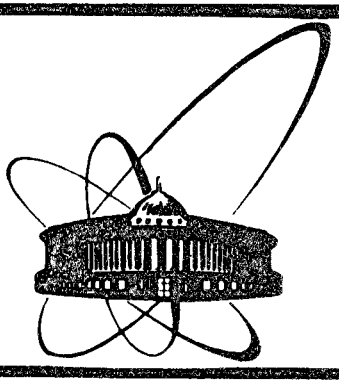

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A PROGRAM FOR CALCULATION OF THE E1, E2 AND M1 TRANSITION PROBABILITIES IN ODD-ODD NUCLEI TAKING THE CORIOLIS MIXING INTO ACCOUNT

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NATURE OF PHYSICAL PROBLEM

It is well known that comparison of experimental reduced transition probabilities with their model-depending predictions is of great importance for studying nuclear structure. Namely, the influence of the Coriolis particle-rotational coupling on electromagnetic transitions between excited states in odd-A deformed nuclei has been the subject of interest in many papers and has been reliably demonstrated [1].

Analogous situation in odd-odd nuclei has also been proved [1].

The program gives a possibility to calculate the E1, E2 and M1 reduced transition probabilities in odd-odd deformed nuclei. The mixed wave functions used result from a least-square fit of energy levels (taking the Coriolis effect into account) to the experimental ones, performed with the modified ODDODDCORI subprogram [2].

METHOD OF SOLUTION

The calculation of the reduced electromagnetic probabilities can be subdivided into two stages. In the first one, the total Hamiltonian (with Coriolis coupling term included) is diagonalised and eigenvalues and eigenvectors are found. This procedure is described in [2]. In the second, the coupling amplitudes obtained in the first stage are used for the calculation of the electromagnetic operators' matrix elements, performed with the present program.

RESTRICTION ON THE COMPLEXITY OF THE PROBLEM

The current version is dimensioned for 40 transitions. For further restrictions see [2].

TYPICAL RUNNING TIME

The running time depends on the number of interacting bands and the number of free parameters above all. Therefore the required time may vary from one to tens of minutes on the CDC-6500 computer.

LONG WRITE-UP

1. Description of the Program

The program calculates the reduced electromagnetic probabilities B(E2), B(M1) and B(E1) for transitions between the

levels in odd-odd deformed nuclei. The calculation of these transition probabilities can be subdivided into two stages:

(i) the obtaining of the eigenvalues and coupling amplitudes of the total nuclear Hamiltonians;

(ii) the calculation of the matrix elements of the electromagnetic operators.

The first part of the problem has been solved in /2/, where the program for calculation of the eigenvalues and eigenvectors of the total odd-odd nuclei Hamiltonian (including Coriolis coupling term) is given. The obtained by /2/ mixing amplitudes are used in the present program for the calculation of the electromagnetic multipole (E1, E2, M1) operators matrix elements.

The calculation procedure is based on the "two particles + + rotor" model with inclusion of the Coriolis coupling /1,4/. According to this model the total Hamiltonian for a deformed odd-odd nucleus can be written as /4/.

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

where H_{int} is the intrinsic part of the Hamiltonian and H_{rot} is the rotational part of the Hamiltonian with the Coriolis member included. The eigenvalues and eigenvectors of (1) are obtained by diagonalisation of the corresponding matrix in the basis of the functions (assuming the axial symmetry)

$$\Psi^{(a)}_{IMK} = \left(\frac{2I+1}{16\pi^2(1+\delta_{K0})}\right)^{1/2} \{ D^I_{MK} \Phi^{(a)}_K + (-1)^{I+K} R_i \Phi^{(a)}_K \} , \tag{2}$$

where D^I_{MK} are the Wigner functions (I is the total angular momentum with projections M and K onto z-axis of lab. system and symmetry axis, respectively), $\Phi^{(a)}_K$ are the intrinsic wave functions - the solution of the Schrödinger equation:

$$H_{int} \Phi^{(a)}_K = E_K \Phi_K . \tag{3}$$

The intrinsic wave function K can be written as a product of the wave functions characterising the intrinsic states of the off neutron and odd proton (see refs. /1,4/):

$$\Phi^{(a)}_K = x^{(\rho_n)}_{\Omega_n} x^{(\rho_p)}_{\Omega_p} , \qquad K = \Omega_n + \Omega_p \tag{4a}$$

$$\Phi^{(a)}_K = x^{(\rho_n)}_{\Omega_n} x^{(\rho_p)}_{\Omega_p} , \qquad K = |\Omega_n - \Omega_p|$$

for $K \neq 0$ and

$$\Phi^{(a)}_K = \frac{1}{\sqrt{2}} \left(x^{(\rho_n)}_{\Omega_n} x^{(\rho_p)}_{-\Omega_p} - \gamma\, x^{(\rho_n)}_{-\Omega_n} x^{(\rho_p)}_{\Omega_p} \right), \quad \Omega_n = \Omega_p \tag{4b}$$

for $K = 0$ $(R_i \Phi^{(a)}_{K=0} = \gamma \Phi^{(a)}_{K=0})$.

In (4) $\kappa^{(\rho_p)}_{\Omega_p}$ and $\kappa^{(\rho_n)}_{\Omega_n}$ are the odd proton and odd neutron wave functions, respectively, $a = (\rho_n, \rho_p)$ denotes the quantum

numbers, which together with projection K determine entirely the intrinsic state of the given odd-odd nucleus.

The diagonalisation of the Hamiltonian (1) matrix gives the eigenvectors in the form of linear combination of the basis functions (2):

$$|IM,\nu> = \sum_{Ka} b^{I\nu}_{aK} |\Psi^{(a)}_{IMK}> , \tag{5}$$

where $b^{I\nu}_{aK}$ are the mixing amplitudes.

The reduced probability for a transition of the type X (X = E or X = M) and of multipolarity L from state $|I\nu>$ to the state $|I'\nu'>$ described by (5) is given by (see, e.g., ref. /4/)

$$B(XL,\ I\nu \to I'\nu') = \frac{1}{2I+1} |<I'\nu'||\mathfrak{M}(X,L)||I\nu>|^2 = \tag{6}$$

$$= \sum_{M'\mu} \Big| \sum_{\substack{Ka \\ K'a'}} b^{I\nu}_{aK} b^{I'\nu'}_{a'K} <I'M'\nu'|\mathfrak{M}(X,L\mu)|IM\nu>| ^2 ,$$

where (X, L) are the electromagnetic multipole operators. Their explicit forms are /1/:

$$\mathfrak{M}(E,L,\mu) = e\, e_{eff}\, Y_{L\mu} \tag{7}$$

$$\mathfrak{M}(M,1\mu) = \left(\frac{3}{4\pi}\right)^{1/2} \frac{eh}{2mc} [(g_s - g_\ell)\hat{s} + (g_\ell - g_R)\hat{j} + g_R \hat{I}]_\mu .$$

where $Y_{L\mu}$ are the spherical functions; $\hat{s}_\mu$, $\hat{j}_\mu$, $\hat{I}_\mu$ are the components of the spin, intrinsic angular and total angular momentum tensor operator, respectively; g_s, g_ℓ and g_R are the spin, orbital momentum and rotational momentum gyromagnetic ratios; $\frac{eh}{2mc}$ is the nuclear magneton. Substituting (7) into (6) and using the properties of Clebsch-Jordan coefficients one can get:

$$B(X1,\ I\nu \to I'\nu') = |B^{X1}_0 + B^{X1}_1|^2 , \tag{8a}$$

where X = E or X = M and (8b)

$$B^{X1}_0 = \sum_{\substack{Ka \\ K'a'}} b^{I\nu}_{aK} b^{I'\nu'}_{a'K} (IK10(I'K) <\Phi^{(a')}_{K'}|\mathfrak{M}(X,10)|\Phi^{(a)}_K> \delta_{KK'}$$

$$B^{X1}_1 = \sum_{\substack{Ka \\ K'a' \\ \pm}} b^{I\nu}_{aK} b^{I'\nu'}_{a'K'} [(IK1 \pm 1\ I'K') <\Phi^{(a')}_{K'}|\mathfrak{M}(X,1\pm1)|\Phi^{(a)}_K> + \tag{8c}$$

$$+ (-1)^{I+K} (I - K1 \pm 1 \cdot I'K') <\Phi^{(a')}_{K'}|\mathfrak{M}(X,1\pm1)|\Phi^{(a)}_{-K}>$$

and

$$B(E2,\ I\nu \to I'\nu') = |B^{E2}_0 + B^{E2}_1 + B^{E2}_2|^2 . \tag{9a}$$

where

$$B_0^{E2} = \sum_{\substack{Ka \\ K'a'}} b_{aK}^{I\nu} b_{a'K'}^{I'\nu'} (IK20 | I'K') \langle \Phi_K^{(a')} | \mathfrak{M}(E20) | \Phi_K^{(a)} \rangle \approx \tag{9b}$$

$$\approx \sqrt{\frac{5}{16\pi}}\, e Q_0 \sum_{Ka} b_{aK}^{I\nu} b_{aK}^{I'\nu'} (IK20 | I'K) \delta_{KK'}$$

$$B_1^{E2} = \sum_{\substack{Ka \\ K'a' \\ \pm}} b_{aK}^{I\nu} b_{a'K'}^{I'\nu'} [(IK2 \pm 1 | I'K') \langle \Phi_{K'}^{(a')} | \mathfrak{M}(E,2\pm1) | \Phi_K^{(a)} \rangle \delta_{K;K\pm1} + \tag{9c}$$

$$+ (-1)^{I+K} (I-K2 \pm 1 | I'K') \langle \Phi_{K'}^{(a')} | \mathfrak{M}(E,2\pm1) | \Phi_{-K}^{(a)} \rangle \delta_{K',-K\pm1}]$$

$$B_2^{E2} = \sum_{\substack{Ka \\ K'a' \\ \pm}} b_{aK}^{I\nu} b_{a'K'}^{I'\nu'} [(IK2 \pm 2 | I'K') \langle \Phi_{K'}^{(a')} | \mathfrak{M}(E,2\pm2) | \Phi_K^{(a)} \rangle \delta_{K',K\pm2} + \tag{9d}$$

$$+ (-1)^{I+K} (I-K2 \pm 2 | I'K') \langle \Phi_{K'}^{(a')} | \mathfrak{M}(E2,\pm2) | \Phi_{-K}^{(a)} \rangle \delta_{K',-K\pm2}.$$

In (9) Q_0 denotes the intrinsic quadrupole moment of odd-odd nucleus. The intrinsic matrix element $\langle \Phi_{K'}^{(a')} | \mathfrak{M}(M,1\mu) | \Phi_K^{(a)} \rangle$ can be written in the form (using (7)):

$$\langle \Phi_{K'}^{(a')} | \mathfrak{M}(M,1\mu) | \Phi_K^{(a)} \rangle = \left(\frac{3}{4\pi}\right)^{1/2} \frac{eh}{2mc} [(g_s - g_\ell) \langle \Phi_{K'}^{(a')} | \hat{s}_\mu | \Phi_K^{(a)} \rangle + \tag{10}$$

$$+ (g_s - g_R) \langle \Phi_{K'}^{(a')} | \hat{j}_\mu | \Phi_K^{(a)} \rangle + g_K K \delta_{K,K'} \delta_{a,a'} \delta_{\mu,0}].$$

$$(\mu = 0, \pm 1).$$

It is possible to express the matrix elements $\langle \Phi_{K'}^{(a')} | \hat{A} | \Phi_K^{(a)} \rangle$ in (8), (9) and (10) by means of intrinsic wave functions for odd proton and neutron:

$$\langle \Phi_{K_1}(a_1) | \hat{A} | \Phi_{K_2}(a_2) \rangle = \delta_{\Omega_{p_1} \Omega_{p_2}} \delta_{\rho_{p_1} \rho_{p_2}} \langle x(\rho_{n_1}) | \hat{A} | x_{\Omega_{n_2}}(\rho_{n_2}) \rangle + \tag{11}$$

$$+ \delta_{\Omega_{n_1} \Omega_{n_2}} \delta_{\rho_{n_1} \rho_{n_2}} \langle x_{\Omega_{p_1}}(\rho_{p_1}) | \hat{A} | x_{\Omega_{p_2}}(\rho_{p_2}) \rangle,$$

where A can be represented by operators: $\mathfrak{M}(E,1\mu), s_\mu, j_\mu$ $(\mu = 0,1)$ or $\mathfrak{M}(E,2\mu)$ $(\mu = 0,1,2)$. A similar expression can be obtained if K_1 or K_2 or both are equal to zero.

The intrinsic matrix elements $\langle x_{\Omega_1}(\rho_1) | \hat{A} | x_{\Omega_2}(\rho_2) \rangle$ can be calculated in the frame of various nuclear models. To be correct one has to take for calculation of $\langle x_{\Omega_1}(\rho_1) | \hat{A} | x_{\Omega_2}(\rho_2) \rangle$ the same nuclear model as for determination of the intrinsic wave function $\Phi_K^{(a)}$ (that means the model used in /2/). The intrinsic matrix elements $\langle x_{\Omega_1}(\rho_1) | \hat{A} | x_{\Omega_2}(\rho_2) \rangle$ are a part of the input data in the program. The input data are further formed by the gyromagnetic ratios g_s, g_ℓ, g_R and by the effective charge e_{eff} (see (7) and (10)).

Table 1
Data cards read by the CORIOP program

Number of card group	Column	Format	Variable name	Comments
1	1 - 2	6I2	NBAND	the number of interacting bands.
	3 / 4		IMAX	the maximum spin for which the energy matrix is still diagonalised
	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
	11-12		ISW2	if not zero, the calculation with the E1, E2 and M1 transition probabilities will be performed
2				see [2]
3				
4				
5				
6		MINIMIZE CALL FCN	3	the MINUIT program control commands (see [2])
7	1 - 2	4I2	LEFROM(I,1)	the band head serial number of the state which the I th transition leaves from
	3 - 4		LEFROM(I,2)	its spin value
	5 - 6		LETO(I,1)	the band head serial number of the state where the I th transition comes

Table 1 (continued)

Number of card group	Column	Format	Variable name	Comments
	7 - 8		LETO(I,2)	its spin value
				a blank card signals the end of this card group
8	1 -10	8F10.2	QOMMNT	quadrupole moment
	11-20		GSP	g_s gyromagnetic ratios for proton
	21-30		GSN	g_s gyromagnetic ratios for neutron
	31-40		GLP	g_l gyromagnetic ratios for proton
	41-50		GLN	g_l gyromagnetic ratios for neutron
	51-60		GR	g_R gyromagnetic ratio
	61-70		EFFCHP	effective charges for proton
	71-80		EFFCHN	effective charges for neutron
				this card group contains one card
9	1 -10	F10.4, 2I2	E11P(I,J)	the rY_{11} operator matrix element between the I and J states
	11-12		I	the serial numbers of states in accordance with the order
	13-14		J	adopted in the quantum numbers of the band heads (for proton states)
				a blank card signals the end of this card group
10	1 -10	F10.4, 2I2	E11N(I,J)	the rY_{11} operator matrix element between the I and J states
			I	the serial numbers of states in accordance with the order
			J	adopted in the quantum numbers of the band heads (for neutron states)
				a blank card again signals the end of this card group
11	1-10	F10.4, 2I2	E10P(I,J)	the cards of the 9 and 10 groups must be repeated with the matrix elements of the left over electromagnetic operators :
			I	
			J	
.	.	.	.	rY_{10} for protons
.	.	.	.	rY_{10} for neutrons
.	.	.	.	r^2Y_{22} for protons
..	.	.	.	r^2Y_{22} for neutrons
				r^2Y_{21} for protons
				r^2Y_{21} for neutrons
				r^2Y_{20} for protons
				r^2Y_{20} for neutrons
				s_+ for protons
				s_+ for neutrons
				s_z for protons
				s_z for neutrons

For given transition $(I\nu \longrightarrow I'\nu')$ the program calculates the reduced probabilities $B(E2, I\nu \longrightarrow I'\nu')$, $B(E1. I\nu \longrightarrow I'\nu')$ and $B(M1, I\nu \longrightarrow I'\nu')$ which are allowed by selection rules.

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

2. INPUT DATA CARDS

The program is written as an FON subroutine for the MINUIT minimization program. The program and the input data cards required are described in ref. [2]. The remaining input cards are read by the present program (see the table). For a more detailed description of the 2,3,4 and 5 card groups see ref. [2].

THE PROGRAM OPTIONS

In addition to the calculation mode described in [2] ISW2=0 means that only the perturbed energy levels and the final set of parameters and the mixed amplitudes will be obtained, while ISW2≠0 means, the complete calculation with the **E1**, **E2** and **M1** reduced transition probabilities will be performed.

3. OUTPUT PRINTS

The input data are reproduced for the value of the FCN parameter IFLAG=3, and final tables are printed as well. Self-explanatory descriptions of the tables are also printed.

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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Программа для вычисления **E1**, **E2** и **M1** приведенных вероятностей с учетом взаимодействия Кориолиса

В работе дана программа для вычисления **E1**, **E2** и **M1** приведенных вероятностей переходов в деформированных нечетно-нечетных ядрах. Программа написана как **FCN** подпрограмма для минимизирующей программы **MINUIT**. Программа основана на модели "две квазичастицы + ротор" с учетом взаимодействия Кориолиса. Чтобы учесть взаимодействие Кориолиса, конструируется и диагонализируется матрица полного гамильтониана. Метод Якоби для диагонализации используется для нахождения собственных значений и функций для всех требуемых значений спина. Одновременно оптимизируются все свободные параметры методом наименьших квадратов к экспериментальным значениям энергий ротационных уровней. При помощи таким способом найденных амплитуд смещения вычисляются **E1**, **E2** и **M1** приведенные вероятности для заданных гамма переходов.

Работа выполнена в Лаборатории теоретической физике и в Лаборатории ядерных проблем ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1982

Hons Z., Kvasil J. E4-82-726

A Program for Calculation of the **E1**, **E2** and **M1** Transition Probabilities in Odd-Odd Nuclei Taking the Coriolis Mixing into Account

A computer program for calculation of the **E1**, **E2** and **M1** reduced transition probabilities in deformed odd-odd nuclei is given. The program is written as an FCN subroutine for the MINUIT minimizing program. The program is based on the "two quasi-particles + rotor" model with inclusion of the Coriolis coupling. 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 eigenvalues and eigenvectors for all spin values required. Simultaneously the adjustment of all the parameters is carried out untill a least-square fit to the experimental energy levels is obtained. With thus obtained coupling amplitudes the required **E1**, **E2** and **M1** gamma transition probabilities are calculated.

The investigation has been performed at the Laboratory of Theoretical Physics and Laboratory of Nuclear Problems, JINR.

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