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Perturbed Nuclear Rotations and K-Mixing in Odd-Mass Nuclei

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Abstract. A particle-plus-rotor Hamiltonian with Coriolis interaction is treated by the contact transformation method. The transformed Hamiltonian is diagonal in the space of the adiabatic rotation functions of a system with separated collective and single particle motion. The obtained energy expression contains terms which mix rotational bands built on single particle states with different values of the third angular momentum projection K. The approach is applied for a description of the ground-state and first excited rotation bands in the nuclei ^{183}W and ^{181}Hf. Very good agreement between theoretical and experimental data is achieved.

1 Introduction

Rotation spectra of many deformed nuclei suggest an interplay between collective and single particle degrees of freedom, as well as, between the rotation and vibration motions [1]. Usually, there is a discrepancy between the experimental rotation spectrum of a given nucleus and the levels of the rigid rotor. It is partially caused by the Coriolis coupling of the single particle motion to the collective rotation. In the present work, we propose an approach to take into account the Coriolis interaction in odd nuclei with axial and reflection symmetric shapes. The formalism is derived in the framework of the rotor plus particle model, in which the Coriolis interaction is included. It is well known that for axially symmetric nuclei the third projections of the total and single particle angular momenta along the symmetry axis are good quantum numbers with equal values, denoted by K. The Coriolis interaction mixes states with different values of K. For the bands with $K = 1/2$ the main contribution of the Coriolis term to the collective energies is diagonal. However, if only the diagonal term is considered the theoretical energy levels systematically appear below the experimental data, especially at high angular momenta. The reason for this deviation is that the band-mixing interaction is neglected [2].

The aim of the present work is to properly take into account the Coriolis mixing effects in rotation spectra of odd mass nuclei. The approach is based on the contact transformation method [3] which is widely used in molecular physics [4]. Some recent considerations in nuclear rotation spectra have also been done [5, 6].

In the next section, the basic frame of the particle plus rotor model with the Coriolis interaction is given. In section 3, the contact transformation approach is given. In section 4, an application of the approach is presented. Some concluding remarks are given in section 5.

2 The Rotor Plus Particle Model

The rotation properties of odd nuclei with axial and reflection symmetric shapes are investigated in the framework of the rotor plus particle model [1]. The most general form of the Hamiltonian is

$$\hat{H} = \hat{H}_p + \hat{H}_{rot} + \hat{H}^{(c)}, \tag{1}$$

where $\hat{H}_p$ is the single particle Hamiltonian, $\hat{H}_{rot}$ is the pure rotation part and $\hat{H}^{(c)}$ is the Coriolis coupling term. The last term represents the interaction between the particle motion and the core rotation. Hamiltonian (1) can be written in more explicit form through the angular momentum operators

$$\hat{H} = \hat{H}_p + \frac{\hbar^2}{2\Im}(\hat{\mathbf{I}}^2 - \hat{I}^2_{z'} - \hat{j}^2_{z'}) + \frac{\hbar^2}{2\Im}\hat{\mathbf{j}}^2 - \frac{\hbar^2}{2\Im}(\hat{j}_+\hat{I}_- + \hat{j}_-\hat{I}_+). \tag{2}$$

When the Coriolis interaction is neglected, the remaining expression is

$$\hat{H}^{(0)} = \hat{H}_p + \hat{H}_{rot}. \tag{3}$$

In this case, the rotation and single particle motion are fully separated. As mentioned in the Introduction, because of the axial symmetry of $H^{(0)}$, the angular momentum projections $I_{z'}$ and $j_{z'}$, usually denoted by K and Ω, are good quantum numbers and their values are equal $K = \Omega$. Thus, the eigenfunctions of $H^{(0)}$ can be written in the form

$$\psi_K = \mathcal{N}\left(D^I_{M,K}\chi_K + (-1)^{I+K}D^I_{M,-K}\mathcal{R}\chi_K\right), \tag{4}$$

where χ_K is the single particle wave function characterized by the quantum number K. The wave function is symmetrized with respect to the rotation $\mathcal{R}$ of the system on angle π about the y-axis in order to take into account the reflection symmetry of the system. Thus, the energy spectrum is given by

$$E(I) = \varepsilon_p(K) + \frac{\hbar^2}{2\Im}(I(I+1) - 2K^2), \tag{5}$$

where $\varepsilon_p(K)$ is the energy of the particle in the state χ_K, and the other part is the energy of a rigid rotor with a moment of inertia $\Im$.

We consider that in the full Hamiltonian $\hat{H}$, the Coriolis coupling term $\hat{H}^{(c)}$ is a perturbation to $\hat{H}^{(0)}$. The Coriolis term $\hat{H}^{(c)}$ is not diagonal with respect to the basis determined by the eigenfunctions (4) of $\hat{H}^{(0)}$. As a result the total Hamiltonian is also not diagonal. However, its eigenfunctions can be expanded in this basis space

$$\Psi_\tau = \sum_K C_K^\tau \psi_K, \tag{6}$$

where the sum, runs over the quantum numbers K of the basis functions. Then, the eigenequation

$$\hat{H}\Psi_\tau = E_\tau \Psi_\tau, \tag{7}$$

turns into a linear system of equations

$$\sum_{K'=1} (H_{KK'} - E_\tau \delta_{KK'}) C_{K'}^\tau = 0, \tag{8}$$

whose solutions are the energies E_τ and the coefficients C_K^τ in (6). The number of equations and the summation range in (8) are determined by the number of the taken basis functions. We should mention that the basis must not necessarily be complete. The so obtained eigenfunctions are the best approximation to the exact eigenfunctions of (1) in the chosen basis [7]. This is the well known direct diagonalization procedure.

The mixing of the wave functions (4) with different K values, physically corresponds to a situation in which the Coriolis interaction mixes different rotation bands. The effects of mixing are usually accounted by the theory of perturbation or by the direct diagonalization. Here, we propose a different approach for description based on the contact transformation method.

3 Contact Transformation and Diagonalization of Coriolis Interaction

The idea of the contact transformation method is to find an unitary operator $\mathcal{U}$ whose action on the full Hamiltonian $\hat{H}$ brings it into a form diagonal with respect to the basis functions ψ_K [3,4]. If such a transformation is applied to $\hat{H}$ and to its eigenfunctions

$$\mathcal{U}\hat{H}\mathcal{U}^\dagger \equiv \hat{H}', \quad \mathcal{U}\Psi_\tau \equiv \psi_K, \tag{9}$$

equation (7) transforms into the equivalent form

$$\hat{H}'\psi_K = E_\tau \psi_K. \tag{10}$$

Apparently, the sets of eigenvalues of the Hamiltonians (7) and (10) are the same. Therefore any eigenvalue E_τ of $\hat{H}$ in (7) corresponds to one eigenvalue of $\hat{H}'$ in (10) which is now characterized by the quantum number K of the basis function ψ_K. Then one can formally write $E_\tau \equiv E_\tau^K$. The eigenfunctions (6) of the original Hamiltonian (1) are determined by $\Psi_\tau = \mathcal{U}^{-1}\psi_K$.

The contact transformation method gives a simple prescription, how to determine the transformation operator $\mathcal{U}$. The unitary transformation can be decomposed into a chain of successive unitary transformations $e^{\hat{T}_i}$, $i = 1, 2, \ldots$

$$\hat{H}' \equiv \ldots e^{\hat{T}_2} e^{\hat{T}_1} \hat{H} e^{-\hat{T}_1} e^{-\hat{T}_2} \ldots, \tag{11}$$

where the operators $\hat{T}_i$ are anti-hermitian. The aim is to eliminate step by step the non-diagonal terms of the transformed operator by properly choosing the operators $\hat{T}_i$. After expanding the exponents in (11), the transformed operator $\hat{H}'$ can be written as a sum of n-fold commutators of the initial Hamiltonian and the operators T_n

$$\begin{aligned} \hat{H}' &= \hat{H}^{(0)} + \hat{H}^{(c)} + [\hat{T}_1, \hat{H}^{(0)}] + [\hat{T}_1, \hat{H}^{(c)}] \\ &+ \frac{1}{2!}[\hat{T}_1, [\hat{T}_1, \hat{H}^{(0)}]] + [\hat{T}_2, \hat{H}^{(0)}] + \ldots . \end{aligned} \tag{12}$$

Here, the expansion is given up to the terms which contribute to the diagonal part of $\hat{H}'$ after the first two transformations. The same expression appears in a matrix form as

$$\begin{aligned} H'_{KK'} = H^{(0)}_{KK'} + H^{(c)}_{KK'} &+ \sum_P (T_{1\,KP} H^{(0)}_{PK'} - H^{(0)}_{KP} T_{1\,PK'}) \\ + &\sum_Q (T_{1\,KQ} H^{(c)}_{QK'} - H^{(c)}_{KQ} T_{1\,QK'}) \\ + &\frac{1}{2!} \sum_R \Bigg(T_{1\,KR} \sum_S (T_{1\,RS} H^{(c)}_{SK'} - H^{(c)}_{RS} T_{1\,SK'}) \\ - &\sum_N (T_{1\,KN} H^{(c)}_{NR} - H^{(c)}_{KN} T_{1\,NR}) T_{1\,RK'} \Bigg) \\ + &\sum_P (T_{2\,KP} H^{(0)}_{PK'} - H^{(0)}_{KP} T_{2\,PK'}) + \ldots, \end{aligned} \tag{13}$$

where $O_{KK'} \equiv \langle \psi_K | \hat{O} | \psi_{K'} \rangle$ is the matrix element of a given operator $\hat{O}$ in the chosen representation ψ_K. In the first step $\hat{T}_1$ can be defined through the equality

$$H^{(c)}_{KK'} = -\sum_P (T_{1\,KP} H^{(0)}_{PK'} - H^{(0)}_{KP} T_{1\,PK'}) \quad K \neq K'. \tag{14}$$

Then, taking into account that $H^{(0)}_{KP} = \epsilon_K \delta_{KP}$ we find

$$T_{1\,KK'} = \frac{H^{(c)}_{KK'}}{\epsilon_K - \epsilon'_K} \quad K \neq K'. \tag{15}$$

The matrix element of the operator T_1 for $K = K'$ is not defined. In the considered basis the Coriolis term has an diagonal part $H^{(c)}_{KK}$ for $K = 1/2$. Therefore H_{KK} should be included in ϵ_K together with the single particle and the rotation energies.

$$\epsilon_K = \varepsilon_p(K) + \frac{\hbar}{2\Im}(I(I+1) - 2K^2) + H^{(c)}_{KK}\delta_{K\frac{1}{2}}. \tag{16}$$

By using (14), the transformed operator $\hat{H}'$ is obtained in the form

$$\begin{aligned} H'_{KK'} &= H^{(0)}_{KK'} + H^{(c)}_{KK'}\delta_{KK'} \\ &- \frac{1}{2}\sum_P (T_{1\,KP}H^{(c)}_{PK'} - H^{(c)}_{KP}T_{1\,PK'}) && (17) \\ &+ \sum_Q (T_{2\,KQ}H^{(0)}_{QK'} - H^{(0)}_{KQ}T_{2\,QK'}) + \ldots, && (18) \end{aligned}$$

which implies the definition of the second operator $\hat{T}_2$ as

$$\sum_Q (T_{2\,KQ}H^{(0)}_{QK'} - H^{(0)}_{KQ}T_{2\,QK'}) = \\ \frac{1}{2}\sum_P (T_{1\,KP}H^{(c)}_{PK'} - H^{(c)}_{KP}T_{1\,PK'}), \quad K \neq K'. \tag{19}$$

It is defined so that to eliminate further non-diagonal terms remaining after the first transformation.

Taking into account equations (15) and (19) and the explicit form of the operator T_1 we have

$$\widetilde{H}'_{KK} = H^{(0)}_{KK} + H^{(c)}_{KK} + \sum_{K' \neq K} \frac{H^{(c)}_{KK'}H^{(c)}_{K'K}}{\epsilon'_K - \epsilon_K}. \tag{20}$$

Then, Eq. (10) can be approximated by

$$\hat{\widetilde{H}}'\psi_K = \widetilde{E}^K_\tau \psi_K, \tag{21}$$

where

$$\widetilde{E}^K_\tau = \widetilde{H}'_{KK}. \tag{22}$$

The notations $\widetilde{E}^K_\tau$ and $\widetilde{H}'_{KK}$ mean that only some parts of the transformed Hamiltonian $\hat{H}'$ is considered.

Equation (20) has the standard form of the energy expression in the regular theory of perturbation. Although both expressions are identical they are derived by two approaches based on different assumptions. The theory of perturbation is based on the assumption that approximate eigenvalues and eigenfunctions can be expanded in series with respect to a small parameter [8]. The condition for convergence requires that every subsequent term in the expansion be smaller than the previous one. This condition is fulfilled when the perturbation is small.

On the other hand, the contact transformation method allows one to find the eigenvalues and the eigenfunctions of a given Hamiltonian in a certain basis without solving the linear system of equations (8). The advantage of the approach is that the transformation operators do not depend on the strength of the perturbation. As mentioned in the beginning of the section, the contact transformation method is based on the expansion of exponential operators in series. Therefore, the accuracy of the method depends on the speed of convergence of the expansion. If the matrix elements of the operators $\hat{T}_i$ are small quantities, then the expansion can be essentially resumed with a small number of terms. It is clear, that the unitarity of the operators depends on the order of the expansion and the smallness of the exponential factor. When the factor is small, a small number of expansion terms is enough to reasonably well approximate the operator.

4 Application to Coriolis Mixed Rotation Bands

In the present approach, the energy expression of the rotation spectrum of a rotor plus particle system with axially and reflection symmetric shape can be taken in accordance to Eqs. (20) and (22) in the form

$$\begin{aligned} E_\tau^K(I) = \varepsilon_p(K) + \frac{\hbar^2}{2\Im}\Bigg[& I(I+1) - 2K^2 \\ - & (-1)^{I+\frac{1}{2}}\delta_{K,1/2}\left(I+\frac{1}{2}\right)\langle\chi_K|\, j_+\, |\mathcal{R}\chi_K\rangle\Bigg] \\ + & 2\left(\frac{\hbar^2}{2\Im}\right)^2 (I-K)(I+K+1)\sum_{K'\neq K}\frac{|\langle\chi_{K'}|\, j_+\, |\chi_K\rangle|^2}{\epsilon_{K'}-\epsilon_K}, \end{aligned} \qquad (23)$$

where χ_K is the wave function of the single particle state on which the rotation band is built. The first line of the above expression is a sum of the single particle energy ε_p and the energy of the pure rotor. The next term is the well known decoupling energy and the last part represents the contribution of the Coriolis mixing to the full energy of the system.

The energy expression (23) is applied for description of the ground state and first excited rotation bands of the nuclei ^{183}W and ^{181}Hf. In both nuclei the ground state band is built on $K = 1/2$ single particle state and the excited band is based on $K = 3/2$. We assume that, both states are mutually mixed without interacting to other excited bands. Then, only one term remains in the sum over

K' in (23). The expression for the energy levels of the ground state band reads

$$\begin{aligned} E_\tau^{1/2}(I) &= \varepsilon_p(1/2) + \frac{\hbar^2}{2\Im}\left[I(I+1) - (-1)^{I+\frac{1}{2}}\left(I+\frac{1}{2}\right)\left\langle \frac{1}{2}\middle| j_+ \middle| -\frac{1}{2}\right\rangle\right] \\ &+ 2\left(\frac{\hbar^2}{2\Im}\right)^2 \frac{(I-\frac{1}{2})(I+\frac{3}{2})}{\epsilon_{3/2}-\epsilon_{1/2}}\left|\left\langle\frac{3}{2}\middle|j_+\middle|\frac{1}{2}\right\rangle\right|^2, \end{aligned} \tag{24}$$

while the energies of the excited band with $K = 3/2$ are

$$\begin{aligned} E_\tau^{3/2}(I) &= \varepsilon_p(3/2) + \frac{\hbar^2}{2\Im} I(I+1) \\ &- 2\left(\frac{\hbar^2}{2\Im}\right)^2 \frac{(I-\frac{3}{2})(I+\frac{5}{2})}{\epsilon_{3/2}-\epsilon_{1/2}}\left|\left\langle\frac{3}{2}\middle|j_+\middle|\frac{1}{2}\right\rangle\right|^2 . \end{aligned} \tag{25}$$

In the Figure 1, the energy levels (24) and (25) for the nucleus ^{183}W are compared with the experimental data. For the band with $K = 1/2$, a theoretical curve obtained by considering only the rotation plus decoupling part of the energy (24) without mixing term is given for comparison. It is seen that the effect of mixing is considerable, especially at the high spin states, where its taking into account provides a very good agreement between the theory and the experiment.

The present approach depends essentially on two parameters, the inertial parameter $\hbar^2/2\Im$ and the quadrupole deformation parameter β_2 for the considered nucleus. Since, we use single particle functions obtained in the framework of

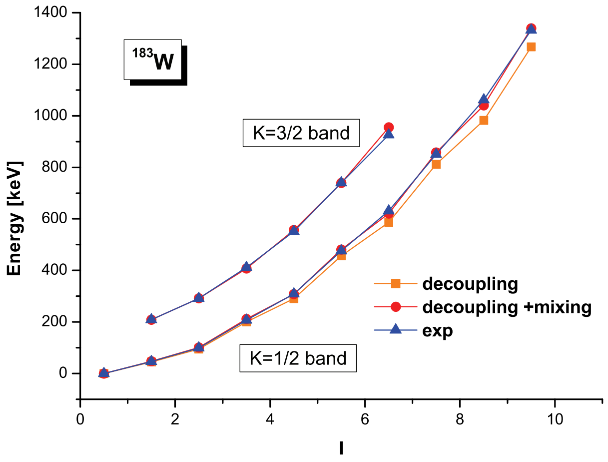

Figure 1. Theoretical and experimental energies [11] of the ground state and excited rotation bands for the nucleus ^{183}W.

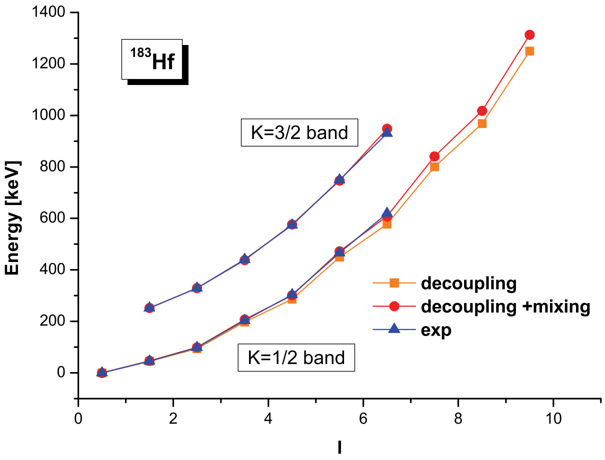

Figure 2. Theoretical and experimental energies [11] of the ground and excited rotation bands for the nucleus ^{181}Hf.

the deformed shell model with Wood-Saxon potential [9], the deformation parameter is related to the single particle potential shape.

The parameters for ^{183}W are as follows: the quadrupole deformation is $\beta_2 = 0.25$; the inertial parameter is $\hbar^2/2\Im = 12.527$ keV for the ground state band and $\hbar^2/2\Im = 18.122$ keV for the excited band . For both bands, the inertial parameter is fitted with respect to the first three levels of the respective band.

The results for the nucleus ^{181}Hf are depicted in Figure 2. They are similar to the results for the nucleus ^{183}W, which is not a surprise considering that both nuclei differ by two protons only. The parameters for ^{181}Hf are slightly different, but still very close to the parameters of ^{183}W. The deformation parameter is $\beta_2 = 0.26$. For the ground-state and exited bands the inertial parameters are $\hbar^2/2\Im = 12.348$ keV and $\hbar^2/2\Im = 16.620$ keV, respectively.

5 Conclusion

In conclusion, the used approach gives a very good agreement between the theory and experiment for the considered nuclei. Although, the effect of the mixing is not very large, it seems that the formalism takes it into account in a proper way. We remark that the present results are obtained with the use of two parameters only.

As mentioned in section 3, the approach is correct if a finite number of terms in the expansion of the operators e^{T_i} can be considered as a good approximation to the exact form of the operators. This condition is fulfilled if the matrix elements of the operators T_i are small. If its value is less than one the convergence is very fast. For an instance, we verified that the numerical value of the matrix element of T_1, Eq.(15), between the states with $K = 3/2$ and $K = 1/2$ at spin $I = 19/2$ for the nucleus ^{183}W is 0.59, which is small enough. The present result corresponds to a physical situation in which the difference between the single particle energies of the bandheads is larger than the energies between the first few levels in the rotation spectra [2, 10]. This feature characterizes the spectra of W, Hf, Er nuclei, as well as some Ra nuclei.

The present work is a test of the approach. It is seen that, the contact transformation method gives reasonable results even by the use of a few terms in the expansion (12). It can be used for analysis of the alignment process of the single particle motion with respect to the collective rotation as well as for a description of the rotation-vibration motion.

Acknowledgments

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