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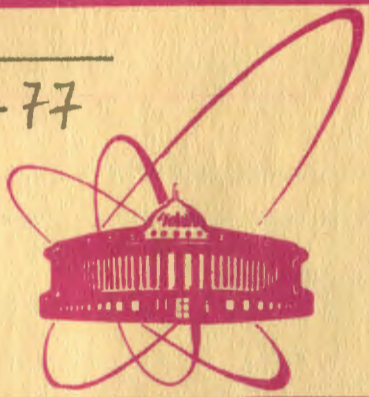

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A PROGRAM FOR CALCULATION OF THE CORIOLIS EFFECT IN ODD-ODD NUCLEI

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NATURE OF PHYSICAL PROBLEM

Many papers have been devoted recently to particle-rotational coupling (Coriolis effect) in odd deformed nuclei (e.g., refs. [1-4]), when the experimental spectrum could be often explained by this coupling. Therefore, one can expect that the Coriolis coupling plays, as well, a significant role in odd-odd deformed nuclei for which a lot of experimental data appeared lately (e.g., refs. [5]). The program gives a possibility of extracting pure intrinsic energy values from experimental data. This is important for testing the theoretical models for intrinsic structure of odd-odd nuclei. The program calculates the perturbed energy levels. It is written as a subroutine to be used with the MINUIT minimization program[6], which makes a least-square fit to the experimental energy levels. Mixed amplitudes of the wave functions are obtained for the final fit.

METHOD OF SOLUTION

In order to take the Coriolis coupling into account, the matrix of the total Hamiltonian is constructed and diagonalized. The Jacobi diagonalization method is used repeatedly in the search for the eigenvalues and coupling amplitudes for all spin values. Simultaneously, the adjustment of all the parameters is carried out until a least-square fit to the experimental energy levels is obtained.

RESTRICTION ON THE COMPLEXITY OF THE PROBLEM

The current version is dimensioned for 20 interacting rotational bands, the maximum spin I=19, and maximum 10 experimental energy levels for each of the interacting rotational bands.

TYPICAL RUNNING TIME

The running time depends on the number of interacting bands and the number of free parameters. Therefore the required time varies from one to several tens of minutes on the CDC 6500 computer.

LONG WRITE-UP

1. Description of the Program

The program is based on the "two particles + rotor" model with inclusion of the Coriolis coupling [7,8]. In order to take into account the Coriolis coupling an energy matrix is constructed and diagonalized. The procedure is similar to that described in ref. [9] for odd nuclei.

The total Hamiltonian for a deformed odd-odd nucleus can be written in the frame of adiabatic approximation:

$$H = H_{int} + H_{rot} , \tag{1}$$

where H_{int} is the intrinsic part of the Hamiltonian and H_{rot} is the rotational Hamiltonian.

$$H_{rot} = \sum_{i=1}^{3} \frac{\hbar^2}{2J_i} R_i^2 = \sum_{i=1}^{3} \frac{\hbar^2}{2J_i} (I_i - j_i)^2 , \tag{2}$$

where $\vec{I}$, $\vec{R}$, $\vec{j}$ are the total, rotational and intrinsic angular momentum operators, respectively.

In case the shape of the deformed core is axially symmetric the inertial parameters fulfil

$$\frac{\hbar^2}{2J_1} = \frac{\hbar^2}{2J_2} = \frac{\hbar^2}{2J}, \quad \text{and} \quad \frac{\hbar^2}{2J_3} = 0$$

so that equation (2) can be rewritten in the form:

$$H_{rot} = H_{rot}^{(0)} + H_j + H_{cor} , \tag{3}$$

where

$$H_{rot}^{(0)} = \frac{\hbar^2}{2J} (I^2 - I_3^2) \tag{4}$$

is the pure rotational term,

$$H_j = \frac{\hbar^2}{2J} \frac{1}{2} (j_+ j_- + j_- j_+) \tag{5}$$

is the recoil term, and

$$H_{cor} = -\frac{\hbar^2}{2J} (I_+ j_- + I_- j_+) \tag{6}$$

is the Coriolis coupling term.

Hamiltonian (1) is used for the construction of the energy matrix in $\sim \mathcal{D}^I_{MK} \phi_K^{(\alpha)}$ basis for a given value of I, where $\mathcal{D}^I_{MK}$ are the Wigner functions (the eigenfunctions of $H_{rot}^{(0)}$) and

$\phi_K(a)$ is the intrinsic wave function - the solution of the Schrödinger equation:

$$H_{int}\,\phi_K^{(a)} = E_{K_a}\phi_K^{(a)}\,, \tag{7}$$

where K is the projection of the intrinsic angular momentum $\vec{j}$ into the symmetry axis of the odd-odd nucleus. The intrinsic wave function $\phi_K^{(a)}$ can be written as a product of the wave functions characterising the intrinsic states of the odd neutron and odd proton (see ref.[10]):

$$\phi_K^{(a)} = x_{\Omega_n}^{(\rho_n)} x_{\Omega_p}^{(\rho_p)}, \quad K = \Omega_n + \Omega_p\,,$$
$$\phi_K^{(a)} = x_{\Omega_n}^{(\rho_n)} x_{-\Omega_p}^{(\rho_p)}, \quad K = |\Omega_n - \Omega_p| \tag{8a}$$

for $K \neq 0$ and

$$\phi_K^{(a)} = \frac{1}{\sqrt{2}}\left(x_{\Omega_n}^{(\rho_n)} x_{-\Omega_p}^{(\rho_p)} - \gamma\, x_{-\Omega_n}^{(\rho_n)} x_{\Omega_p}^{(\rho_p)}\right), \quad \Omega_n = \Omega_p \tag{8b}$$

for $K = 0$. In (8) $x_{\Omega_p}^{(\rho_n)}$ and $x_{\Omega_n}^{(\rho_p)}$ are the odd-proton and odd-neutron wave functions, respectively, $a \equiv (\rho_n, \rho_p)$ denotes the quantum numbers, which together with projection K determine entirely the intrinsic state of given odd-odd nucleus.

The diagonal elements of the energy matrix of Hamiltonian (1) are as follows:

$$H_{Ka}(I)_{Ka} = E_{Ka} + \frac{\hbar^2}{2J_a}\{I(I+1) - K^2\} + \frac{\hbar^2}{2J_a}\sum_{a_i} \langle \phi_K(a)|j_+|\phi_{K_i}(a_i)\rangle^2 \tag{9}$$

and the nondiagonal elements:

$$H_{K_1 a_1}(I)_{K_2 a_2} = -\frac{1}{2}\left(\frac{\hbar^2}{2J_1} + \frac{\hbar^2}{2J_2}\right)\{\sqrt{(I+K_2)(I-K_2+1)}\,\delta_{K_1,K_2-1}\langle\phi_K(a_2)|j_+|\phi_{K_1}(a_1)\rangle +$$
$$+ \sqrt{(I-K_2)(I+K_2+1)}\,\delta_{K_1,K_2+1}\langle\phi_{K_1}(a_1)|j_+|\phi_{K_2}(a_2)\rangle +$$
$$+ \frac{1}{2\sqrt{2}}\sqrt{I(I+1)}\,\delta_{K_1,0}\delta_{K_2,1}(1+(-1)^I\gamma_{a_1})^2\langle\phi_{K_2}(a_2)|j_+|\phi_{K_1}(a_1)\rangle + \tag{10}$$
$$+ \frac{1}{2\sqrt{2}}\sqrt{I(I+1)}\,\delta_{K_1,1}\delta_{K_2,0}(1+(-1)^I\gamma_{a_2})^2\langle\phi_{K_1}(a_1)|j_+|\phi_{K_2}(a_2)\rangle\}.$$

The matrix elements $\langle\phi_{K_1}(\alpha_1)|j_+|\phi_{K_2}(\alpha_2)\rangle$ can be expressed by means of the matrix elements of intrinsic wave functions $x_\Omega(\rho)$ for odd neutrons and protons:

$$\langle\phi^{(\alpha_1)}_{K_1}|j_+|\phi^{(\alpha_2)}_{K_2}\rangle =$$

$$=\delta_{\Omega_{p_1}\Omega_{p_2}}\langle x_{\Omega_{n_1}}(\rho_{n_2})|j_+(n)|x_{\Omega_{n_2}}(\rho_{n_2})\rangle\beta_{\rho_{n_1}\rho_{n_2}}\delta_{\rho_{n_1}\rho_{n_2}} + \qquad (11)$$

$$+\delta_{\Omega_{n_1},\Omega_{n_2}}\langle x_{\Omega_{p_1}}(\rho_{p_1})|j_+(p)|x_{\Omega_{p_2}}(\rho_{p_2})\rangle\beta_{\rho_{p_1},\rho_{p_2}}\delta_{\rho_{n_1}\rho_{n_2}} .$$

A similar expression can be obtained if one from K_1 and K_2 is equal to zero. The attenuation parameters β_{ρ_1,ρ_2} are introduced to adjust the coupling strength when it is necessary from the point of view of the applied model. These parameters can be considered as free parameters in the program. The intrinsic Coriolis matrix elements $\langle x_{\Omega_1}|j_+|x_{\Omega_2}\rangle$ can be calculated in the frame of various nuclear models, for instance, the Nilsson single-particle model [11], or the independent quasiparticle model [7,10], or the quasiparticle + phonon model [7]. The intrinsic Coriolis matrix elements are a part of the input data in the program. Since all the presently used intrinsic nuclear models are not precise enough to give the values of intrinsic energies E_{K_α} with sufficient accuracy, the program enables to fit them. It is also a reason for treating the inertial parameters as free parameters for each rotational band. Since this assumption is not theoretically clear, a possibility is given in the program to keep all inertial parameters equal to each other and to fit only the one common to every rotational band.

The energy matrix is constructed by the program from the elements given by equations (9) and (10). In order to obtain the perturbed rotational energy levels this matrix is repeatedly diagonalized for all the spin values I included. The program simultaneously adjusts the values of free parameters: E_{K_α}, $\frac{h^2}{2J_\alpha}$, β_{ρ_1,ρ_2} for all included rotational bands until a least square fit to the experimental energy levels is made. The minimized value is:

$$x^2 = \sum_{i=1}^{n} w_i (E_i^{th} - E_i^{exp})^2 , \qquad (12)$$

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* The energy range can be chosen so that all the energies are referred to the lowest level of the ground rotational band.

where n is the number of experimental levels, E_i^{th} and E_i^{exp} denote the calculated and experimental energy levels, respectively, and w_i is the weighting factor which is assumed to be an inverse square of the experimental error.

The program gives perturbed energy levels as well as the final set of parameters. This mixed amplitudes of the wave functions are printed for the final fit.

The program is written in FORTRAN. Instructions for use are given in section 2.

2. Input Data Cards

The program is written as an FCN subroutine for the MINUIT minimization program. The program and the input data cards required are described in ref.[12]. The remaining input cards are read by the FCN subroutine (see the table). The input parameter cards read by the MINIUT program must preserve the same order in which the band head asymptotic quantum number cards are read by the FCN subroutine, and at the same time the intrinsic energy levels must be read first; the inertial parameters, second; and at the end of the free parameter card string, the attenuation factors.

The number of attenuation factor cards must be equal to the number of different intrinsic Coriolis matrix elements. The FCN subroutine links the attenuation factors with the intrinsic Coriolis matrix elements in the order of their appearance in the fourth card group (see the table).

2.1. The Program Options

In addition to the calculation mode (ISW1=0) when all inertial parameters can be treated as free ones, independently of each other, there exists a possibility of adjusting only one inertial parameter common for all rotational bands (ISW1≠0). In this case the FCN subroutine takes the X(NBAND+1) parameter as a common one and the rest of the inertial parameters on the MINUIT input cards must be fixed.

3. Output Prints

The input data are reproduced for the value of the FCN parameter IFLAG=3, final tables are printed as well. Self-explanatory descriptions of the tables are also printed. In addition to it, if MATDIA≠0, the energy matrix before diagonalization

Table

Data cards read by the ODDODDCORI subprogram

Number of card group	Column	Format	Variable name	Comments
1	2	3	4	5
1		5I2		
	1-2		NBAND	The number of interacting bands. NBAND must be less than 21.
	3-4		IMAX	The maximum spin value for which the energy matrix is still diagonalized. IMAX must be less than 20.
	5-6		MATDIA	If not zero, the energy matrix before diagonalization is printed if simultaneously IFLAG=3.
	7-8		NUMITR	If not zero, the number of diagonalizing steps is printed if simultaneously IFLAG=3.
	9-10		ISW1	If not zero, one common inertial parameter is fitted for all bands (that X(NBAND+1)). This card group contains one card.
2		10I3		The asymptotic quantum numbers of the band heads: $K\gamma\Omega_p[Nn_z\Lambda]_p\Omega_n[Nn_z\Lambda]_n$.I is the band head serial number.
	1-3		KNNZLA(I,1)	K - the value of the angular momentum component along the nuclear symmetry axis.
	4-6		KNNZLA(I,2)	γ - this value is +1 or -1 only for the band with K=0. If K$\neq$0 then γ must be zero.

Table (continued)

1	2	3	4	5
	7-9		KNNZLA(I,3)	$2\Omega_p$- the doubled value of the angular momentum component of the proton state along the nuclear symmetry axis.
	10-12		KNNZLA(I,4)	N
	13-15		KNNZLA(I,5)	n_z } The asymptotic quantum numbers of the proton state
	16-18		KNNZLA(I,6)	Λ
	19-21		KNNZLA(I,7)	$2\Omega_n$- the doubled value of the angular momentum component of the neutron state along the nuclear symmetry axis
	22-24		KNNZLA(I,8)	N
	25-27		KNNZLA(I,9)	n_z } the asymptotic quantum numbers of the neutron state
				Λ
				The Ω_p must be always positive. The cards must be in the order of increasing K. This card group contains NBAND cards.
3				The experimental energy levels.
	1-2	I2	KORDER	The serial number of the band corresponding to the asymptotic quantum numbers' serial number of the band head, adopted in the previous item.
		2F10.2,		
	1-10	I2	EEXP (KORDER, J)	The experimental energy level.
	11-20		EEXP(KORDER, (J+1)	Its error.

Table (continued)

1	2	3	4	5
	21-22		IEXP(KORDER, J+2)	Its spin value. The number of the experimental energy levels for concrete KORDER value must not exceed 10. Every card group corresponding to one band must be finished by a card containing an arbitrary negative real at the first ten columns. A blank card signals the end of this card group. The whole card number of this group: twice number of the bands with known experimental levels + the number of all known experimental levels + 1
4		F10.4, 2I2		Intrinsic Coriolis matrix elements among the proton states.
	1-10		AMATPR(I,J)	The value of the matrix element between the I and JI states.
	11-12		I	The serial numbers of states, in accordance with the order adopted in the quantum numbers of the band heads.
	13-14		J	One blank card signals the end of this card group.
5		F10.4, 2I2		Intrinsic Coriolis matrix elements among the neutron states.
	1-10		AMATNT(I,J)	The description of this card group is analogous to that of the previous one.
	11-12		I	
	13-14		J	A blank card again signals the end of this card group.

is printed when IFLAG=3 and if NUMITR≠0, the number of diagonalization steps performed by the KIM subroutine to reach a defined zero (put into the DISTAN variable) in non-diagonal matrix element is printed, too. By changing the DISTAN value one affects the running time. The FCN subroutine prints neither the input values of the parameters nor the resulting ones.They are printed only by the MINUIT Program.

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