap Δ of neutrons as a function of $\langle J_1 \rangle$ for ^{166}Yb, ^{168}Yb and ^{170}Yb.

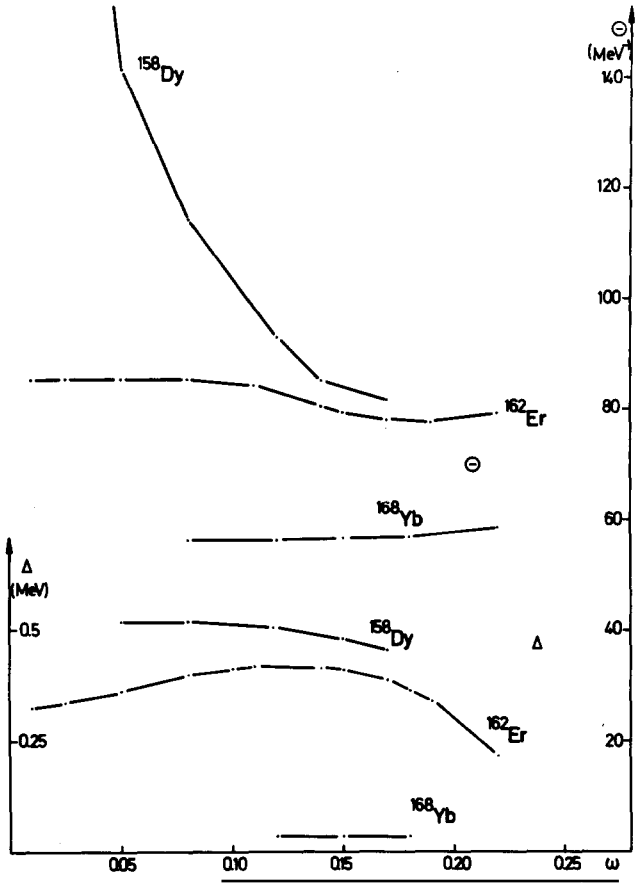

Fig. 3. Moments of inertia and energy gaps for rotational bands of negative parity in ^{158}Dy, ^{162}Er and ^{168}Yb.

Table 3

Spherical single particle energies and coupling constants. The values given for t_{nlj} correspond to ^{162}Er. Those for other nuclei are slightly different because of the factor $A^{-1/3}$ in $\hbar\omega = 41/A^{1/3}$ MeV.

Protons		Neutrons		
nlj	t_{nlj}	nlj	t_{nlj}	
$1g_{9/2}$	−5.002	$1i_{13/2}$	−0.250	$Q_{nn} = -0.034$ MeV/b^4
$1g_{7/2}$	−0.677	$2g_{9/2}$	5.842	$Q_{pp} = -0.034$ MeV/b^4
$2d_{5/2}$	0.0000	$1h_{11/2}$	−5.979	$Q_{np} = -0.089$ MeV/b^4
$2d_{3/2}$	2.422	$2f_{1/2}$	−1.579	$G_n = -0.139$ MeV
$3S_{1/2}$	2.708	$1h_{9/2}$	−0.790	$G_p = -0.190$ MeV
$1h_{11/2}$	0.955	$3p_{3/2}$	1.467	$b = (\hbar/m\omega)^{1/2}$ oscillator length
$1h_{9/2}$	6.205	$2f_{5/2}$	1.918	
		$3p_{1/2}$	2.933	

1) Energy levels and moments of inertia of rotational bands in even nuclei. This includes the "back-bending" effect [40], see figs. 2a, 2b, 2c, 3.
2) Energy levels, moments of inertia and decoupling factors of rotational bands in odd mass nuclei, figs. 4, 5, 6, 7.

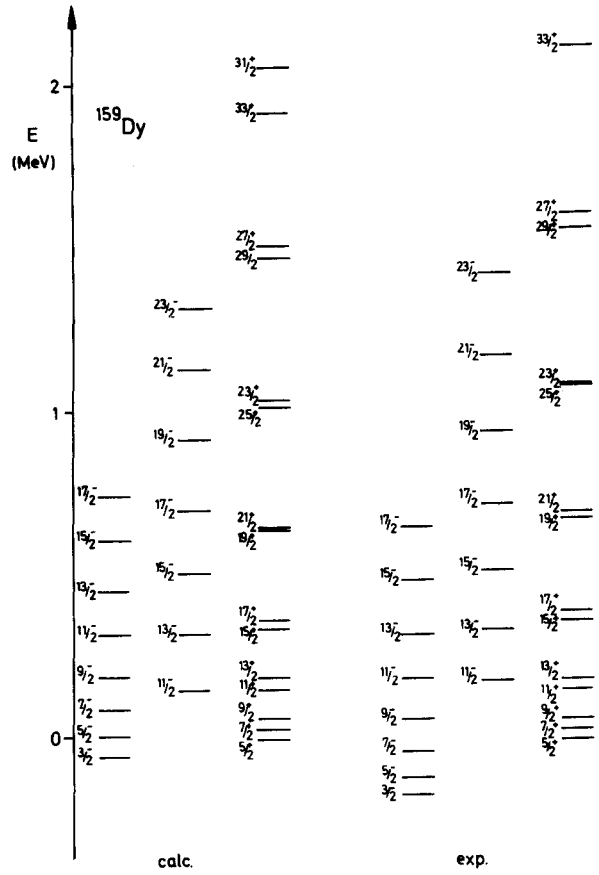

Fig. 4. Experimental and calculated energy levels of ^{159}Dy [45, 37].

3) Intrinsic quadrupole moments $Q_0 = \sqrt{\frac{16\pi}{5}}\langle T^2 Y_2^0\rangle$ and $Q_2 = \sqrt{\frac{16\pi}{5}}\langle r^2 Y_2^2\rangle$ of even and odd mass nuclei, figs. 8a, 8b.
4) Occupation probabilities, energy gaps and single-particle wavefunctions, table 4, figs. 2d, 9a, 9b, 9c, 10a, 10b.
5) Quadrupole moments, fig. 11.

Before these results can be discussed, a few words must be said about the somewhat different methods of calculating the quantities listed above. The various methods differ essentially only in two respects; the sophistication with which conservation laws are treated and the flexibility of the intrinsic wavefunction. Whereas the results of ref. [37] have been obtained in a fully selfconsistent way but with angular momentum and particle number conservation treated in the cranking and BCS approximation respectively, the results depicted in fig. 2b [38] and 2c [41] have been obtained with a refined treatment of particle number [38, 41] and angular momentum conservation [38]. The price one pays in the latter cases is that selfconsistency is replaced by a variation with respect to a few parameters like deformations and energy gaps. Moreover the intrinsic wavefunctions of ref. [38] are always axially symmetric ($J_3|\Phi\rangle = 0$).

Despite such differences some general features emerge from the material presented.

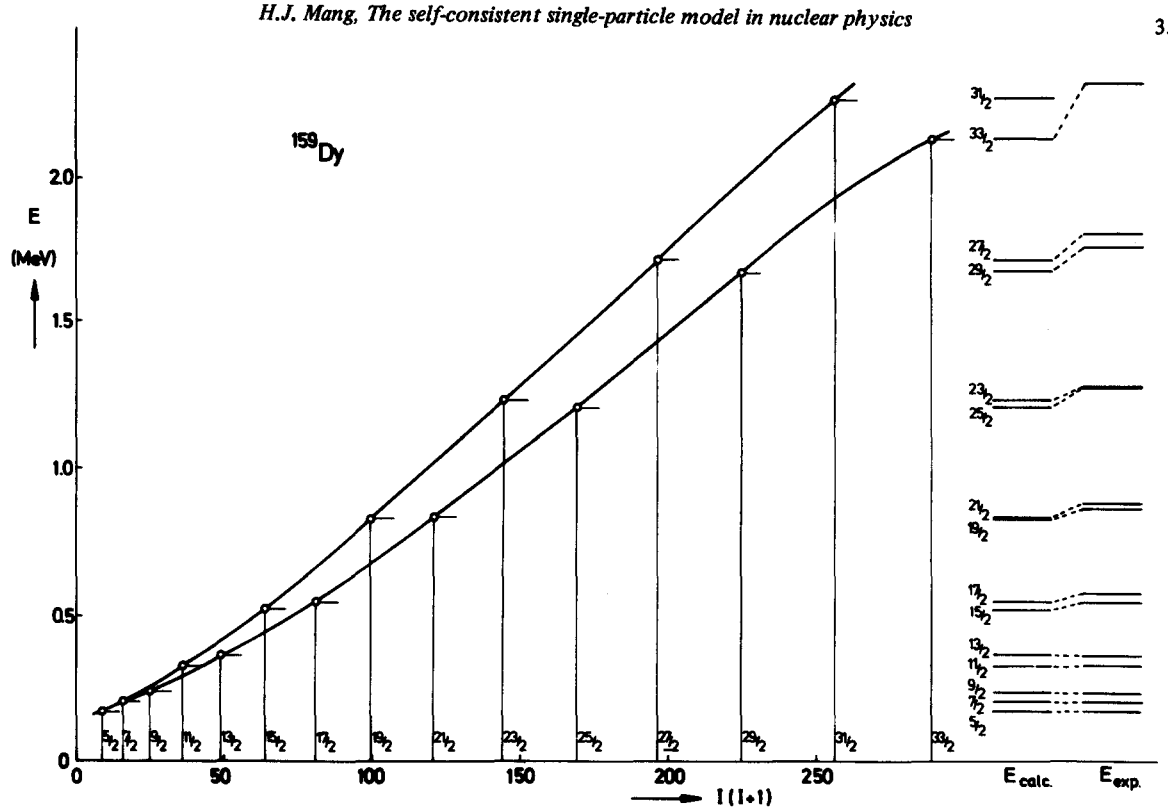

Fig. 5a. Energy of the rotational band of positive parity in ^{159}Dy versus $J(J+1)$ [37, 45].

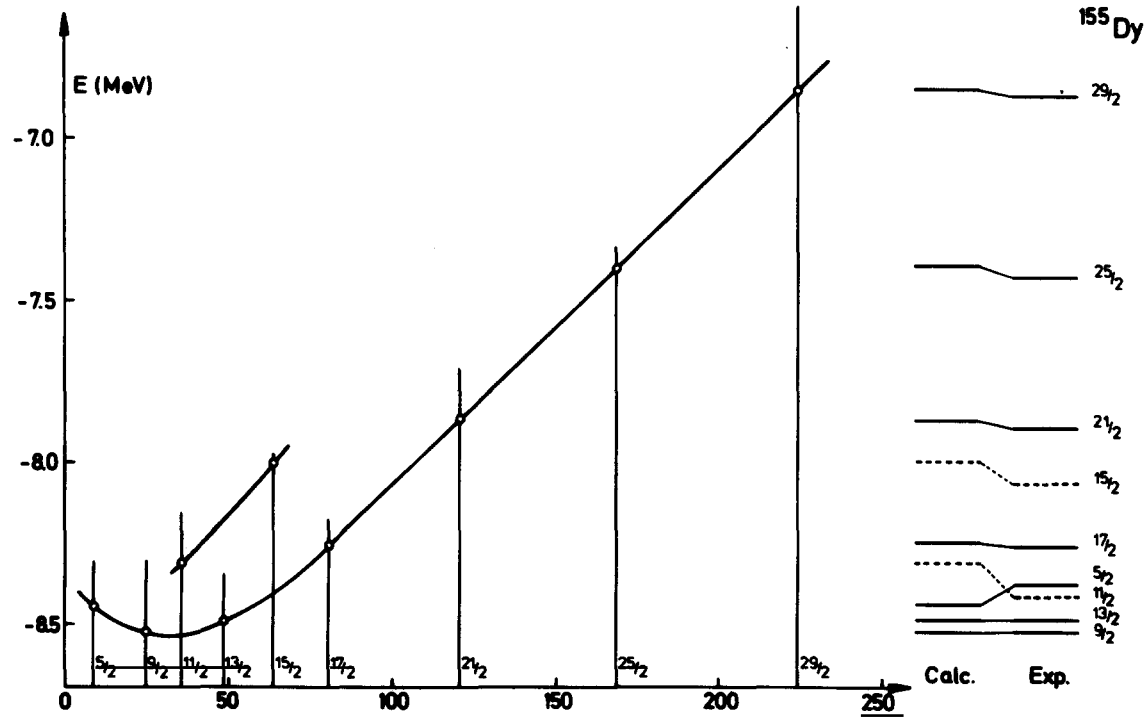

Fig. 5b. Energy of the rotational band of positive parity in ^{155}Dy versus $J(J+1)$ [37, 45].

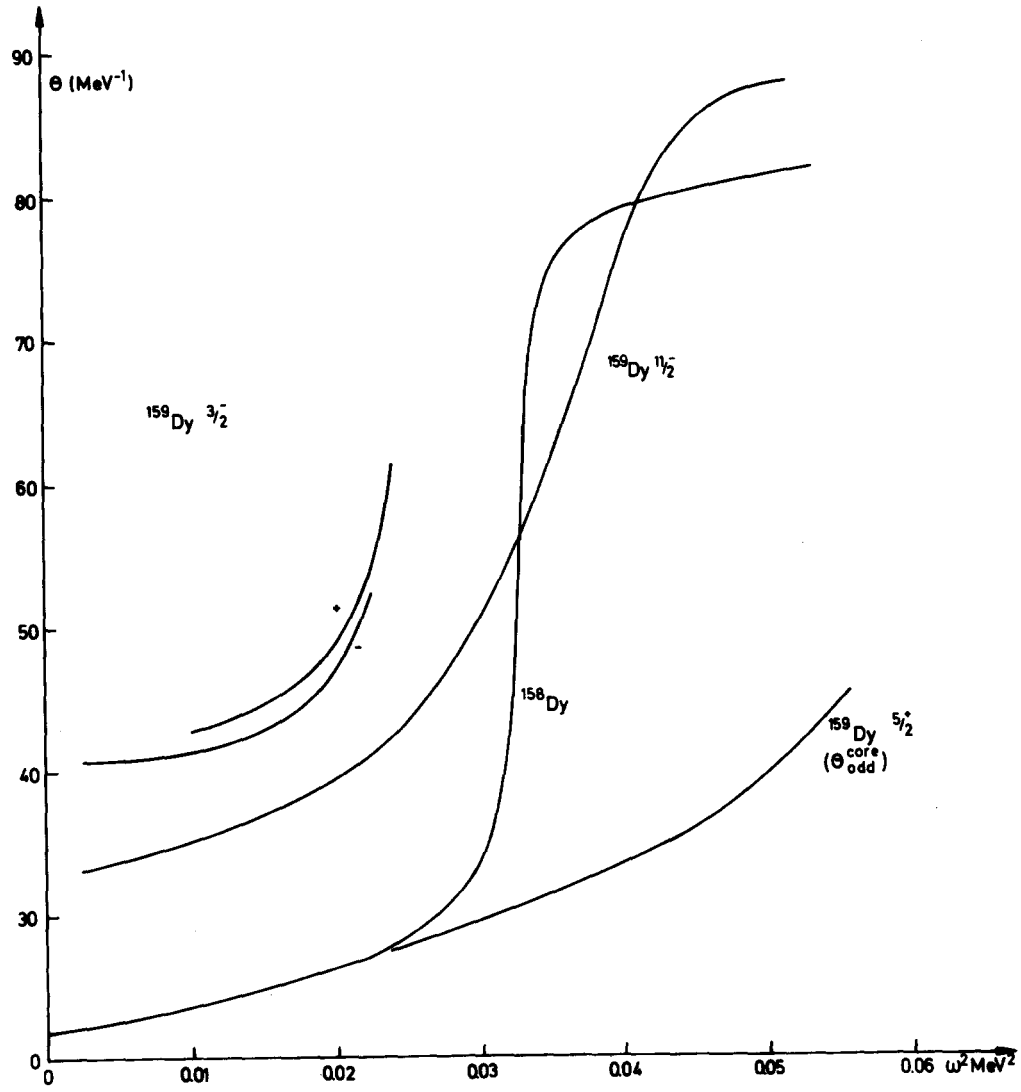

Fig. 6. Moments of inertia versus ω^2.

The often rapid increase of the moment of inertia of groundstate rotational bands is caused by two effects. The Coriolis antipairing which reduces the energy gap with increasing angular momentum on the one hand and the alignment of two quasi-particles along the axis of rotation on the other hand. In the case presented in figs. 2a and 2c back-bending occurs because the energy gap of one pair of quasi-particles – the one that aligns – goes to zero much faster than the rest of the energy gaps. Of course, one could have asked the question whether projection of particles number could not change the picture obtained in ref. [37] substantially [31]. In order to answer such a question the simplified calculation with inclusion of particle number projection of ref. [41] was performed (fig. 2c). Instead of varying the HFB-wavefunction $|\Phi\rangle$ only the energy gap of neutrons Δ_N was varied. The results given in fig. 2c and 2d fully confirm the conclusions drawn from the self-consistent calculation without projection of particle number.

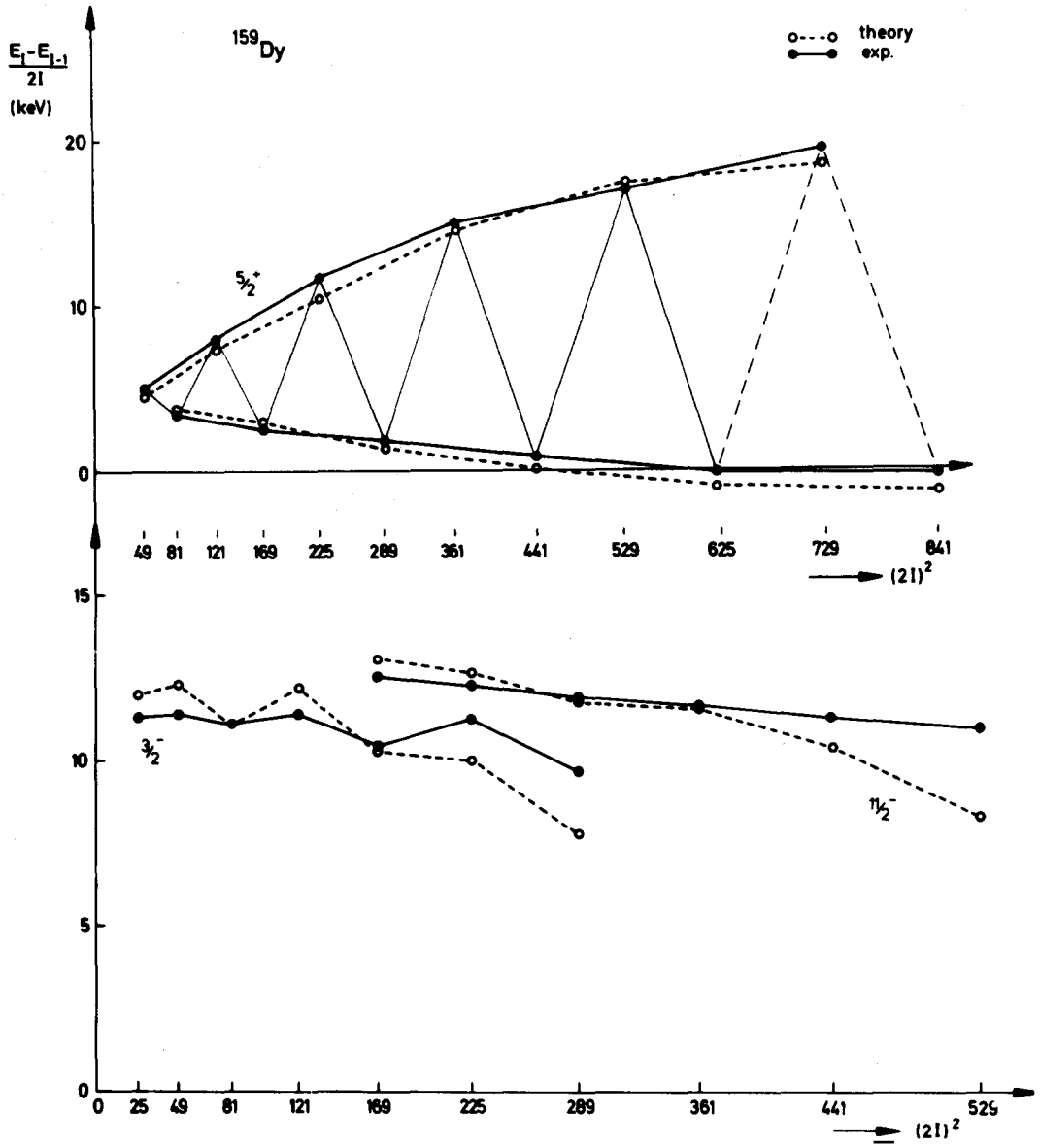

Fig. 7. The quantity $(E_J - E_{J-1})/2J$ as a function of $(2J)^2$ for the three bands of ^{159}Dy.

Another important feature concerns the rotational bands of negative parity. Their moments of inertia are rather constant and large from the beginning [42] with the exception of ^{158}Dy. This indicates that they can be interpreted as two quasi-particle bands. The quasi-particle of positive parity aligns quite easily and ensures at the same time, by blocking the aligned state, that the moment of inertia of the core remains practically constant. It is worthwhile to note that the usual relation between energy gap and moment of inertia is inverted for these bands as can be seen in fig. 3. The

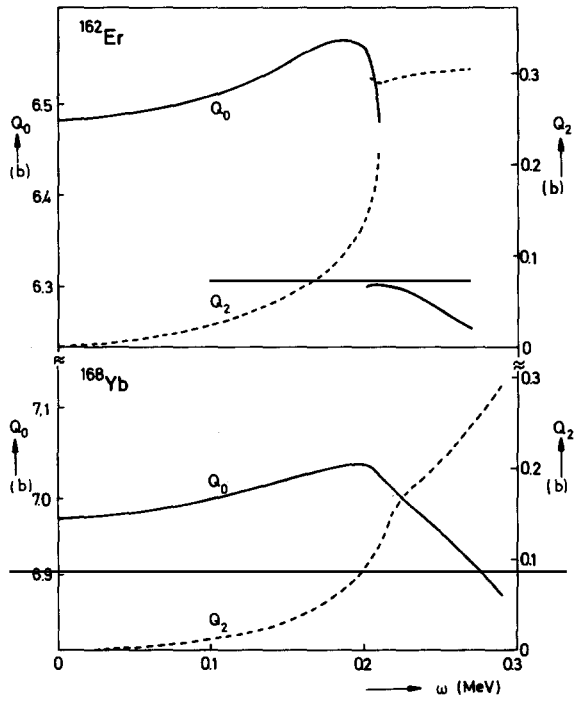

Fig. 8a. Intrinsic quadrupole moments $Q_0 = \sqrt{16\pi/5}\langle\Phi|r^2 Y_2^0|\Phi\rangle$ and $Q_2 = \sqrt{16\pi/5}\langle\Phi|r^2 Y_2^2|\Phi\rangle$ versus ω for ^{163}Er and ^{168}Yb.

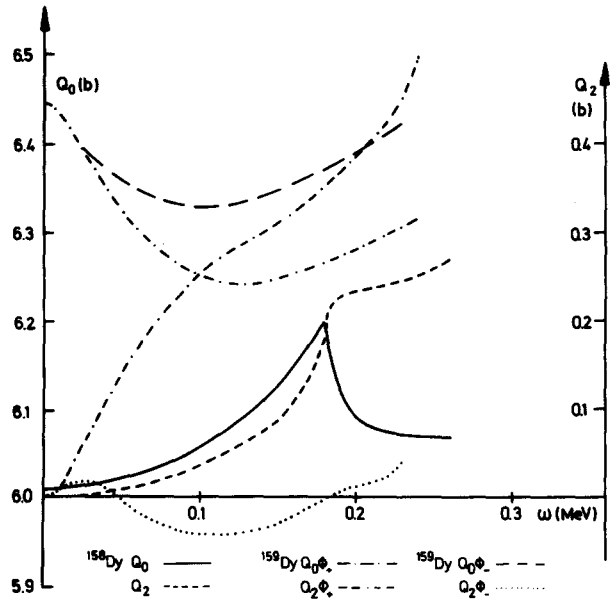

Fig. 8b. Intrinsic quadrupole moments Q_0 and Q_2 versus ω^2 for ^{158}Dy and ^{159}Dy ($5/2^+$ band).

reason is that a large energy gap favors the alignment of a one quasi-particle state. This shows up also in rotational bands of odd mass nuclei.

Turning to these nuclei one realizes right away that one of the problems to be discussed is band mixing [43] and attenuation factors [44]. The best examples are bands of positive parity in some of the lighter rare earth elements like ^{159}Dy and ^{155}Dy [45]. Clearly calculated and experimental values of the excitation energies are in astonishingly good agreement, indeed, in much better agreement than was seen in even nuclei. The reason is that the odd particle dominates the structure of the levels up to spins of approximately 21/2. Only beyond this point one notices that the contribution of the core to the moment of inertia increases too rapidly. Consequently calculated levels lie below the experimental ones. The wavefunctions of the odd particle of even parity (figs. 9a, 9b) show very clearly the alignment and finally decoupling from the collective rotation. For angular momenta greater than 19/2 the wavefunction and the contribution to the angular momentum $\langle J_1\rangle$ are practically constant which means that the particle is completely decoupled from the rotation. For ^{155}Dy the effect is even more pronounced than for ^{159}Dy because there, the band is a $1/2^+$ band from the outset. There can be no doubt that no additional attenuation of the Coriolis matrix elements is needed in order to explain the experimental data [37, 46]. The $11/2^-$ band in contrast behaves quite normal and its moment of inertia is very similar to the one of the neighbouring even nucleus ^{158}Dy. The minor changes result from changes in pairing correlations because of the blocking effect. It is worthwhile to mention that a compar-

Table 4

Occupation number V_K^2, energy gap parameter $\Delta_{K\bar{K}}$, single particle energies h_{KK} and matrix elements of the angular momentum J^1_{KK} of some single particles states K, which diagonalize the density matrix ρ for different values of the cranking frequency ω; a) ^{162}Er, b) ^{168}Yb.

a) ^{162}Er

	K	V_K^2	$\Delta_{K\bar{K}}$(MeV)	h_{KK}(MeV)	J^1_{KK}
($\omega = 0.0$	1	0.899	0.906	−1.200	0.0
$\langle J_1\rangle = 0$)	2	0.833	0.907	−0.812	0.0
	3	0.520	0.902	−0.036	0.0
	4	0.112	0.891	1.094	0.0
	5	0.029	0.873	2.436	0.0
($\omega = 0.200$	1	0.939	0.657	−0.810	1.983
$\langle J_1\rangle = 7.16$)	2	0.926	0.738	−1.183	0.123
	3	0.437	0.625	−0.133	−1.067
	4	0.068	0.697	1.046	−0.733
	5	0.020	0.718	2.430	−0.183
($\omega = 0.206$	1	0.998	0.104	−0.497	5.230
$\langle J_1\rangle = 16.02$)	2	0.960	0.463	−1.063	0.169
upper	3	0.148	0.369	0.419	0.263
	4	0.012	0.447	1.943	−0.065
	5	0.004	0.465	3.810	−0.049
($\omega = 0.270$	1	1.000	0.026	−0.477	5.510
$\langle J_1\rangle = 20.25$)	2	0.981	0.301	−0.849	0.801
	3	0.103	0.233	0.171	−0.499
	4	0.006	0.317	2.019	−0.093
	5	0.002	0.321	3.764	−0.069

b) ^{168}Yb

	K	V_K^2	$\Delta_{K\bar{K}}$(MeV)	h_{KK}(MeV)	J^1_{KK}
($\omega = 0.0$	1	0.971	0.760	−2.130	0.0
$\langle J_1\rangle = 0$)	2	0.956	0.769	−1.720	0.0
	3	0.882	0.780	−0.928	0.0
	4	0.331	0.766	0.274	0.0
	5	0.044	0.770	1.710	0.0
($\omega = 0.200$	1	0.989	0.465	−2.176	0.317
$\langle J_1\rangle = 9.90$)	2	0.982	0.471	−1.745	−0.052
	3	0.978	0.381	−0.836	2.114
	4	0.125	0.358	0.068	−1.704
	5	0.017	0.464	1.653	−0.469
($\omega = 0.210$	1	0.994	0.329	−2.044	0.868
$\langle J_1\rangle = 10.90$)	2	0.991	0.266	−0.965	2.204
	3	0.989	0.345	−1.717	−0.168
	4	0.063	0.233	−0.047	−0.220
	5	0.009	0.342	1.622	−0.464
($\omega = 0.270$	1	1.000	0.012	−0.860	5.020
$\langle J_1\rangle = 17.02$)	2	1.000	0.029	−2.090	0.309
	3	1.000	0.027	−1.466	−0.750
	4	0.000	0.012	1.418	0.083
	5	0.000	0.027	−0.161	−3.838

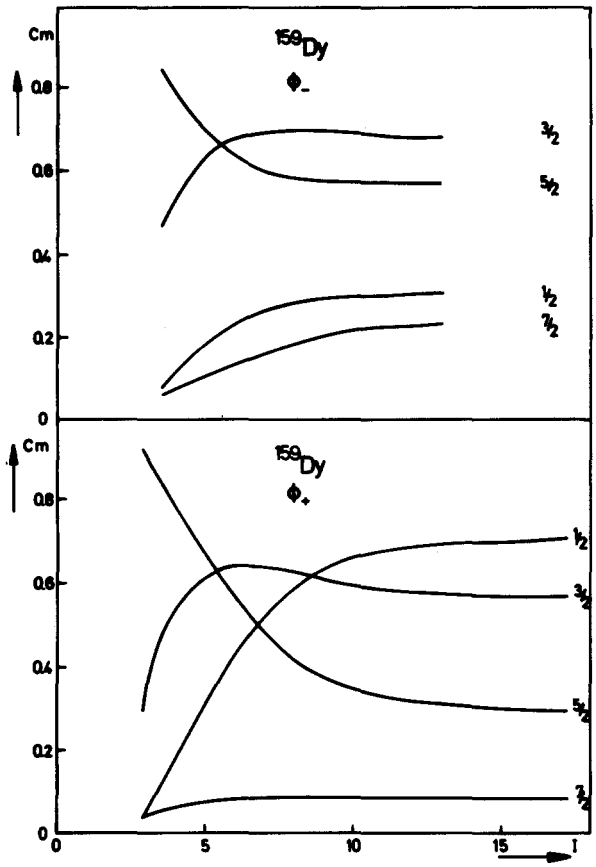

Fig. 9a. Amplitudes $c_m(i_{13/2})$ of the single particle state of the odd nucleon in the even parity band of ^{159}Dy as a function of $I = \sqrt{\langle J_1 \rangle^2 + \langle J_3^2 \rangle}$.

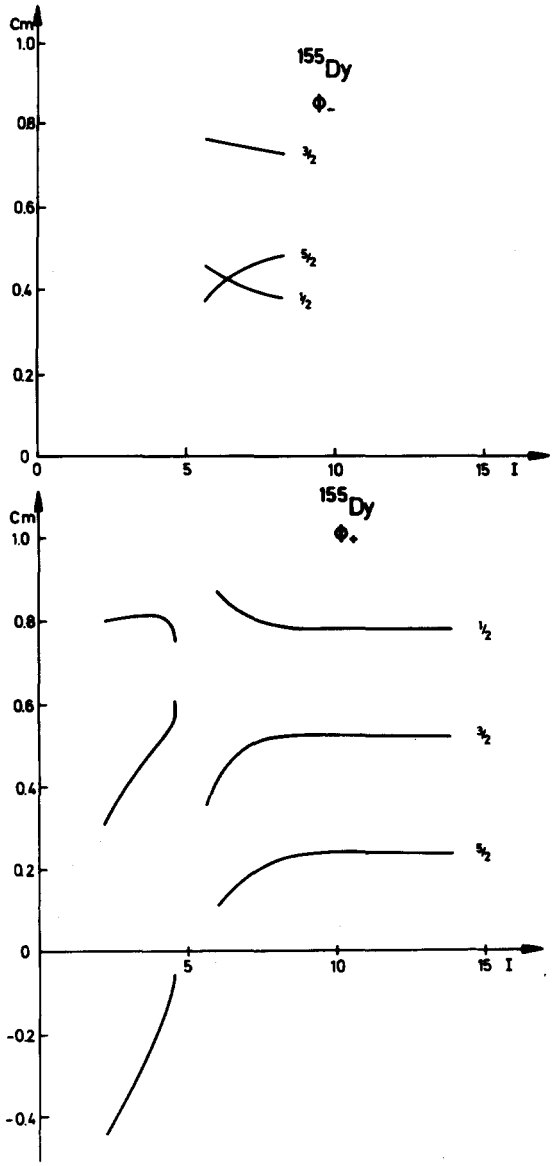

Fig. 9b. The same as in fig. 9a for ^{155}Dy.

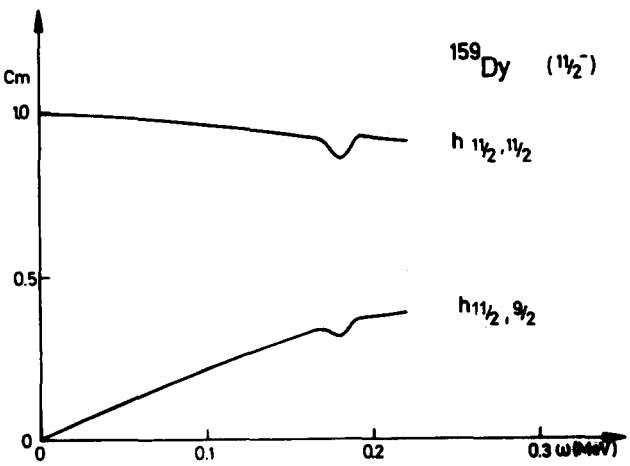

Fig. 9c. Amplitudes of the single particle state of the odd nucleon in the $11/2^-$ band of ^{159}Dy as a function of ω

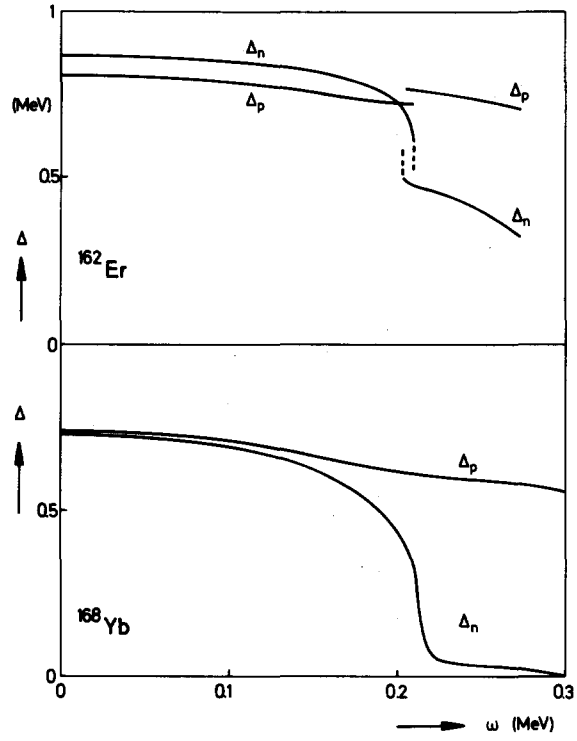

Fig. 10a. Energy gap Δ as a function of ω for ^{162}Er and ^{168}Yb. The values Δ_p, Δ_n correspond to an averaged energy gap for protons and neutrons respectively.

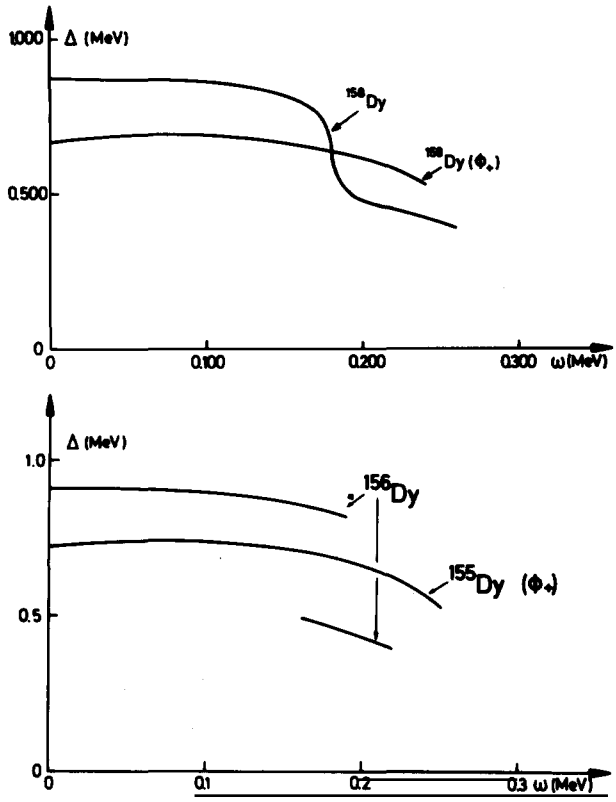

Fig. 10b. Energy gaps of ^{155}Dy, ^{156}Dy, ^{158}Dy, ^{159}Dy versus ω.

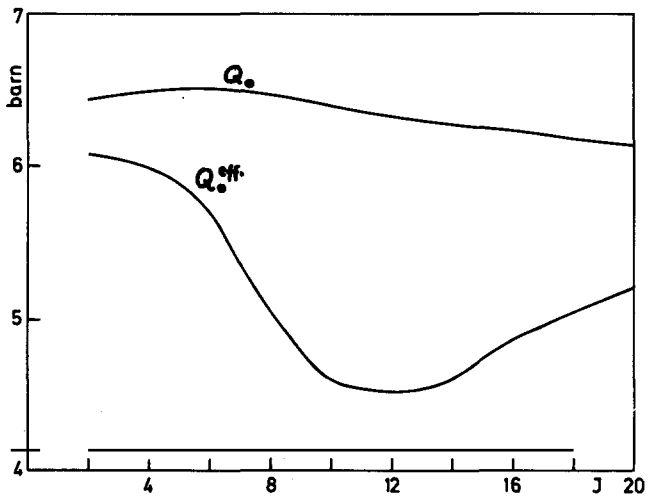

Fig. 11. Calculated effective quadrupole moment Q_0^{eff} and intrinsic quadrupole moment Q_0 as a function of J for ^{162}Er. The smooth curves are only drawn to guide the eye.

ison of the moment of inertia of the "even core" in the $5/2^+$-band with the moment of inertia of ^{158}Dy clearly shows the effect of blocking the state of the "easily alignable particle". Finally the $3/2^-$ band lies somewhat in between the two extremes. It is slightly disturbed by the mixing with a $1/2^-$ band. Before going on, a brief comment is in order, on why no attenuation factors are necessary in a self-consistent calculation. This is most clearly seen by comparing the Coriolis coupling term in the self-consistent treatment and in the conventional particle plus rotor model. The terms to be compared are

$$\omega j_1 \text{ and } \boldsymbol{j}\cdot\boldsymbol{J}/\Theta_{\text{rotor}}$$

$$\text{or } j_1\langle J_1\rangle/\Theta_{\text{s.c.}} \text{ and } \boldsymbol{j}\cdot\boldsymbol{J}/\Theta_{\text{rotor}}$$

($\Theta_{\text{s.c.}}$ = selfconsistent moment of inertia).
The essential difference is that in the selfconsistent treatment $\Theta_{\text{s.c.}}$ appears in the denominator instead of Θ_{rotor}. If the matrix elements of j_1 are large then they also contribute significantly to $\Theta_{\text{s.c.}}$ which is then large [47] in particular much larger than Θ_{rotor}. Thus the coupling term is drastically reduced.

Concerning the intrinsic quadrupole moments Q_0 and Q_2 one may say that in general the variation of Q_0 and Q_2 with angular momentum is of the same order of magnitude as can be read off figs. 8a, 8b directly. Spectroscopic quadrupole moments were calculated with the formulas given in section 4. As far as deviations from the adiabatic limit are concerned there are two possible sources. First angular momentum projection may give rise to additional terms beyond the ones obtained in the adiabatic limit. Moreover changes in the intrinsic wavefunction with angular momentum may lead to a dependence of moments on angular momentum [47]. These two effects can be separated qualitatively in the following manner:

In the adiabatic approximation when the wavefunction is written as

$$|JM\rangle = \sqrt{\frac{2J+1}{8\pi^2}}\, D^J_{M0}|\Phi_0\rangle$$

the reduced matrixelement of the quadrupole operator is given by

$$\langle J\|r^2 Y_2\|J\rangle = \frac{2J+1}{5}\, C(JJ2;00)\,\langle\Phi_0|r^2 Y^0_2|\Phi_0\rangle\,.$$

Therefore an effective intrinsic quadrupole moment Q_0^{eff} is defined by

$$Q_0^{\text{eff}} = \frac{5}{2J+1}\,\frac{\langle J\|r^2 Y_2\|J\rangle}{C(JJ2;00)}\,\sqrt{\frac{16\pi}{5}}$$

where $\langle J\|r^2 Y_2\|J\rangle$ is computed with the help of eqs. (4.52) and (4.55).

Results for ^{162}Er are given in fig. 11 [47] and show clearly that the effect of angular momentum projection is quite substantial in particular for high angular momenta.

For transition rates no results are yet available but there the situation is even more complicated by the incomplete overlap of the intrinsic wavefunctions of initial and final state which may be as low as 0.8 for angular momenta $J_i = 14$ and $J_f = 12$.

Summing up one may conclude that the results obtained up to now warrant further systematic studies of nuclear structure within the selfconsistent single particle model, hopefully with more realistic effective forces and in a less restricted single particle configuration space.

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