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F.R.May, L.Münchow

REMOVAL OF SPURIOUS CONTRIBUTIONS FROM ROTATIONAL EXCITATIONS

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* Central Institute for Nuclear Research, Rossendorf, GDR.

1. INTRODUCTION

Strong Coriolis band mixing effects are known from the study of decoupled bands in deformed odd-mass nuclei [1,2] and from the angular momentum alignment structures, found in a lot of transitional nuclei [3,4]. Certainly, band coupling is essential [5] for the explanation of back-bending. All these facts forced the interest to a more fundamental understanding of the Coriolis interaction concept.

Different attempts have been made for a microscopic description of the Coriolis interaction in odd-mass nuclei. A fruitful way is the direct derivation in the RPA framework, started by N.I.Pyatov [6] and recently continued by K.Hara [7] and by I.Hamamoto [8]. The latter authors gave expressions for dynamical attenuation factors, connected with the admixture of three quasiparticle states. A shortcoming of the RPA is the logical inconsistence to use the small angle approximation for situations where strong nonadiabatic effects are to be described. Therefore, a full legitimacy has the angular momentum projection method where this limitation is not required. This method has been recently proved to be useful both for a semi-phenomenological description [9], and for a more microscopic description of strong nonadiabatic effects like back-bending[10]. A shortcoming of this method, however, is the use of a nonorthogonal basis which has its origin in the admixture of spurious states. Firstly, I.N.Mikhailov and coworkers[11] and the authors[12] showed that diagonalizing in a perturbation approximation, the nonorthogonal states lead to a Coriolis-like coupling. In the paper[13] we demonstrated, that for even-even nuclei the same procedure leads to the exclusion of spurious contributions and to the introduction of the Thouless moment of inertia. This work is closely connected with a former investigation of J.Corbett[14]. Physically related to these results are the papers of H.J.Mang and coworkers[15] who derived the cranking formalism starting from angular momentum projection.

In[11,12] the main task was to derive the Coriolis interaction and an attenuation factor. A more close investigation shows, however, that this is not the whole thing. Like the case of even-even nuclei[13] this attenuation is due to spurious admixtures and just compensates diagonal spurious contributions. This is shown in chapter 2 using internal and collective coordinates. In chapter 3 mainly the same result is obtained by the usual direct method of projection for odd-mass nuclei. The latter gives the foundation for a numerical diagonalization of nonorthogonal projected states.

2. MIXING OF PROJECTED BANDS AND CORIOLIS INTERACTION

For the description of rotational bands in deformed nuclei we use the set of basic vectors

$$|IMK> = \frac{1}{N_{IK}^{1/2}} \int d\Omega \, \overset{*}{D}{}^{I}_{MK}(\Omega) R(\Omega)|K> \qquad (2.1)$$

with $\Omega = (\alpha\beta\gamma)$ - Euler angles, $R(\Omega) = R_z(\alpha) R_y(\beta) R_z(\gamma)$

- rotation operator, $|K>$ - deformed A - particle state with J_z - quantum number K,

$$N_{IK} = 4\pi^2 \int_0^{\pi} d\beta \sin\beta <K|R_y(\beta)|K> d^I_{KK}(\beta).$$

The basis (2.1) is overcomplete, thus

$$<IMK|IMK'> = \frac{4\pi^2}{N_{IK}^{1/2} \, N_{IK'}^{1/2}} \int_0^{\pi} d\beta \sin\beta \, d^I_{KK'}(\beta) <K|R_y(\beta)|K'> \neq 0. \qquad (2.2)$$

Orthogonal eigenstates are obtained from the superposition

$$|IM\nu> = \sum_K C^K_{I\nu} |IMK> \qquad (2.3)$$

leading to the eigenvalue problem

$$\sum_{K'} <IMK|H - E_{I\nu}|IMK'> C^{K'}_{I\nu} = 0. \qquad (2.4)$$

This procedure we call "band mixing" and will demonstrate, that it is a generalization of the Coriolis coupling concept.

To see the reason of the nonorthogonality (2.2) and to establish the relation to Coriolis coupling we use in this chapter the coordinate representation for deformed states

$$|K\rangle = \Psi_K(r_{1\alpha}, r_{2\alpha}, \dots) \equiv \Psi_K(r_{i\alpha}) \tag{2.5}$$

with $\alpha = (x, y, z)$ - components of the i-th particle position vector $\vec{r}_i$ on the axes of the laboratory system. The state $|K\rangle$ is assumed to be an eigenfunction of the deformed shell model Hamiltonian

$$H'|K\rangle = E_K|K\rangle, \qquad H' = T + V'. \tag{2.6}$$

To describe rotations we introduce a body-fixed system, the coordinate axes of which are given by the unit vectors $\vec{e}_a$ $(a = 1,2,3)$. Then

$$r_{i\alpha} = \sum_a R_{\alpha a} r'_{ia}, \qquad R_{\alpha a}(\vec{e}_\alpha \vec{e}_a) = R_{\alpha a}(\Omega) \tag{2.7}$$

with $\Omega = (\alpha\beta\gamma)$ - Euler angles, determining the position of the body-fixed system relative to the laboratory system. The Euler angles $\Omega = (\alpha\beta\gamma)$ and the internal coordinates r'_{ia} may be tracted as independent new coordinates, if a constraint is imposed on r'_{ia}. A possible one is the requirement

$$Q'_{ab} = \sum_i r'_{ia} r'_{ib} = Q'_a \delta_{ab}. \tag{2.8}$$

After this, the kinetic energy reads /16, 17/

$$T = \frac{1}{2m}\sum_{ia} p'^2_{ia} + \frac{1}{2\mathcal{J}}(J^2 - J_3^2) - \frac{1}{2\mathcal{J}}(J_+J'_- + J_-J'_+) + \frac{1}{2\mathcal{J}}(J'^2_1 + J'^2_2) \tag{2.9}$$

with $p'_{ia} = -i\frac{\partial}{\partial r'_{ia}}$ - component of the internal particle momentum on axis a, J_a - component of the total angular momentum on the axis a acting only on Euler angles, $J'_a = \sum_i (r'_{ib} p'_{ic} - r'_{ic} p'_{ib})$ - component of the internal angular momentum on axis a.

In eq. (2.9) the operator equation

$J_3 = J'_3$

is assumed to be fulfilled. Some additional terms to eq. (2.9), expressed by the so-called Nataf operator are omitted, they do not influence our result in a qualitative way. From the requirement (2.8) the moment of inertia $\mathcal{J}$ in formula (2.9) equals

$$\mathcal{J} = m\frac{(Q_3 - Q_2)^2}{Q_3 + Q_2}. \tag{2.10}$$

The deformed shell model potential V' becomes angle-dependent due to the violation of rotational invariance. For small angles one obtaines an anisotropic axial symmetric oscillator potential /17/

$$\begin{aligned} V' &= \frac{m}{2}\{\sum_i (x_i^2 + y_i^2)\omega_2^2 + \sum_i z_i^2 \omega_3^2\} = \\ &= \frac{m}{2}\{\sum_i (r'^2_{i1} + r'^2_{i2})\omega_2^2 + \sum_i r'^2_{i3}\omega_3^2 + (Q_3 - Q_2)(\omega_2^2 - \omega_3^2)\beta^2\} = \\ &= V'_{in} + \frac{1}{2}\mathcal{J}\omega^2\beta^2 \end{aligned} \tag{2.11}$$

with $\omega = \sqrt{2}\,\omega_0$ - the energy of the rotational - vibration quant. From eqs. (2.9) and (2.11) the deformed shell model Hamiltonian H' contains the rotational-vibration part

$$H_{RV} = H_{ROT} + \frac{1}{2}\mathcal{J}\omega^2\beta^2, \tag{2.12}$$

where

$$\begin{aligned} T_{ROT} = \frac{1}{2\mathcal{J}}(J^2 - J_3^2) = -\frac{1}{2\mathcal{J}}\Big(\frac{1}{\sin\beta}\frac{\partial}{\partial\beta}\big(\sin\beta\frac{\partial}{\partial\beta}\big) + \\ + \frac{1}{\sin^2\beta}\big(\cos^2\beta\frac{\partial^2}{\partial\gamma^2} + \frac{\partial^2}{\partial\alpha^2} - 2\cos\beta\frac{\partial^2}{\partial\alpha\partial\gamma}\big)\Big). \end{aligned} \tag{2.13}$$

The eigenfunctions $|K\rangle = \Psi_K(r_{i\alpha})$ may be written as

$$\Psi_K(r_{i\alpha}) = \sum_{K',n} c_n^{KK'} \Phi^{(n)}_{KK'}(\Omega) \Psi_K(r'_{ia}), \qquad (2.14)$$

where

$$H_{RV} \Phi^{(n)}_{KK'}(\Omega) = E^{(n)}_{KK'} \Phi^{(n)}_{KK'}(\Omega). \qquad (2.15)$$

From the assumption of axial symmetry we have

$$J_z \Psi_K(r_{i\alpha}) = K \Psi_K(r_{i\alpha}),$$

but this does not mean that also the z-component on the body-fixed axis J_3 is conserved because the Coriolis interaction in eq. (2.9) mixes internal states with different K-values. Setting in eq. (2.15)

$$\Phi^{(n)}_{KK'}(\alpha\beta\gamma) = e^{iK\alpha} \Phi^{(n)}_{KK'}(\beta) e^{iK'\gamma} \qquad (2.16)$$

we obtain for small angles β the equation

$$\left[\frac{1}{2\mathcal{J}}\left(-\frac{1}{\beta}\frac{\partial}{\partial\beta} - \frac{\partial^2}{\partial\beta^2} + \frac{(K-K')^2}{\beta^2}\right) + \frac{1}{2}\mathcal{J}\omega^2\beta^2\right] \Phi^{(n)}_{KK'}(\beta) = E^{(n)}_{KK'} \Phi^{(n)}_{KK'}(\beta) \qquad (2.17)$$

with the solution

$$\Phi^{(n)}_{KK'}(\beta) = N^{-1/2}_{KK'} \cdot x^{|\rho|} \cdot e^{-x^2/2} \sum_{\ell=0}^{n} a_\ell x^\ell, \quad x = \frac{\beta}{\beta_0}, \quad \beta_0 = \sqrt{\frac{1}{\mathcal{J}\omega}}, \quad \rho = \pm(K-K'),$$

$$a_{\ell+2} = \frac{2\ell - 2n}{(\ell+1)(\ell+2) + (2\rho+1)\ell + 2} a_\ell, \quad \ell = 0,2,\ldots,n-2, \quad n = 0,2, \qquad (2.18)$$

$$E^{(n)}_{KK'} = (n + 1 + |\rho|)\omega.$$

The structure of deformed shell model states $\Psi_K(r_{i\alpha})$ may be interpreted using eq. (2.14). Different internal states are admixed to it by the Coriolis coupling. This point of view has formerly been discussed by S.Frauendorf /18/.

As the frequency of rotational vibrations ω is large compared to single particle excitations

$$(E_{K'} - E_K) \ll \omega,$$

perturbation theory may be used. From

$$J_- |\Phi^{(0)}_{KK}(\Omega)\rangle = (J_1 - iJ_2)|\Phi^{(0)}_{KK}(\Omega)\rangle =$$

$$= \exp[i\gamma(-i\frac{1}{\beta}\frac{\partial}{\partial\gamma} - \frac{\partial}{\partial\beta} + \frac{i}{\beta}\frac{\partial}{\partial\alpha})]|\Phi^{(0)}_{KK}(\Omega)\rangle = \qquad (2.19)$$

$$= \frac{1}{\beta_0}|\Phi^{(0)}_{KK+1}(\Omega)\rangle$$

one obtains from eq. (2.15), applying the Coriolis interaction to eq. (2.9)

$$H_C = -\frac{1}{2\mathcal{J}}(J_+ J'_- + J_- J'_+)$$

as a perturbation,

$$\Psi_K(r_{i\alpha}) = \Phi^{(0)}_{KK}(\Omega)\Psi_K(r'_{ia}) + \frac{1}{2\mathcal{J}\beta_i} \frac{\langle K+1|J'_+|K\rangle}{E_{K+1} - E_K + \omega} \Phi^{(0)}_{KK+1}(\Omega)\Psi_{K+1}(r'_{ia}). \qquad (2.20)$$

To get the connection with angular momentum projection, we start from eq. (2.1)

$$|IMK\rangle = \frac{1}{N^{1/2}_{IK}} \int d\Omega' \overset{*}{D}{}^{I}_{MK}(\Omega') R(\Omega') \Psi_K(r_{i\alpha}).$$

Then for the first term in eq. (2.20) we obtain /19/

$$R(\Omega')\Phi^{(0)}_{KK}(\Omega)\Psi_K(r'_{ia}) = \sum_{I',M'} c_{I'} \overset{*}{D}{}^{I'}_{MK}(\Omega) D^{I'}_{M'K}(\Omega')\Psi_K(r'_{ia}),$$

$$c_{I'} = \frac{2I'+1}{2} N^{-1/2}_{KK} \int_0^\pi d\beta \sin\beta\, d^{I}_{KK}(\beta)\Phi^{(0)}_{KK}(\beta) = \frac{2I'+1}{2} N^{-1/2}_{KK'} \beta_0^2$$

and a similar result for the second term; thus finally

$$|IMK\rangle = \Psi_K(r'_{ia}) D^{*I}_{MK}(\Omega) + \frac{1}{2\mathcal{J}} \frac{\langle K+1|J'_+|K\rangle}{E_{K+1}-E_K+\omega}\sqrt{(I-K)(I+K+1)}\,\Psi_{K+1}(r'_{ia}) D^{*I}_{MK+1}(\Omega) \qquad (2.21)$$

and likely, for a deformed state with $J_z = K+1$

$$|IMK+1\rangle = \Psi_K(r'_{ia}) D^{I}_{MK+1}(\Omega) + \frac{1}{2\mathcal{J}} \frac{\langle K|J'_-|K+1\rangle}{E_K-E_{K+1}+\omega}\sqrt{(I-K)(I+K+1)}\,\Psi_K(r'_{ia}) D^{*I}_{MK}(\Omega)\,. \qquad (2.22)$$

From eqs. (2.21) and (2.22) we conclude, that projected states $|IMK\rangle$, $|IMK+1\rangle$ contain components with different internal states $\Psi_{K+1}(r'_{ia}), \Psi_K(r'_{ia})$ caused by Coriolis coupling of the internal motion to spurious rotational-vibration modes. Just the spurious components manifest themselves in the non-orthogonality of projected states $|IMK\rangle$ and $|IMK+1\rangle$

$$\langle IMK|IMK+1\rangle = \frac{1}{2\mathcal{J}}\langle K|J'_-|K+1\rangle\sqrt{(I-K)(I+K+1)}\times \qquad (2.23)$$

$$\times\left\{\frac{1}{E_K-E_{K+1}+\omega} + \frac{1}{E_{K+1}-E_K+\omega}\right\}.$$

Now we show that in the case of two bands $|IMK\rangle$, $|IMK+1\rangle$ and weak coupling the solution of the eigenvalue eq. (2.4) leads to a compensation of spurious components from projected states and instead of them to the Coriolis admixture of proper internal-rotational states. Let

$$|IM\nu\rangle = |IMK\rangle + c^{\nu}_{KK+1}|IMK+1\rangle \qquad (2.24)$$

then

$$c^{\nu}_{KK+1} = -\frac{\langle IMK|H-E_{I\nu}|IMK+1\rangle}{\langle IMK+1|H-E_{I\nu}|IMK+1\rangle}\,. \qquad (2.25)$$

The complete Hamiltonian reads

$$H = T_{in} + T_{ROT} + H_C + V(r'_{ia}, r'_{ib}),$$

further, in the lowest order

$$E_{I1} = \langle IMK|H|IMK\rangle = E^i_K,$$

e.g., from eq. (2.25)

$$c^{1}_{KK+1} = \frac{\langle IMK|(H-E^i_K)|IMK+1\rangle}{E^i_K - E^i_{K+1}}\,.$$

Using formulae (2.21), (2.22), this leads to

$$c^{1}_{KK+1} = -\frac{1}{2\mathcal{J}}\frac{\langle K|J'_-|K+1\rangle}{E^i_K - E^i_{K+1}}\sqrt{(I-K)(I+K+1)}\left(1-\frac{E^i_{K+1}-E^i_K}{\omega}\right). \qquad (2.26)$$

From eqs. (2.24) and (2.21) we obtain after all

$$|IM1\rangle = \Psi_K(r'_{ia}) D^{*I}_{MK}(\Omega) + \frac{1}{2\mathcal{J}}\frac{\langle K|J'_-|K+1\rangle}{E^i_{K+1}-E^i_K}\sqrt{(I-K)(I+K+1)}, \qquad (2.27)$$

e.g., the above stated result.

Finally, a remark concerning the usual Gaussian overlap approximation should be made. As is well known[20] in even-even nuclei the relation

$$\langle K=0|\,R_y(\bar{\bar{\beta}})|K=0\rangle = \exp\left(-\frac{\bar{\bar{\beta}}^2}{2}\langle 0|J^2_y|0\rangle\right) \qquad (2.28)$$

leads to the adiabatic $I(I+1)$-rotator spectrum. This expression follows at once, if in eq. (2.21) only the first term with the oscillator in the ground state is considered

$$\Psi_{K=0}(r_{i\alpha}) = N_{00}^{-1/2} e^{-x^2/2} \Psi_K(r'_{ia}).$$

For small angles β this assumption leads to

$$<0|R_y(\beta)|0> = N_{00}^{-1} <e^{-x^2/2}| e^{-\tilde{\tilde{\beta}}\frac{\partial}{\partial\beta}} | e^{-x^2/2}> = e^{-\tilde{\tilde{\beta}}^2/4\beta_0^2}. \quad (2.29)$$

Further,

$$<0|J_y^2|0> = \frac{1}{2\beta_0^2}\,, \quad <0|\beta^2|0> = \frac{\beta^2}{2}$$

hence the angular momentum-angle uncertainty relation for oscillator states

$$<0|J_y^2|0><0|\beta^2|0> = \frac{1}{4}$$

holds which shows together with eq. (2.29) that the Gaussian approximation (2.28) comes out. From

$$\beta_0^2 = \frac{1}{2<0|J_y^2|0>} \equiv \frac{1}{4j}$$

the coupling matrix element in eq. (2.25) is

$$<IMK|H-E_{I\nu}|IMK+1> = -\frac{1}{2\mathcal{J}}<K|J'_-|K+1>\sqrt{(I-K)(I+K+1)}\left(1-\frac{E^i_{K+1}-E^i_K}{4j}\mathcal{J}\right) \quad (2.30)$$

- an expression, formerly obtained by direct calculation for even-even and odd-mass nuclei [12,13].

A practical shortcoming of the coordinate method of this chapter is the difficulty to fulfill the constraint (2.8) at any step of the calculation. Also, it is difficult to establish the contact with the usual theory of deformed single particle states. Therefore, in the next chapter the direct method for the calculation of projection integrals is applied.

3. DIRECT INVESTIGATION OF BAND MIXING IN ODD-MASS NUCLEI

We shall apply the general ideas of chapter 2 to the case of two bands $|IMK>$, $|IMK+1>$ of an odd-mass nucleus using deformed Nilsson states and pairing interaction. The case of an even-even nucleus has been analysed formerly in similar lines [13].

The basic states

$$|IMk> = \frac{1}{N_{Ik}^{1/2}} \int d\Omega D^{I*}_{MK}(\Omega) R(\Omega)|k>$$

are again the starting point, where $|k>$ is the one quasi-particle state

$$|k> = \alpha^+_{K\sigma}|0> \quad (3.1)$$

(K, σ) - Nilsson quantum numbers, $|0>$ - BCS - vacuum of the even-even core.

A direct evaluation of the wave function is not useful in this method and we shall calculate the matrix elements to solve the eigenvalue problem (2.4). Firstly, we obtain diagonal matrix elements $<IMk|H|IMk>$ and will see, that due to spurious components in the wave function there appears a rotational energy contribution from the odd particle [21]. As

$$<IMk|H|IMk> = \frac{4\pi^2}{N_{Ik}} \int_0^\pi d\beta \sin\beta\, d^I_{KK}(\beta) <k|HR_y(\beta)|k> \quad (3.2)$$

one has to obtain the overlap integral $h_{kk}(\beta) \equiv <k|HR_y(\beta)|k>$. From

$$R_y(\beta)\alpha_k^+ R_y^{-1}(\beta) = \sum_{k'} d_{k'k}(\beta)\, \xi^{(+)}_{kk'} \alpha^+_{k'}, \quad \xi^{(\pm)}_{kk'} = u_k v_{k'} \pm u_{k'} v_k \quad (3.3)$$

it follows that

$$h_{kk}(\beta) = \langle 0|\alpha_k R_y(\beta) H \alpha_k^+|0\rangle = \langle 0|H R_y(\beta)|0\rangle + \sum_{k'} \langle 0|\alpha_k [H, \alpha_{k'}^+] R_y(\beta)|0\rangle d_{k'k}(\beta). \tag{3.4}$$

To continue we have to use a concrete expression for the Hamiltonian. Within the pairing plus Q-Q-model

$$H = E_0 + \sum_k E_k \alpha_k^+ \alpha_k - \frac{\chi}{2} \sum_\mu (-)^\mu Q_{-\mu} Q_\mu \tag{3.5}$$

we obtain from eq. (3.4)

$$h_{kk}(\beta) = \langle 0|H R_y(\beta)|0\rangle + E_k \langle 0|R_y(\beta)|0\rangle - \chi \sum_{k'} \xi^{(-)}_{kk'} \left[q^{1}_{kk'} \langle 0|Q_{-1} R_y(\beta)|0\rangle + q^{-1}_{kk'} \langle 0|Q_1 R_y(\beta)|0\rangle\right], \tag{3.6}$$

where

$$q^{\mu}_{kk'} = \langle k|r^2 Y_{2\mu}|k'\rangle .$$

Further, using the relations

$$\langle 0|Q_{\pm 1} R_y(\beta)|0\rangle = \mp \frac{1}{4}\sqrt{6}\,\sin\beta \langle 0|Q_0|0\rangle \langle 0|R_y(\beta)|0\rangle \tag{3.7}$$

and

$$\langle 0|\alpha_k Q_{\pm 1} \alpha_{k'}^+|0\rangle = -\frac{1}{\sqrt{6}} \frac{E_{k'} - E_k}{\chi \langle 0|Q_0|0\rangle} \xi^{(+)}_{kk'} j^{\pm}_{kk'} \tag{3.8}$$

one gets for small angles β the expression

$$h_{kk}(\beta) = [E_0 + E_k + (h_{1c} + h_1')\beta^2]\, e^{-j\beta^2} \tag{3.9}$$

with

$$h_{1c} = -\frac{1}{2} \langle 0|(H - E_0) J_y^2|0\rangle ,$$

$$h_1' = -\frac{1}{2} \sum_{k'} \xi^{(+)2}_{kk'} \left[|\langle \phi_{k'}|j_y|\phi_k\rangle|^2 \delta_{K'K+1} + |\langle \phi_k|j_y|\phi_{k'}\rangle|^2 \delta_{K'K-1}\right](E_{k'} - E_k), \tag{3.10}$$

$$j = \frac{1}{2}\langle k|J_y^2|k\rangle = \frac{1}{2}\langle 0|J_y^2|0\rangle + \frac{1}{2}\sum_{k'} \xi^{(+)2}_{k'k} \left[|\langle \phi_{k'}|j_y|\phi_k\rangle|^2 \delta_{K'K+1} + |\langle \phi_k|j_y|\phi_{k'}\rangle|^2 \delta_{K'K-1}\right] \equiv j_0 + j' . \tag{3.11}$$

Assuming finally a large dispersion $j > 1$, from eq. (3.2) we get in the lowest order the rotational energy

$$E^{dia}_{I\nu} \equiv \langle IMk|H|IMk\rangle = E_0 + E_k - \frac{1}{2\mathcal{J}_k}\langle k|J^2|k\rangle + \frac{1}{2\mathcal{J}_k}[I(I+1) - K^2] \tag{3.12}$$

with

$$\frac{1}{2\mathcal{J}_k} = \frac{1}{2\mathcal{J}_0}\left(1 - \frac{2j'}{j_0}\right) + \frac{1}{8 j_0^2}\left(1 - \frac{2j'}{j_0}\right) \times \sum_{k'} (E_{k'} - E_k)\, \xi^{(+)2}_{k'k} \left[|\langle \phi_{k'}|j_y|\phi_k\rangle|^2 \delta_{K'K+1} + |\langle \phi_k|j_y|\phi_{k'}\rangle|^2 \delta_{K'K-1}\right].$$

Formula (3.12) shows, that the projected energy of the one quasi-particle state $|k\rangle$ automatically contributes to the rotational energy, if terms of the order j'/j_0 are included. The expression for the inverse moment of inertia $1/2\mathcal{J}_k$, however, is not the result one expects by adding one particle to the core. It rather leads to an enlarging of the rotational energy, compensated somewhat by the factor $(1-2j'/j_0)$ in front of the $1/2\mathcal{J}_0$ -core-term. As we shall see, the removal of nonorthogonality by the method, introduced in chapter 2, helps to obtain a more meaningful result. For the diagonalization the coupling matrix element $\langle IMk|H-E_{Ik}|IMk+1\rangle$ in the case of two bands is needed. Similar to eq. (3.2) we have

$$\langle IMk|H|IMk+1\rangle = \frac{1}{N_{Ik}^{1/2}\, N_{Ik+1}^{1/2}} \int_0^{\pi} d\beta \sin\beta\, d^I_{KK+1}(\beta) \langle k|HR_y(\beta)|k+1\rangle \qquad (3.13)$$

and

$$\langle k|HR_y(\beta)|k'\rangle = \xi^{(+)}_{kk'} d_{kk'}(\beta)\{\langle 0|HR_y(\beta)|0\rangle + E_k \langle 0|R_y(\beta)|0\rangle\} - \qquad (3.14)$$

$$-\frac{\chi}{2}\sum_{k''} \xi^{(+)}_{k''k'} d_{k''k'}(\beta) \langle k|Q_-|k''\rangle \langle 0|Q_- R_y(\beta)|0\rangle,\quad Q_- = Q_1 - Q_{-1}.$$

Using relations (3.7) and (3.8), we obtain the simple result

$$\langle k|HR_y(\beta)|k'\rangle = \xi^{(+)}_{kk'} d_{kk'}(\beta)\{\langle 0|HR_y(\beta)|0\rangle + \frac{1}{2}(E_k + E_{k'})\langle 0|R_y(\beta)|0\rangle\}. \qquad (3.15)$$

Within the Gaussian overlap approximation

$$\langle 0|HR_y(\beta)|0\rangle = (E_0 + h_{1c}\beta^2)\exp(-j\beta^2),\quad \langle 0|R_y(\beta)|0\rangle = \exp(-j\beta^2),$$

$$d_{kk+1}(\beta) = -i\beta\langle\phi_k|j_y|\phi_{k+1}\rangle,\qquad d_{kk}(\beta) = 1,$$

$$d^I_{KK+1}(\beta) = \frac{\beta}{2}\sqrt{(I-K)(I+K+1)},\qquad d^I_{KK}(\beta) = 1$$

we get from eqs. (3.13) and (3.14)

$$\langle IMk|H|IMk+1\rangle = -\frac{1}{2\mathcal{J}_0}\langle k|J_-|k+1\rangle\sqrt{(I-K)(I+K+1)}\left(1-\mathcal{J}_0\frac{E_{k+1}+E_k}{4j_0}\right), \qquad (3.16)$$

$$\langle IMk|IMk+1\rangle = \frac{1}{4j_0}\langle k|J_-|k+1\rangle\sqrt{(I-K)(I+K+1)}.$$

For small perturbation we may put in the nondiagonal matrix element $E_{Ik} = E_k$ for the energy of the coupled $|IMK\rangle$ -band, then

$$\langle IMk|H-E_{I\nu}|IMk+1\rangle = -\frac{1}{2\mathcal{J}_0}\langle k|J_-|k+1\rangle\sqrt{(I-K)(I+K+1)} \times \qquad (3.17)$$

$$\times\left(1 - \frac{E_{k+1}-E_k}{4j_0}\mathcal{J}_0\right)$$

- the same expression as obtained in chapter 2 by the coordinate method. Expression (3.17) is similar to the Coriolis-coupling matrix-element, the only difference is the "attenuation" factor $1 - \frac{E_{k+1}-E_k}{4j_0}\mathcal{J}_0$ which comes from spurious admixtures and disappears at the end of calculation. The correction to the energy follows from the formula

$$E_{I\nu} = E^{dia}_{I\nu} - \frac{|\langle IMk|H-E_{I\nu}|IMk+1\rangle|^2}{E_{k+1}-E_k}, \qquad (3.18)$$

which gives together with eqs. (3.12) and (3.17)

$$E_{I\nu} = E_0 + E_k - \frac{1}{2\mathcal{J}_k}\langle k|J^2|k\rangle + [I(I+1)-K^2][\frac{1}{2\mathcal{J}_0}(1-\frac{\mathcal{J}'}{\mathcal{J}_0})+ \tag{3.19}$$
$$+\frac{1}{8j_0^2}(\frac{1}{2}-\frac{j'}{j_0})(E_{k+1}-E_k)\xi^{(+)2}_{k+1\,k}|\langle\phi_{k+1}|j_y|\phi_k\rangle|^2 -$$
$$-\frac{K}{(2\mathcal{J}_0)^2}|\langle k|J_-|k+1\rangle|^2(1-\frac{E_{k+1}-E_k}{4j_0}\mathcal{J}_0)^2,\ \mathcal{J}'=\frac{2|\langle k|J_y|k+1\rangle|^2}{E_{k+1}-E_k}.$$

The first part of the effective inverse moment of inertia

$$\frac{1}{2\mathcal{J}_0}(1-\frac{\mathcal{J}'}{\mathcal{J}_0}) = \frac{1}{2(\mathcal{J}_0+\mathcal{J}')}$$

is an expression, expected from the influence of a pure Coriolis interaction on the motion of the odd particle. It is also known from the cranking model. The second term is the small remaining part of the projection rotational energy which is not compensated exactly in the approximation scheme of this chapter.

To see the reason for this we calculate the matrix element $\langle IMk|H|IMk\rangle$ using eq. (2.21). If $\Psi_K(r'_{ia})$ is assumed to describe an odd-mass nucleus, one gets, in the limit $(E_{k+1}-E_k) \ll \omega$

$$\langle IMk|H|IMk\rangle = E_0 + E_k + \frac{1}{2\mathcal{J}}[I(I+1)-K^2] + \tag{3.20}$$
$$+\frac{(E_{k+1}-E_k)|\langle k|J'_y|k+1\rangle|^2}{16j^2}(I-K)(I+K+1) - \frac{1}{2\mathcal{J}}\frac{2j'}{j}(I-K)(I+K+1),$$

e.g., the contribution to the inverse moment of inertia $1/2\mathcal{J}$ from the odd particle is

$$\frac{(E_{k+1}-E_k)|\langle k|J'_y|k+1\rangle|^2}{16j^2}$$

rather then

$$\frac{(E_{k+1}-E_k)|\langle k|J'_y|k+1\rangle|^2}{8j^2}(1-\frac{2j'}{j_0})$$

obtained in formula (3.12) (the pairing factor neglected). Actually, the factor $(1-2j'/j_0)$ can be of the order of $\frac{1}{2}$ so that the correct result of chapter 2 comes out. A more accurate numerical calculation of the relevant matrix elements will probably remove this small discrepancy.

The main result of this investigation is the derivation of the Coriolis interaction in a microscopic way showing also that for weak nonadiabatic effects in the frame of one quasi-particle states no attenuation appears. Further, starting from the obtained analytical results it appears to be meaningful to do numerical calculations in the scheme of chapter 3 in order to cover higher order contributions.

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