ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
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ИССЛЕДОВАНИЙ

Дубна

E4 - 4523

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A GENERALIZED TREATMENT OF THE ROTATION-PARTICLE COUPLING IN ODD-MASS DEFORMED NUCLEI

ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

1969

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Submitted to Nucl. Phys.

1. Introduction

In recent years, an increasing number of experimental data indicates that the simple adiabatic description of low-energy spectra of odd-mass deformed nuclei based on the Nilsson model is valid to a certain extent only. In particular, a very large mixing of single-particle states from different harmonic oscillator shells (N -mixing) has been observed in the Gd , Dy and Er nuclei. Another example is the mixing associated with the Coriolis force (K -mixing). Both effects have been discussed in detail in a number of papers (see, e.g. refs. /1-3/). Hence we face the necessity to improve the single-particle description.

Recently, the theoretical treatment, using the Woods-Saxon's type of potential /4,5/ has been proved to be very useful in the analysis of the mixing of states from different major shells /6/. A systematic analysis of the K -mixing induced through Coriolis coupling of rotational bands was developed by Bohr and Mottelson in terms of the perturbation expansion /7,8/. However, when K -mixing becomes of importance one has to use the nonadiabatic rotational model. For the two interacting rotational bands with $\Delta K = 1$

the problem has been solved by Kerman[9]. A more general case has been investigated by Brockmeier et al.[10], and, more recently, by Bunker and Reich[11]. But their least-squares fits to energy levels require a considerable number of input parameters.

In the present works, we shall describe a method by which an exact diagonalization of the Coriolis coupling term can be made and shall show results of some initial calculations. The outline of this method has been reported recently by one of the authors (M. Ch.)[12].

2. Theoretical Consideration

The Hamiltonian of the problem for the axially-symmetric nucleus can be written in the form[7,9]

$$H = H_{s.p.} + H_{rot} + H_C , \tag{1}$$

where $H_{s.p.}$ describes the single-particle motion, H_{rot} is the rotational energy, and H_C represents the Coriolis force, which gives rise to a coupling between rotational bands. This term is of the form

$$H_C = -\frac{\hbar^2}{2J}[I_+ j_- + I_- j_+] \tag{2}$$

with the usual definition

$$I_\pm = I_x \pm i I_y , \quad j_\pm = j_x \pm i j_y .$$

We solve the problem by diagonalizing the matrix of H using a certain set $\chi_{\nu K}$ of eigenfunctions of $H_{s.p.}$ in the (ν, K) representation. Here, K is the angular momentum component along the nuclear symmetry axis and ν stands for the set of asymptotic quantum numbers N, n_z, Λ. We denotes by $\epsilon_{\nu K}$ the corresponding single-particle energies.

We may write the symmetrized non-adiabatic wave function in the following form

$$|IM> = \sum_{\nu,K} C^{I}_{\nu K} \, | IM\nu K>, \tag{3}$$

where

$$| IM\nu K> = \sqrt{\frac{2I+1}{16\pi^2}} \{ D^{I}_{MK} \, \chi_{\nu K} + \tag{4}$$

$$+ (-)^{I+\ell+K} \, D^{I}_{M,-K} \, \chi_{\nu \tilde{\tilde{K}}} \}.$$

Here, $\chi_{\nu\tilde{\tilde{K}}}$ is defined as the time-reversed of $\chi_{\nu K}$. The phase factor in eq. (4) includes the orbital quantum number ℓ.

The K-mixing amplitudes $C^{I}_{\nu K}$ are supposed to be real and normalized as follows

$$\sum_{\nu,K} (C^{I}_{\nu K})^2 = 1. \tag{5}$$

In general case we can take into account the mixing of states with $\Delta K \le I - 1/2$. Now, the eigenstates of H can be classified by I, $I_z = M$ and parity π. In some cases the approximate quantum numbers (ν, K) can be used as well.

In our treatment the moment of inertia J is considered as a spin-independent parameter, which can be chosen for each nucleus from comparison with experimental data. Thus, the full spin dependence is believed to be provided by the mixing amplitudes $C^{I}_{\nu K}$, which are to be calculated for each spin value.

The eigenvalues of the Hamiltonian (1) may be written as follows:

$$\mathcal{E}(IM) = \langle IM \mid H \mid IM \rangle$$

$$= \sum_{\nu,K} (C^{I}_{\nu K})^2 \left[\epsilon_{\nu K} - \frac{\hbar^2}{2J} K^2 \right] \tag{6}$$

$$+ \frac{\hbar^2}{2J} \{ I(I+1) + (-)^{I+1/2} \quad (I+1/2)\, a(I) \}$$

with definition

$$(-)^{I+1/2} \; (I+1/2)\, a(I) = - \langle IM \mid I_+ j_- + I_- j_+ \mid IM \rangle . \tag{7}$$

Eq. (7) presents the generalized definition of the decoupling parameter for any spin value. A more detailed expression for $a(I)$ reads

$$(-)^{I+1/2} \quad (I+1/2)\, a(I) = - \sum_{\nu,K} \sum_{\nu',K'} C^{I}_{\nu K}\, C^{I}_{\nu' K'}$$

$$\times \langle IM\nu K \mid I_+ j_- + I_- j_+ \mid IM\, \nu' K' \rangle = - \sum_{\nu K} \sum_{\nu' K'} C^{I}_{\nu K} C^{I}_{\nu' K'}$$

$$\times \; \{ 2\sqrt{(I-K)(I+K+1)} \quad \delta_{K', K+1} \langle \chi_{\nu K} \mid j_- \mid \chi_{\nu' K'} \rangle \tag{8}$$

$$+ (-)^{I+1/2} \; (I+1/2)\, \delta_{K,1/2} \delta_{K',1/2} \, (-)^{\ell} \langle \chi_{\nu K} \mid j_+ \mid \chi_{\nu' \bar{K}} \rangle \} .$$

The summation in eqs. (6) and (8) extends over single-particle states of the same partity and with $\Delta K \leq I - 1/2$.

In case of $I = 1/2$ and for a single level with $K = 1/2$ the generalized definition (7) coincides with the usual one, given by Nilsson/13/. The interaction of two or more levels with $K = 1/2$ brings the change of the decoupling parameter for any spin value. On the other hand, the notion of the decoupling parameter extends now on any rotational band. The fluctuation of the mean value of $C^{I}_{\nu K}$ and $a(I)$ within a rotational band will show to what extent the phenomenological formulae for the rotational energy can be used. In practice, even though the distortion caused by the Coriolis force is strong, sometimes the nuclear states possessing approximately the same mean value of $a(I)$ can be considered as belonging to a "rotational" band and described by means of phenomenological formulae, e.g. of the type established by Bohr and Mottelson/7,8/.

3. Static Pairing

There is an additional interaction, so far neglected, associated with the pairing force. In the second quantization formalism it is

$$H_{pair} = - G \sum_{\nu,\nu' > 0} a^{+}_{\nu} a^{+}_{\tilde{\nu}} a_{\tilde{\nu}'} a_{\nu'}, \tag{9}$$

where a^{+}_{ν} and a_{ν} are the creation and annihilation operators respectively, G is the strength of the pairing force, $\tilde{\nu}$ denotes the time-reversed state of ν .

Now we can start from the solution of the pairing correlations and then superimpose the Coriolis force. The use of the static pairing approximation implies that the solution for the energy gap Δ and chemical potential λ , obtained for the ground state of even-

-even nucleus can be utilized to calculate the single-quasi-particle energies in the neighboring odd-mass nucleus. Thus, to take into account the static pairing, the general formalism, developed in the previous section, is to be changed in the following manner

i) The single-particle states $\chi_{\nu K}$ are replaced by single quasi-particle ones $a^{+}_{\nu K}|0>$, the latter being the solutions of the equation

$$(H_{s.p.}-\lambda N+H_{pair})\,a^{+}_{\nu K}\,|0> = E_{\nu K}\,a^{+}_{\nu K}|0>. \tag{10}$$

Here, N denotes the particle number operator, and $|0>$ is the vacuum state. The single-quasi-particle energies are defined as

$$E_{\nu K}=[\Delta^{2}+(\epsilon_{\nu K}-\lambda)^{2}]^{1/2} \tag{11}$$

ii) The single-quasi-particle energies $E_{\nu K}$ are used in all the formulae instead of single-particle ones.

iii) The matrix elements $<\chi_{\nu K}|j_{\pm}|\chi_{\nu' K'}>$ are to be multiplied by the factor

$$M_{\nu K,\nu' K'}=u_{\nu K}\,u_{\nu' K'}+v_{\nu K}\,v_{\nu' K'}\quad , \tag{12}$$

where $v^{2}_{\nu K}$ ($u^{2}_{\nu K}$) is the filling (emptiness) number of the state (ν K) .

Using the static pairing approximation we neglect the following most important effects:

i) the blocking effect,

ii) the Coriolis force antipairing effect,

iii) the coupling of the quasi-particle to pairing vibrations of the core, generated by pairing force.

These effects will be taken into account properly elsewhere.

4. Details of Calculation

In order to find the mixing amplitudes $C^I_{\nu K}$ and energies $\mathcal{E}(IM)$ we minimize the latter

$$\frac{\partial}{\partial C^I_{\nu K}} \{ \mathcal{E}(IM) - \omega(I) [\sum_{\nu', K'} (C^I_{\nu' K'})^2 - 1] \} = 0. \qquad (13)$$

Using eqs. (6), (8), (13) and the results of the previous section, we obtain a basic set of equations which together with eq. (5) determines $C^I_{\nu K}$ and $\omega(I)$

$$C^I_{\nu K} \{ E_{\nu K} + \frac{\hbar^2}{2J} [I(I+1) - K^2] - \omega(I) \} =$$

$$= \frac{\hbar^2}{2J} \sum_{\nu', K'} C^I_{\nu' K'} F_{\nu K, \nu' K'}(I) M_{\nu K, \nu' K'}, \qquad (14)$$

where $F_{\nu K, \nu' K'}$ is given by

$$F_{\nu K, \nu' K'} = \langle IM \nu K \mid I_+ j_- + I_- j_+ \mid IM \nu' K' \rangle . \qquad (15)$$

The Lagrangian multiplier $\omega(I)$ introduced in the above equation, must coincide with the mean value of $\mathcal{E}(IM)$.

In calculating, we have used the single-particle energies and the wave functions for the deformed Saxon-Woods potential, calculated by means of the method suggested by Gareev et al.[5] Thus, the mixing of states from different major shells has been taken into account properly. For the pairing interactions in rare-earth nuclei, we have used the same values of G determined from the experimental even-odd mass difference by Gareev et al.[14] namely,

$$G_N = \frac{23-26}{A}\ \mathrm{MeV}\ , \quad G_Z = \frac{29-32}{A}\ \mathrm{MeV}. \tag{16}$$

In their calculation the pairing force was allowed to scatter among 40 single-particle states nearest to the Fermi surface.

In the case of strong K-mixing of several bands such a choice of the pairing force strength G cannot be justified however, due to the interaction between pairing and nuclear rotation. This interaction may result in either decrease or increase of the G value, depending on concrete properties of the interacting states[15]. In the next section we will show that the renormalization of G value is necessary to bring into agreement the calculated and experimental energies.

5. Results and Discussion

Recently in a number of papers (see e.g., refs.[1-3]) it has been pointed out that the effects of Coriolis coupling are especially pronounced among the positive parity states of rare-earth nuclei with neutron numbers 91, 93, 95 and 97. Actually the single-particle scheme in this region (a portion of it is reproduced in fig.1) is very complicated due to the "crossing" of several states from $N=4$ and 6 shells[5]. Of particular interest is the strong N-mixing of pairs of states $\{1/2^+[660],\ 1/2^+[400]\}$ and $\{3/2^+[651],\ 3/2^+[402]\}$. Moreover, the matrix elements $F_{\nu K,\nu' K'}(I)$ between states, originating from the $i_{13/2}$ spherical state are very large, that causes an appriciable distortion of the rotational bands, based on the states mentioned. A relevant case is the anomalous "rotational" band in ^{161}Er observed recently by Ryde et al.[16] by means of $(\alpha, 3n)$ reaction. Some levels of the same "rotational" band have been found by Gromov et al.[17] through β -decay study of ^{161}Tm. Ryde et al.[16] had observed a cascade of quadrupole transitions between states with $\Delta I = 2$. It is proposed the "rotational" band, consisting of states with even values of $I - 1/2$, the $9/2^+$ state being the lowest of the band.

One can construct such a rotational band, based on a state with $K = 1/2$, provided the decoupling parameter $a > 8$. The theory predicts that the single-particle decoupling parameter $a_{s.p.}$ for the state $1/2^+ [660]$ is less than seven. The suggested experimental value $a_{exp} = 9.1 \pm 0.3$ by far exceeds the single-partcile value. Utilizing the method described in the previous sections we carried out the calculations for ^{161}Er varying deformation δ , inertial parameter $\hbar^2/2J$ and pairing force strength G_N. The number of single-particle states involved in the K-mixing process was varied as well.

Due to the large value of the decoupling parameter the rotational band, based on the $1/2^+ [660]$ state splits into two bands of states with even and odd numbers of $I - 1/2$, the band with odd numbers $I - 1/2$ being shifted up. Electric quadrupole transitions connect the states inside of each band, while the interband $M1$ -transitions cannot be seen because of the large spin-difference of states. On the other hand the K-mixing of states originating from the $i_{13/2}$ spherical state is very strong, that brings an additional distortion of the rotational band, based on the $1/2^+ [660]$ state. Owing to the strong Coriolis coupling the rotational bands, based on the states $3/2^+ [651]$ and $5/2^+ [642]$ also split into parts with even and odd numbers of $I - 1/2$.

The calculations performed show that it is possible to form the anomalous "rotational" band in ^{161}Er either on the $1/2^+[660]$ or on the $5/2^+[642]$ states. The structure of the "rotational" band on the $1/2^+[660]$ state is very complicated due to the strong coupling with the $3/2^+[651]$ and $3/2^+[402]$ states, which is responsible for the significant increase of the decoupling parameter value, and results in the lowering of states with even numbers of $I-1/2$, the state with $I=9/2$ being the lowest one. The energy spacing between the states with $I=9/2$, $13/2$ and $17/2$ becomes much smaller if we involve the state $5/2^+[642]$ into K-mixing process. It occured that with $G_N=23/A$ MeV (this value is obtained from odd-even mass difference) it is impossible to fit the calculations to the experimental energy difference $\mathcal{E}(I+2)-\mathcal{E}(I)$ by any variation of neither the deformation δ nor the inertial parameter $\hbar^2/2J$. Fig.2 shows the results of calculation with $\delta=0.304$ (at this point the state $3/2^+[651]$ contains approximately 50% of the state $3/2^+[402]$ and vice versa). The dependence of $\mathcal{E}(I)$ on deformation δ is important only for the two or three-bands mixing. The inclusion of additional states in the diagonalization of the matrix of the Coriolis term made this dependence very smooth. However, in order to fit our five-bands mixing results to experimental data we have to reduce the pairing force strength by approximately 30% (see Fig.2). The effects from the addition of the states $7/2^+[633]$ and $9/2^+[624]$ are also shown in Fig.2.

The complete theoretical energy diagram of the positive parity states in ^{161}Er, tentatively distributed over "rotational" bands, is given in Fig.3. Each "rotational" band consists of states, which have the close mean values of $a(I)$ x/ as is shown in the lower

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x/ It is interesting to note that the sum of all $a(I)$ for a given I is the same for each spin value and equal to the sum of unperturbed $a_{s.p.}$ for the states $1/2+[660]$ and $1/2^+[400]$.

part of Fig.3. The only normal rotational band is that one built on the $1/2^+[400]$ state.

In almost all the states within the "rotational" band built on the $3/2^+[651]$ state the main component does not exceed 50% of the total norm. The state $3/2^+[402]$ is also strongly mixed with the others. Apparently neither the $3/2^+[651]$ nor the $3/2^+[402]$ rotational bands could be properly identified in the spectra of ^{161}Er. This result is in agreement with experimental data obtained by Tjøm and Elbek /18/

The amplitudes of the low-energy "rotational" states, associated with the $1/2^+[660]$ orbital are listed in Table 1. This band is strongly mixed with all, but $1/2^+[400]$, bands, the leading component $[C^{I}_{[660]\,1/2}]^2$ being less than 0.5 for most states with even number of $I - 1/2$. The $\Delta K=2$ admixture is very large, especially in the lowest states of the band. Moreover, the decrease of the pairing force strength G_N for this band is mainly due to the inclusion of the $5/2^+[642]$ state into the diagonalization matrix.

The Coriolis coupling distorts the rotational band built on the $5/2^+[642]$ state. The states with the odd-numbers of $I - 1/2$ are distinguished in this band and may be identified with those observed in the spectra of ^{161}Er (see Fig.4). Five - bands mixing with $G_N = 23/A$ MeV gives a satisfactory fit to the experimental energy spectrum. But in this case not all the possible $\Delta K=1$ or 2 effects are taken into account. The inclusion of the states $7/2^+[633]$ and $9/2^+[624]$ necessitates the decrease of G_N to bring into agreement the calculated and experimental energies. Table 2 lists the results obtained for some states of the band discussed.

It may be concluded that the theory predicts the existence of at least two groups of low-energy states in the spectra of ^{161}Er, each might be identified with the observed anomalous "rotational" band. /16/

The strong Coriolis coupling profoundly affects the E2-transition probability ratios within the rotational band as is demonstrated in Table 3.

The authors would like to thank Professor V.G.Soloviev for his interest in this work. One of us (N.P.) would like to thank Professor A.Bohr and Dr. S.Wahlborn for the stimulating and clarifying discussions of the problem. We are grateful to Dr. K.Ja. Gromov for discussions and to Drs. H.Ryde, S.Hjorth and K.Hagemann for discussion and making available the experimental results prior to publication. Thanks are due to Drs. S.Ivanova, F.Gareev and H.Schulz for generous access to some computer programmes. The valuable programming assistance of Dr . A.Korneichuk is also gratefully acknowledged.

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Received by Publishing Department
on June 4, 1969.

TABLE I

Energies, decoupling term a(I) values and K-mixing amplitudes $C^{I}_{\nu K}$ for the "rotational" band built on the I/2$^+$[660] state in ^{I6I}Er. Five-bands calculation is carried out with $\hbar^2/2J$=I7 keV, δ=0.304 and G_N=I6/A MeV (Δ_N=0.438 MeV, λ_N = -5.4 MeV). The levels below the energy 2.5 MeV are listed

I^{π}	$\mathcal{E}$(I) [keV]	a(I)	$C^{I}_{\nu K}$				
			I/2$^+$ [660]	I/2$^+$ [400]	3/2$^+$ [65I]	3/2$^+$ [402]	5/2$^+$ [642]
I/2$^+$	757	6,29	0,949	-0,3I4	---	---	---
3/2$^+$	II87	8,75	0,954	-0,I50	-0,I80	0,I90	---
5/2$^+$	374	5,39	0,639	-0,I34	0,477	-0,429	-0,403
7/2$^+$	I737	I0,I6	0,904	-0,I59	-0,272	0,279	0,075
9/2$^+$	0	9,03	0,423	-0,086	0,437	-0,400	0,680
II/2$^+$	2438	I0,65	0,874	-0,I59	-0,3I2	0,3I7	0,II3
I3/2$^+$	80	I0,57	0,55I	-0,III	0,458	-0,429	0,538
I7/2$^+$	270	II,07	0,6I4	-0,I23	0,456	-0,432	0,46I
2I/2$^+$	587	II,28	0,649	-0,I29	0,45I	-0,430	0,4I6
25/2$^+$	I035	II,38	0,672	-0,I33	0,446	-0,428	0,387
29/2$^+$	I6I6	II,43	0,687	-0,I36	0,44I	-0,425	0,367

TABLE 2

Energies, decoupling term a(I) values and K-mixing amplitudes $C^{I}_{\nu K}$ for some states of the "rotational" band built on the 5/2$^+$[642] state in ^{I6I}Er. Seven-bands calculation is carried out with $\hbar^2/2J$=I5 keV, δ=0.304 and G_N=I5/A MeV (Δ_N = 0.370 MeV, λ_N=-5.387 MeV)

I^{π}	$\mathcal{E}$(I) keV	a(I)	$C^{I}_{\nu K}$						
			I/2$^+$[660]	I/2$^+$[400]	3/2$^+$[65I]	3/2$^+$[402]	5/2$^+$[642]	7/2$^+$[633]	9/2$^+$[624]
7/2$^+$	0	-5,37	0,093	-0,020	0,289	-0,254	0,902	0,I7I	---
II/2$^+$	84	-7,65	0,I36	-0,030	0,350	-0,3I2	0,830	0,267	0,035
I5/2$^+$	273	-8,59	0,I60	-0,036	0,373	-0,337	0,785	0,3I7	0,059
I9/2$^+$	574	-9,07	0,I75	-0,039	0,384	-0,350	0,755	0,347	0,080
23/2$^+$	I0I0	-9,35	0,I84	-0,04I	0,389	-0,356	0,733	0,373	0,099
27/2$^+$	I522	-9,53	0,I9I	-0,043	0,39I	-0,359	0,7I7	0,39I	0,II5

Table 3

Ratios of B(E2) values within the "rotational" band built on the I/2$^+$[660] state, calculated with δ =0.304, G_N=I6/A MeV and $\hbar^2/2J$ =I7 keV, are compared with that according to Alaga rule

B(E2, I+2 → I)/ B(E2, I3/2 → 9/2)					
I	9/2	I3/2	I7/2	2I/2	25/2
Theory	I	2.8	4.0	5.0	5.6
Alaga	I	I.05	I.07	I.09	I.II

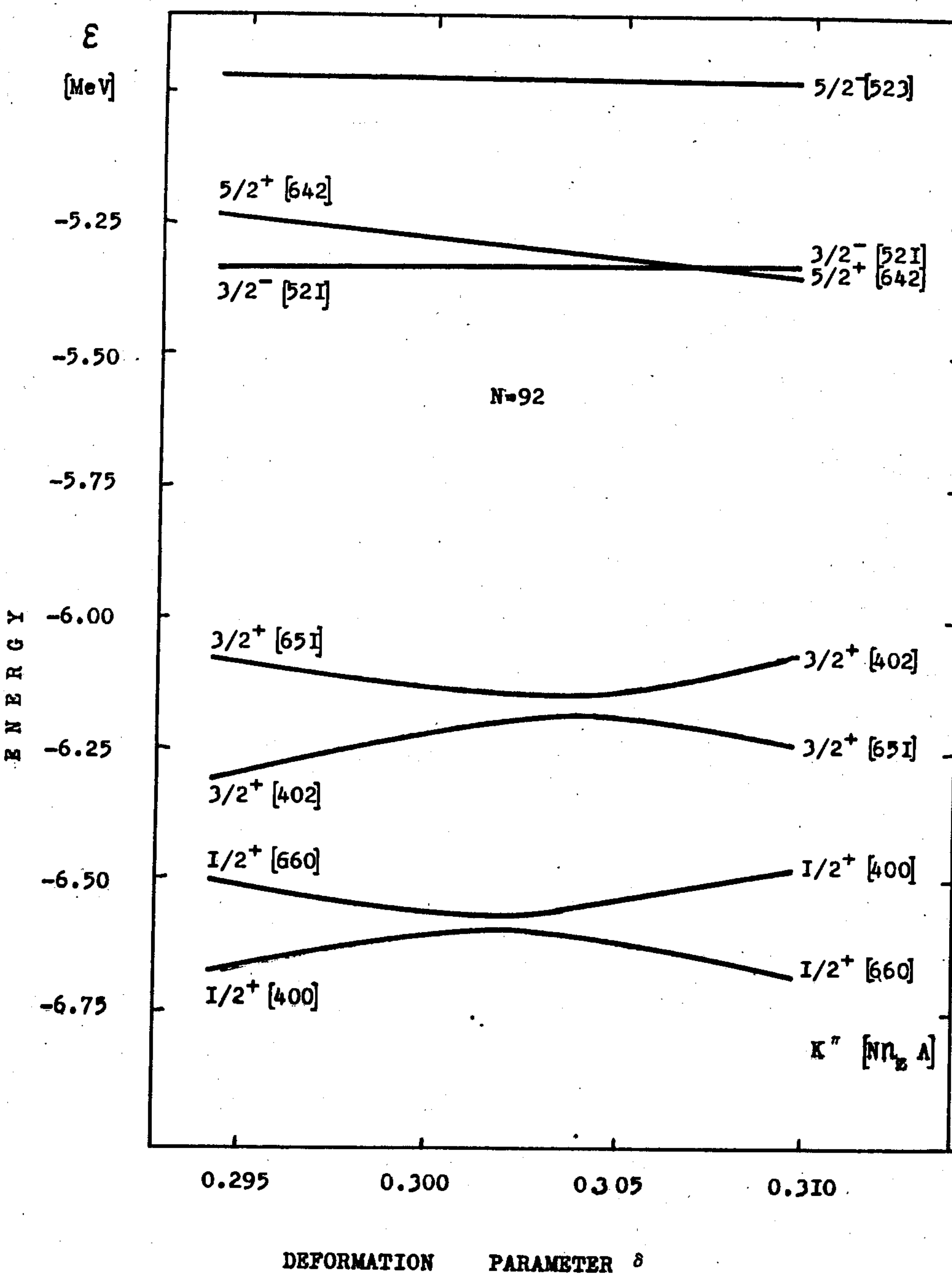

Fig.1. Woods-Saxon diagram, showing the "crossing" of some orbitals in the rare-earth region/5/.

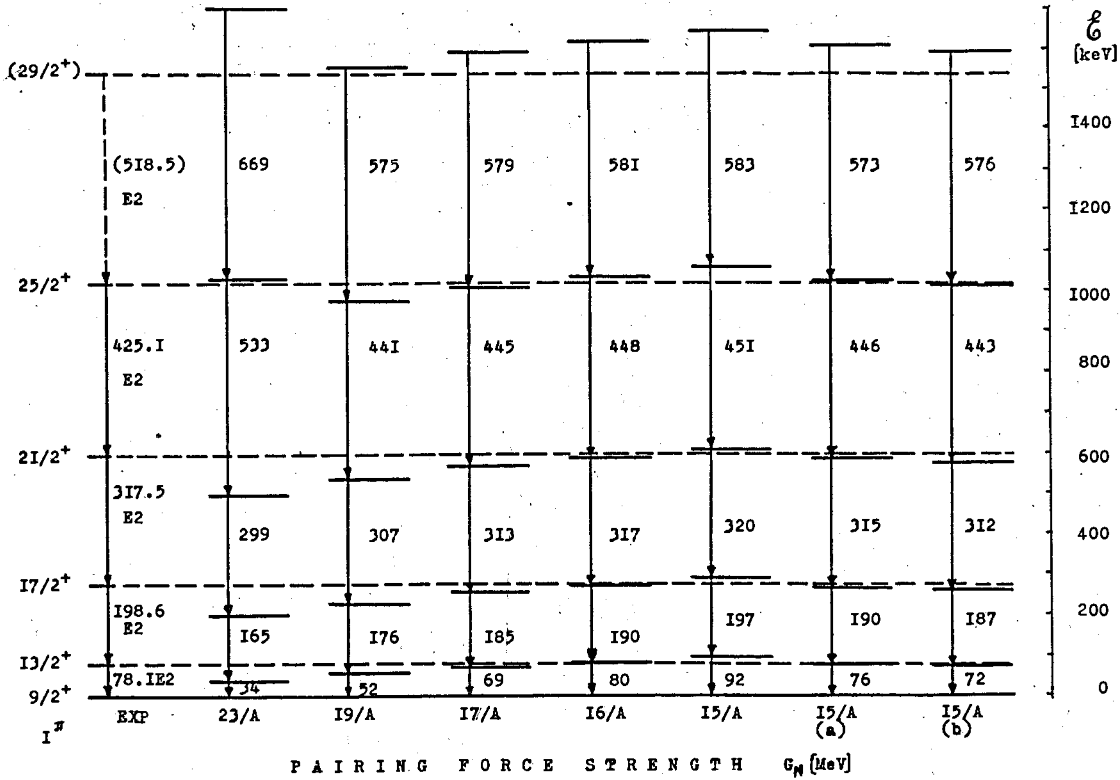

Fig.2. Anomalous "rotational" band in ^{161}Er built on the $1/2^+$ 660 state, comparison between experiment/16/ (dashed lines) and calculations (solid lines) for various G_N and δ =0.304. Five-bands mixing results are shown in the second to sixth rows (the states $1/2^+$[660] , $1/2^+$ [400], $3/2^+$[651], $3/2^+$ [402] and $5/2^+$[642] are mixed). (a) Six-bands mixing results (the state $7/2^+$ [633] is added). (b). Seven-bands mixing results (the state $9/2^+$ [624] is added). The inertial parameter used is $\hbar^2/2J$ =17 keV.

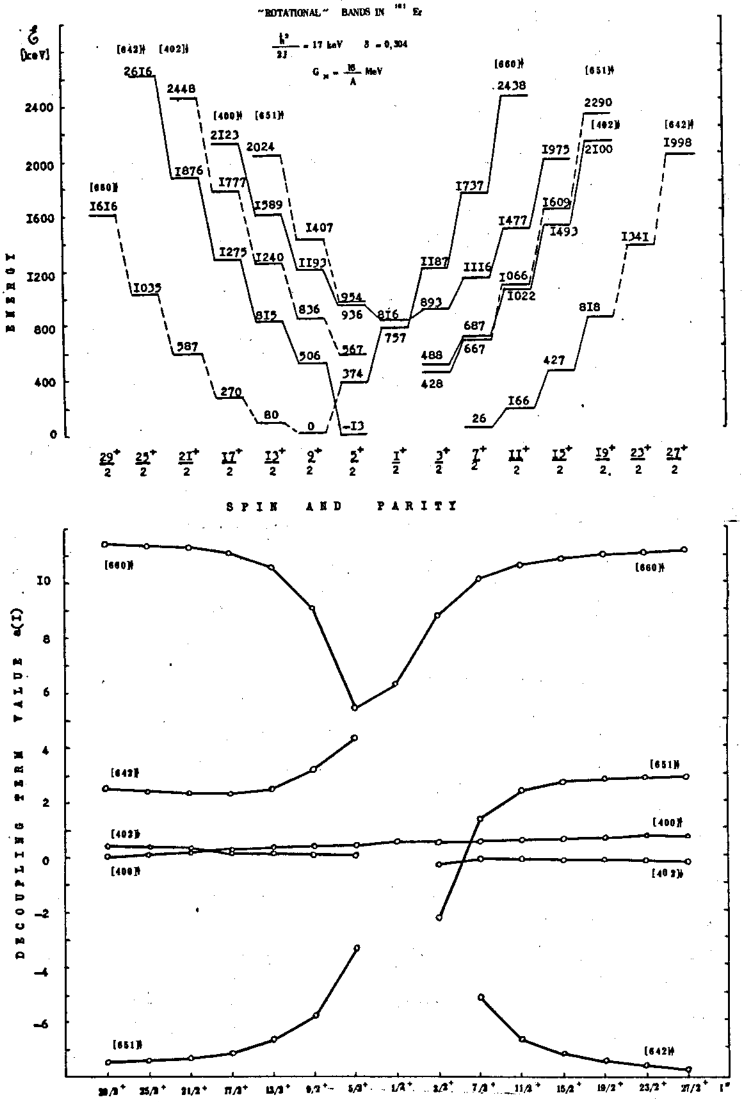

Fig.3. Positive parity states in ^{161}Er according to the five-bands mixing calculation (above) and the decoupling term a(I) versus the spin value (below). The distribution over the "rotational" bands mush be considered as tentative. The dashed line connects the strongly mixed states, the leading component if which is less than 50% of the total norm.

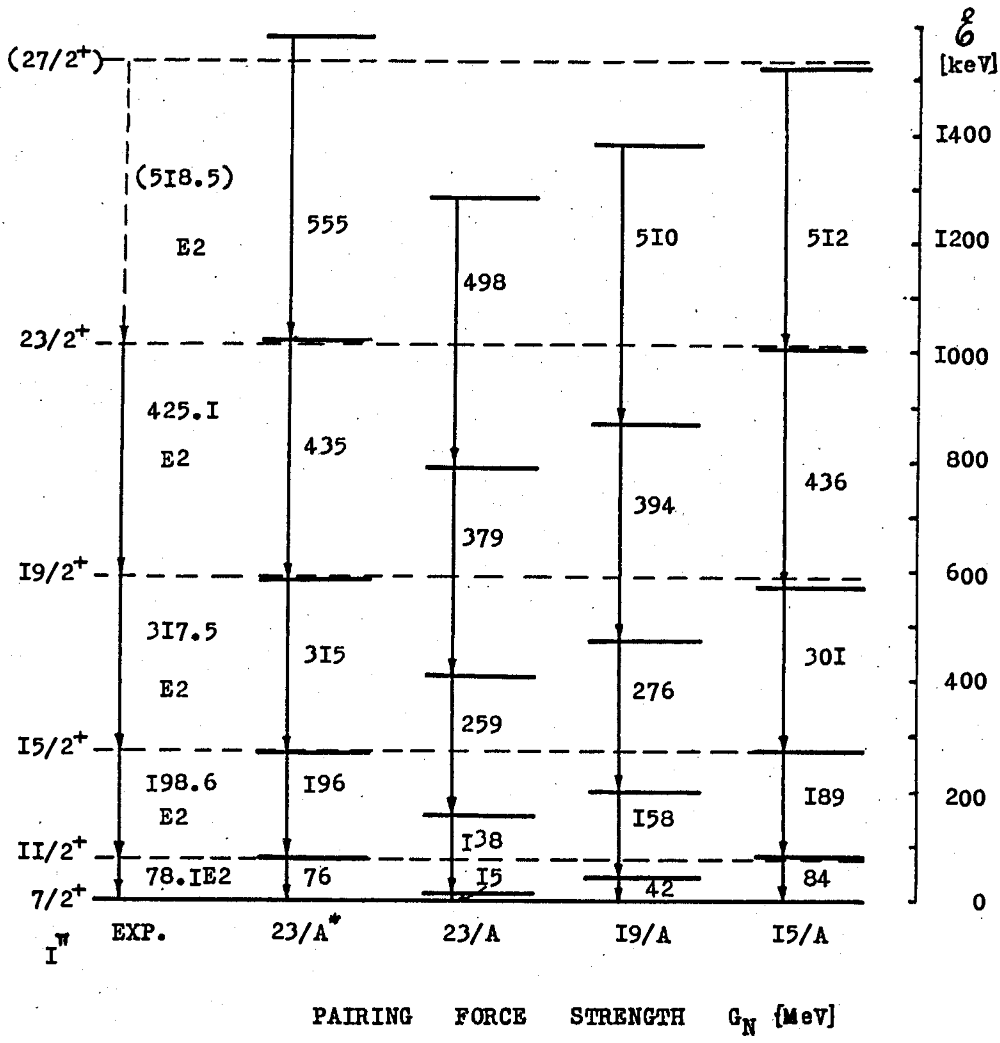

Fig.4. "Rotational" band in ^{161}Er built on the $5/2^+$[642] state, comparison between experiment/16/(dashed lines) and seven-bands mixing calculation (solid lines, the last three rows). Five-bands mixing calculation is shown in the row, marked by asterisk. The parameters used were δ =0.304 and $\hbar^2/2J$ = 15 keV.