PARTICLE-ROTOR MODEL DESCRIPTION OF DEFORMED NUCLEI

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1. Introduction

An appropriate theoretical basis for the study of strongly deformed nuclei is provided by the many-particles plus rotor (MPR) model.[1,2] The main difficulty with this model is the description of the correlated motion of the valence nucleons in the intrinsic deformed field. Although the residual interaction is usually assumed to be a simple pairing force, the large number of particles and levels which have to be taken into account make a complete-basis diagonalization very impractical, if not unfeasible. This has caused the BCS theory to become the most widely used approach to this problem. The errors inherent in this approximation may well result, however, in a poor description of the intrinsic structure, thus making it difficult to assess the real scope of the MPR model.

We are currently handling this problem by making use of a new method for treating pairing correlations in deformed nuclei. This method, which we call chain-calculation method (CCM), provides the natural framework for a sequence of number-conserving approximations. We have shown[3-5] that it has the power to reduce the complexity of multi-level, multi-particle pairing problems drastically while yielding practically exact results.

In this paper, we apply the MPR model to the nucleus ^{163}Er considering twenty-one valence neutrons distributed over eighteen twofold degenerate single-particle levels. We first treat the pairing Hamiltonian by means of the CCM and then diagonalize the recoil term within the set of seniority-one states. As a final step the Coriolis term is taken into account. Along the same lines we have also performed a calculation where the pairing correlations are treated in the BCS approximation.

In Sec. 2 we give an outline of the essentials of the MPR model. In Sec. 3 we describe the salient features of the CCM and evidence its practical value. In Sec. 4 we discuss the recoil term and give the relevant matrix elements. The Coriolis coupling is then discussed in Sec. 5. In Sec. 6 we present some results of our study of ^{163}Er. It is shown that, in contrast to the results of the BCS approximation, we obtain a good agreement with experiment without any ad-hoc attenuation factor of the Coriolis term. A brief summary is given in Sec. 7.

2. Many-Particles plus Rotor Model

In the strong coupling representation the model Hamiltonian describing a system of N valence particles coupled to an axially-symmetric rotor is written

$$H_{MPR} = H_I + H_{intr} + H_c, \tag{1}$$

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where

$$H_I = A(\boldsymbol{I}^2 - I_3^2), \tag{2}$$

$$H_{intr} = H_0 + H_{pair} + H_{rec}, \tag{3}$$

$$H_{rec} = A(\boldsymbol{J}^2 - J_3^2), \tag{4}$$

$$H_c = -A(I_+ J_- + I_- J_+), \tag{5}$$

with standard notation. The recoil term H_{rec} is of particular relevance in the MPR model,[2,6] as it contains both one-body and two-body terms. In fact, the angular momentum $\boldsymbol{J}$ due to the valence particles has the form

$$\boldsymbol{J} = \sum_{i=1}^{N} \boldsymbol{j}(i), \tag{6}$$

which implies that H_{rec} becomes

$$H_{rec} = A\left[\sum_{i=1}^{N} \boldsymbol{j}^2(i) - \left(\sum_{i=1}^{N} j_3(i)\right)^2 + 2\sum_{i<k} \boldsymbol{j}(i)\cdot\boldsymbol{j}(k)\right]. \tag{7}$$

The intrinsic deformed field H_0 is described by a nonspheroidal axial and reflection symmetric Woods-Saxon potential.[7] The eigenstates of $H_I + H_{intr}$ can be written in the form

$$\Psi^I_{M\Omega\tau} = \sqrt{\frac{2I+1}{16\pi^2}}\left[D^I_{M\Omega}(\omega)\chi_{\Omega\tau} + (-)^{I+\Omega} D^I_{M-\Omega}(\omega)\chi_{\bar{\Omega}\tau}\right], \tag{8}$$

where the intrinsic wave functions $\chi_{\Omega\tau}$ are solutions to the eigenvalue equation

$$(H_0 + H_{pair} + H_{rec})\chi_{\Omega\tau} = \mathcal{E}_{\Omega\tau}\chi_{\Omega\tau}. \tag{9}$$

Once Eq. (9) is solved the Coriolis term can be diagonalized in this representation. In the next three sections we shall discuss in some detail our treatment of the intrinsic Hamiltonian and of the Coriolis coupling.

3. Treatment of Pairing Correlations by means of the CCM

The Hamiltonian $H = H_0 + H_{pair}$ is written as

$$H = \sum_{\nu} \epsilon_\nu \hat{N}_\nu - \sum_{\nu\nu'} G_{\nu\nu'} A^\dagger_\nu A_{\nu'}, \tag{10}$$

where

$$\hat{N}_\nu = a^\dagger_\nu a_\nu + a^\dagger_{\bar{\nu}} a_{\bar{\nu}}, \tag{11}$$

$$A^\dagger_\nu = a^\dagger_\nu a^\dagger_{\bar{\nu}}. \tag{12}$$

The index ν stands for all quantum numbers specifying the single-particle states while $\bar{\nu}$ denotes the time reversal partner. In cases where Ω is essential, ν will represent only the asymptotic quantum numbers $[Nn_3\Lambda]$.

In our approach the wave function for a system with N identical particles is given the form

$$| N, \beta, L\rangle = \sum_{\nu\gamma} c^L_{\nu\beta\gamma}(N) A^\dagger_\nu \mid N-2, \gamma, L\rangle, \tag{13}$$

where the index L stands for the quantum numbers of the blocked levels and ν runs only over the unblocked ones. The indices β and γ specify the states with N and $N-2$ particles, respectively. It is precisely the use of (13) which leads to solving the N-particle problem through a chain calculation across systems differing by two in nucleon number.

It should be noted that inherent in this formalism is the use of an overcomplete set of basis vectors $A^\dagger_\nu|N-2,\gamma,L\rangle$. To single out a linearly independent set of states we analyze the metric matrix, whose elements are defined as

$$d^L_{\nu\gamma\nu'\gamma'}(N-2) = \langle N-2, \gamma, L \mid A_\nu A^\dagger_{\nu'} \mid N-2, \gamma', L\rangle, \tag{14}$$

through the Cholesky decomposition of symmetric positive definite matrices. An account of our procedure for removing the redundant states may be found in Ref. 8. It is therefore to be understood that the sum in (13) is restricted to pairs of indices $(\nu\gamma)$ corresponding to linearly independent basis vectors. Making use of expansion (13) in the Schrödinger equation,

$$H|N,\beta,L\rangle = E_{L\beta}(N)|N,\beta,L\rangle, \tag{15}$$

leads straightforwardly to the formulation of the eigenvalue problem in the form

$$\sum_{\nu'\gamma'}\Big\{\sum_{\nu''\gamma''}[\bar{d}^L(N-2)]^{-1}_{\nu\gamma\nu''\gamma''} H^L_{\nu''\gamma''\nu'\gamma'}\Big\} c^L_{\nu'\beta\gamma'}(N) = E_{L\beta}(N)\, c^L_{\nu\beta\gamma}(N), \tag{16}$$

where

$$H^L_{\nu''\gamma''\nu'\gamma'} = \langle N-2,\gamma'', L|A_{\nu''} H A^\dagger_{\nu'}|N-2,\gamma',L\rangle \tag{17}$$

and $\bar{d}^L$ denotes the metric matrix obtained from the original matrix by removing rows and columns corresponding to redundant states according to the above mentioned procedure.

The elements of the metric matrix (14) as well as those of the Hamiltonian matrix (17) are calculated by making use of the explicit expression of the wave function $|N-2,\gamma,L\rangle$ in the occupation-number representation,

$$|N-2,\gamma,L\rangle = \sum_{n_1\ldots n_l} K^L_{n_1\ldots n_l\gamma}(N-2)(A^\dagger_1)^{n_1}\ldots(A^\dagger_l)^{n_l}|N_0,L\rangle, \tag{18}$$

where $n_i = 0$ or 1, and $n_1+n_2+\cdots+n_l = (N-2-N_0)/2, l$ being the number of doubly degenerate single-particle levels and N_0 the number of unpaired particles (of course, for blocked levels $n_i = 0$). The explicit expression of the elements of the metric matrix as well as those of the Hamiltonian matrix may be found in Ref. 5.

The coefficients $K^L_{n_1\ldots n_l\beta}(N)$ are related to the c^L 's through

$$K^L_{n_1\ldots n_l\beta}(N) = \sum_{\nu\gamma} c^L_{\nu\beta\gamma}(N) K^L_{n_1\ldots n_{\nu-1}0n_{\nu+1}\ldots n_l\gamma}(N-2)\delta_{n_\nu 1}. \tag{19}$$

The solution of the N-particle problem can therefore be obtained by a chain calculation starting from N_0 and proceeding by adding pairs of particles up to the desired value of N.

The formalism given above is exact to the extent that all the existing core states $|N-2,\gamma,L\rangle$ are taken into account. Its practical value, however, resides in the fact that it provides the framework for a sequence of number-conserving approximations which are obtained by truncating the expansion (13). We call $k-th$ order theory the approximation scheme in which the core states are restricted to the lowest k states. We have verified[3-5] that the use of very low orders of approximation (typically fourth or fifth order) produces extremely accurate results for at least the three or four lowest states. Clearly, this brings about an enormous reduction in the size of the matrices to be diagonalized. In fact, they are at most of the order $k \times l$. It is possible, however, to further simplify our chain-calculation approach by restricting the sums on the r.h.s. of (18). Of course, the main question is how to perform this truncation without spoiling the accuracy of the method. We shall not touch on this point here, but refer the reader to Ref. 5 for a detailed discussion. To evidence the degree of accuracy that can be attained by our approach we report, however, some representative results of an application to a system of sixteen particles in as many doubly degenerate single-particle levels (the single-particle level scheme may be found in Ref. 5). The pairing strength G (we use the usual constant pairing force) is 0.20 MeV and we consider states in which all the particles are distributed in time-reversed pairs over the available orbitals (in the following we shall denote these seniority-zero type states as $v=0$ states).

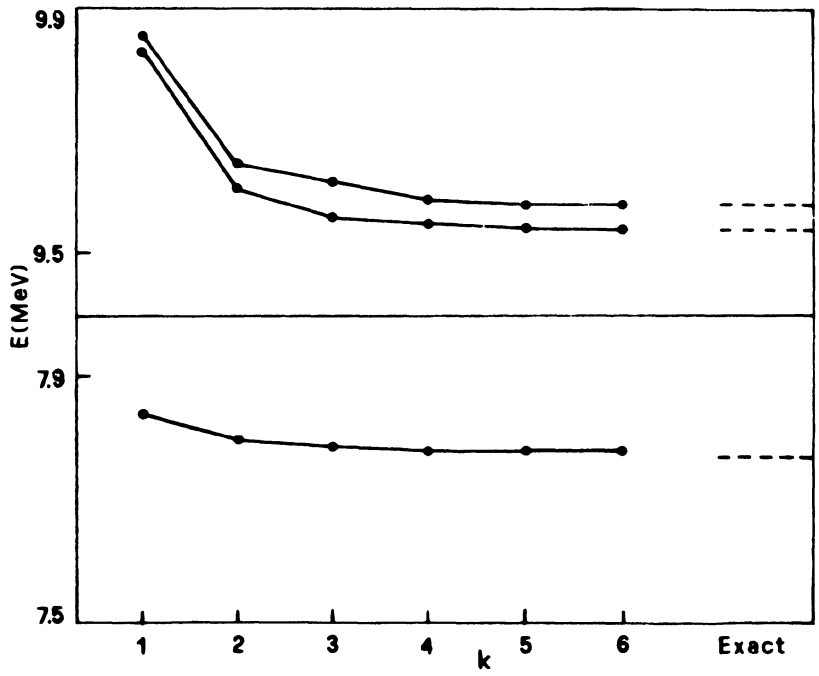

Figure 1. *Energies of the three lowest $v=0$ states for a system of 16 particles distributed among as many single-particle levels. The results are plotted as a function of the order of approximation k. The number of configurations included in the calculation is 4000. See text for details.*

Fig. 1 shows the energy of the three lowest $v = 0$ states obtained at orders of approximation ranging from 1 to 6 with inclusion of 4000 configurations (they are 11440 in all) in (18). We see that the fifth-order theory yields results which are quite close to the exact ones. In fact, the ground-state energy is only 10 keV higher than the exact one while for both the two excited states the difference is 3 keV. Regarding the reduction in the size of the energy matrices, the fifth order calculation involves the diagonalization of an 80×80 matrix, whereas the total number of $v = 0$ states is 12870.

The above example shows that our chain-calculation approach makes it possible to treat multi-level pairing-force problems in a simple but extremely accurate way.

4. The Recoil Term

The recoil term (7) in second quantization reads

$$H_{rec} = A\Big[\sum_{\nu\nu'} F_{\nu\nu'} a^{\dagger}_{\nu} a_{\nu'} + \sum_{\nu_1\nu_2\nu_3\nu_4} R_{\nu_1\nu_3} R_{\nu_4\nu_2} a^{\dagger}_{\nu_1} a^{\dagger}_{\nu_2} a_{\nu_4} a_{\nu_3}\Big], \tag{20}$$

where

$$F_{\nu\nu'} = \langle\nu|\boldsymbol{j}^2 - j_3^2|\nu'\rangle, \tag{21}$$

$$R_{\nu'\nu'} = \begin{cases} \langle\nu|j_-|\nu'\rangle & \text{if } \Omega_\nu < \Omega_{\nu'}, \\ \langle\nu'|j_-|\nu\rangle & \text{if } \Omega_\nu > \Omega_{\nu'}, \\ \langle\overline{\nu}|j_-|\nu'\rangle & \text{if } \Omega_\nu = \Omega_{\nu'} = \frac{1}{2}. \end{cases} \tag{22}$$

Here we focus attention on the treatment of odd-A nuclei. In this case we diagonalize H_{rec} within the set of $v = 1$ states obtained by treating the Hamiltonian (10) as described in the previous section. The intrinsic wave function has therefore the form

$$\chi_{\Omega\tau} = \sum_{\beta\mu} f^{\Omega}_{\beta\tau\mu} |\beta, \mu\Omega\rangle. \tag{23}$$

Here and in the following the label μ refers to the quantum numbers of the blocked level.

The matrix elements of H_{rec} between $v = 1$ states are given by

$$\langle\beta, \mu\Omega|H_{rec}|\beta', \mu'\Omega\rangle = A\Big\{\delta_{\mu\mu'}\Big[2\sum_{\nu>0} F_{\nu\nu} T^{\mu\mu'}_{\beta\beta'\nu} - \sum_{\nu,\nu'>0} R^2_{\nu\nu'} T^{\mu\mu'}_{\beta\beta'\nu\nu'}\Big] +$$

$$[1 - (1 - \delta_{\beta\beta'})\delta_{\mu\mu'}] F_{\mu\mu'} S^{\mu\mu'}_{\beta\beta'} - \sum_{\nu>0} R_{\nu\mu'} R_{\nu\mu} S^{\mu\mu'}_{\beta\beta'\nu}\Big\}, \tag{24}$$

where the quantities S and T are expressed in terms of the coefficients (19). Their explicit expressions may be found in Ref. 9.

Let us now discuss briefly the effects produced by the recoil term. We first consider the diagonal matrix elements. The first two sums in Eq. (24) represent the so-called core contribution.[6,10] In fact, they are just the expectation value of the recoil term with respect to the even-mass nucleus, whose $N - 1$ valence particles are distributed over all the available levels except the blocked one. This contribution, being almost independent of the level blocked by the unpaired particle, does not significantly affect the spectrum of the odd nucleus. The remaining two terms in Eq. (24) are the contribution of the unpaired particle. The third one reduces to the single-particle matrix element $F_{\mu\mu}$ ($S^{\mu\mu}_{\beta\beta} = 1$) while the quantity

$\sum_{\nu>0} R^2_{\nu\mu} S^{\mu\mu}_{\beta\beta\nu}$ represents the correction arising from the other valence nucleons. The latter is strongly dependent both on the nature of the level μ and on the pairing correlations.

As regards the off-diagonal matrix elements, they may have $\beta \neq \beta'$ and/or $\mu \neq \mu'$. We have found, in agreement with the results of other authors,[2] that the matrix elements with $\mu \neq \mu'$ are very small. Through the matrix elements with $\beta \neq \beta'$ different eigenstates of the pairing Hamiltonian may be brought into the intrinsic wave function. In this way the recoil term affects the pair distribution of particles.[11,12] This effect may be particularly important when the involved levels originate from the so-called intruder states (in the case considered in this paper this is the spherical $i_{13/2}$ state).

5. The Coriolis Coupling

The matrix elements of the Coriolis term (5) are given by

$$\langle \Psi^I_{M\Omega\tau} | H_c | \Psi^I_{M\Omega'\tau'} \rangle = -A \Big\{ \sum_{\mu\mu'} \Big[(I+\Omega')(I-\Omega'+1) \Big]^{\frac{1}{2}} R_{\mu\mu'} \delta_{\Omega'\Omega+1}$$

$$+ \Big[(I-\Omega')(I+\Omega'+1) \Big]^{\frac{1}{2}} R_{\mu'\mu} \delta_{\Omega'\Omega-1} + (-)^{I+\frac{1}{2}} (I+\frac{1}{2}) R_{\mu\mu'} \delta_{\Omega\frac{1}{2}} \delta_{\Omega'\frac{1}{2}} \Big\} P^{\Omega\Omega'}_{\tau\mu\tau'\mu'}, \qquad (25)$$

where

$$P^{\Omega\Omega'}_{\tau\mu\tau'\mu'} = \sum_{\beta\beta'} f^{\Omega}_{\beta\tau\mu} f^{\Omega'}_{\beta'\tau'\mu'} S^{\mu\mu'}_{\beta\beta'}. \qquad (26)$$

The matrix elements (25) are written as the product of two factors. The first one corresponds to the contribution of the odd particle while the second one takes into account the many-particle correlations induced from both the pairing and the recoil interaction. Since the quantities $P^{\Omega\Omega'}_{\tau\mu\tau'\mu'}$ are all ≤ 1, they produce an attenuation of the Coriolis coupling.

6. MPR Model Study of ^{163}Er

We report here some results of a study of the nucleus ^{163}Er within the framework of the MPR model. A similar study by Engeland[13] is based on an exact diagonalization of the intrinsic Hamiltonian in a model space including only a rather limited number of Nilsson levels. We have considered twenty-one valence neutrons distributed over eighteen single-particle levels. As already mentioned in Sec. 2, the intrinsic deformed field has been described by a nonspheroidal axial and reflection symmetric Woods-Saxon potential. The parameters of the potential and the single-particle level scheme are given in Ref. 9.

As for the pairing strength G we have used a value of 0.191 MeV which gives an odd-even mass difference P_n for neutrons,

$$P_n = \frac{1}{2} \left[B\left(^{164}Er\right) + B\left(^{162}Er\right) - 2B\left(^{163}Er\right) \right], \qquad (27)$$

in agreement with the experimental value 0.970 MeV. It should be noted that the recoil term contributes to P_n about 240 keV. For the rotational parameter A we take the value 14 keV which comes close to that corresponding to the $11/2^-[505]$ band, which is essentially rotational in character.

In Fig. 2 we show the spectrum of the lowest positive-parity band (originating from the $i_{13/2}$ shell-model state) obtained by using our treatment of pairing correlations, which,

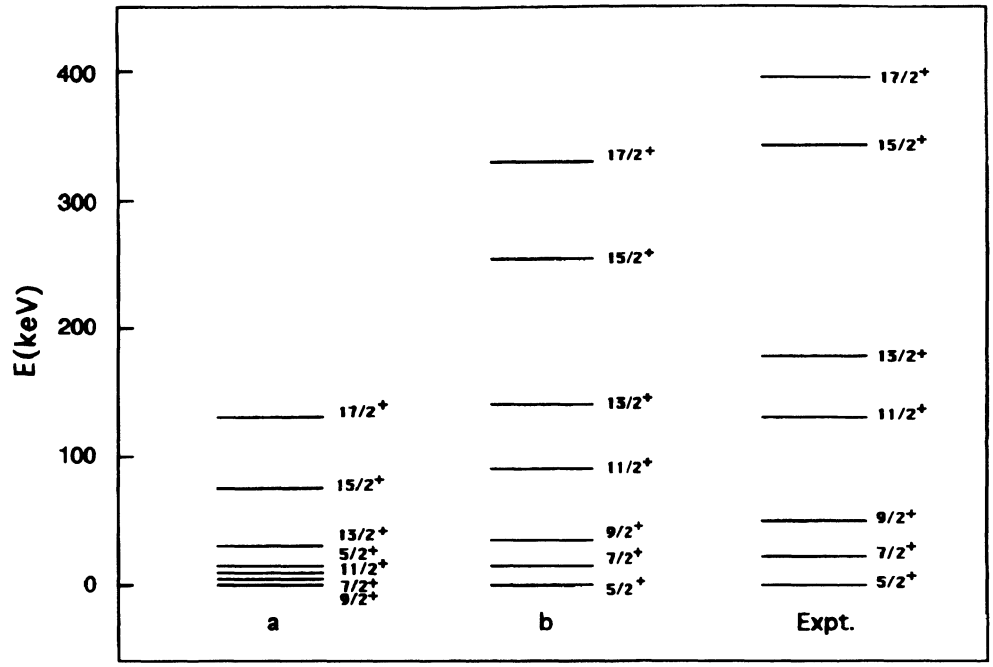

Figure 2. *The spectrum of ^{163}Er obtained by using the CCM: a) without recoil, b) with recoil.*

as pointed out in Sec. 3, is practically exact. We see that the right level ordering and an overall satisfactory agreement with experiment is obtained without any attenuation factor. The comparison between case a) and b) shows the relevance of the recoil term.

By using the same single-particle spectrum and the same rotational parameter we have also performed a calculation where the pairing correlations have been treated in the BCS approximation. As in the calculation based on the CCM, the value of the pairing strength, $G = 0.197$ MeV, has been determined by reproducing the experimental value of P_n while the recoil term has been diagonalized within the set of one quasi-particle states. In Fig. 3 we show the spectrum obtained in this approximation. The comparison between case a) and b) evidences again the role of the recoil term in the MPR model. However, as we see from the spectrum c), a satisfactory agreement with experiment can only be obtained by introducing an ad-hoc attenuation factor.

As regards the spectra of the negative-parity bands $3/2^-[521], 5/2^-[523]$ and $11/2^-[505]$, which are practically purely rotational, a very good agreement with experiment is obtained from both calculations.

Let us now discuss briefly the origin of the difference in the spectra of the positive-parity band obtained from our method and the BCS approximation. As already mentioned, in the final step of the MPR-model calculations the Coriolis interaction is diagonalized in the set of basis states (8). Therefore the difference between the CCM and the BCS results may arise from the differences in the values of the intrinsic energies which appear in the diagonal matrix elements as well as from the attenuation factors $P^{\Omega\Omega'}$ in the off-diagonal ones (25). For ^{163}Er the latter do not differ significantly in the two cases, while rather large differences show up in the intrinsic energies, as it appears from Table 1 (the intrinsic states are characterized

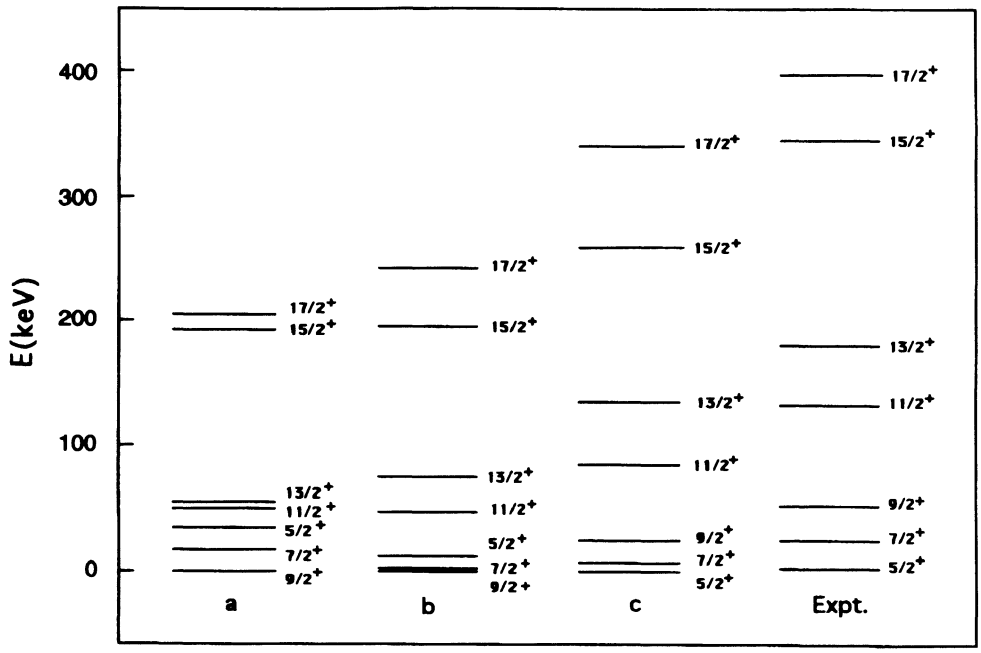

Figure 3. *The spectrum of ^{163}Er obtained in the BCS approximation: a) without recoil, b) with recoil, c) with recoil, Coriolis attenuation of 0.9.*

by $[Nn_3\Lambda]$, since, as already mentioned in Sec. 4, there is no appreciable mixing of states corresponding to different blocked levels). Indeed, from this table we see an increase in the intrinsic energy spacings $\mathcal{E}_{[633]7/2} - \mathcal{E}_{[642]5/2}$ and $\mathcal{E}_{[651]3/2} - \mathcal{E}_{[642]5/2}$ of 334 keV and 254 keV, respectively, from the BCS to our treatment of pairing correlations. This reduces the Coriolis coupling bringing the final energy spectrum of the decoupled band in agreement with experiment.

Table 1. *Values of the intrinsic energies $\mathcal{E}_{\mu\Omega} - \mathcal{E}_{[642]5/2+}$ (keV).*

Odd particle state $\mu\Omega$	$\mathcal{E}^{\mathrm{CCM}}$	$\mathcal{E}^{\mathrm{BCS}}$
$[660]\frac{1}{2}^+$	1470	1187
$[651]\frac{3}{2}^+$	946	692
$[642]\frac{5}{2}^+$	0	0
$[633]\frac{7}{2}^+$	905	571
$[624]\frac{9}{2}^+$	2488	2138

Finally, in Table 2 we compare the band-head energies with experiment. It appears that while a very good agreement is obtained from the calculation based on the CCM, the BCS results show rather large discrepancies. Since the Coriolis coupling has little influence on the

Table 2. *Values of the band-head energies (keV) obtained from the CCM and from the BCS method.*

Band head	E^{CCM}	E^{BCS}	E_{expt}
$\frac{5}{2}^-$	0	0	0
$\frac{5}{2}^+$	85	214	69
$\frac{3}{2}^-$	87	86	112
$\frac{11}{2}^-$	435	338	444

band-head energies (all the considered bands have $\Omega \neq \frac{1}{2}$), the results of Table 2 are again a consequence of the differences in the values of the intrinsic energies.

7. Summary

In this paper we have applied a new method for treating pairing correlations in deformed nuclei to the study of the nucleus ^{163}Er within the framework of the many-particles plus rotor model. While involving a limited amount of computational work this method yields extremely accurate results.

The results of our calculation have turned out to be in good agreement with experiment without any ad-hoc attenuation factor of the Coriolis term. This is not the case when the pairing correlations are treated by the usual BCS method. In fact, we have found out that use of this approximation makes it necessary to introduce an attenuation factor of 0.9. The primary reason for this is the inaccuracy in the values of the intrinsic energies.

In conclusion, the results of our study of ^{163}Er point to the fact that, once the intrinsic structure is properly treated, the MPR model provides an appropriate framework for the description of deformed nuclei.

Acknowledgements

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