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ОБЪЕДИНЕННЫЙ  
ИНСТИТУТ  
ЯДЕРНЫХ  
ИССЛЕДОВАНИЙ

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E4 - 3453



F.A.Gareev, L.I.Vinokurov, B.N.Kalinkin

ONE-PARTICLE STATES  
OF DEFORMED NONAXIAL NUCLEI

ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

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5342/1 p2.

## 1. Introduction

Problems related to the improvement of the one-particle level schemes have recently drawn attention of physicists engaged in studying the nuclear structure. These schemes underlie all theoretical approaches claiming to the explanation of main regularities in nuclei from the microscopic point of view.

The one-particle level schemes are to be improved for the following reasons.

It is well known that the peripheral collisions are very important in direct reactions. Therefore, it is necessary for the model wave functions of nucleus states involved in the transition to have right behaviour on the boundary and the periphery of the nucleus.

In analysing the nuclear structure it is very important to take into account the right behaviour of the wave functions. There are data which indicate that the correlative forces acting between nucleons are especially effective in the surface layer of the nucleus<sup>1,2</sup>.

This region gives the largest contribution in the electromagnetic transitions of high multipolarity  $\lambda > 2$ , as well as in forbidden beta transitions since in these cases the radial part of the transition operator is a sharply increasing function of the coordinate.

All the investigations of deformed nuclei were actually based on the model one-particle states obtained in the paper by Nilsson<sup>3</sup> which played a great role in nuclear spectroscopy.

However the wave functions of these states are not accurate in the abovementioned sense because they are the solution of the Schrodinger equation with oscillator potential, which strongly differs from the realistic potential on the boundary and the periphery of the nucleus.

In addition, the relative position of the levels in the Nilsson scheme with a noticeable changing of the mass number  $A$  remains unaffected (it is only the energy scale that changes). In the realistic potential the relative position and even the level sequence may essentially alter.

To get more correct wave functions and the one-particle energies of deformed nuclei it is necessary to start from the anisotropic Saxon-Woods potential which reflects, to a larger degree, the real situation.

A number of paper <sup>4,5,6,7,8</sup> is devoted to the solution of this problem for axially-symmetrical deformed nuclei.

In the present paper we generalize the method suggested in refs. <sup>5,6</sup> to the case of nonaxial deformed nuclei and consider the main regularities in the behaviour of one-particle levels. This problem is very important in the study of the nucleus equilibrium shape. The calculations performed are based on the Newton approximation <sup>9</sup>, being a generalization of the Nilsson scheme <sup>3</sup> and therefore in this case too are not correct enough.

## 2. Solution of the Schrodinger equation

Following the paper of Gareev, Ivanova and Kalinkin<sup>5</sup> we assume that the mean radius  $R$  of a deformed nucleus is determined by the formula:

$$R = R_0 \left[ 1 + a_0 \frac{Y^0}{2} + a_2 \left( \frac{Y^2}{2} + \frac{Y^{-2}}{2} \right) \right] = \quad (1)$$

$$= R_0 \left[ 1 + (2\pi)^{-1/2} a_0 P_2 + 2(2\pi)^{-1/2} a_2 P_2^{(2)} \cos 2\phi \right];$$

$$a_0 = \beta \cos \gamma; \quad a_2 = 2^{-1/2} \beta \sin \gamma \quad (2)$$

$R_0$  being the radius of an equally large sphere <sup>10</sup>.

The Schrodinger equation is written in the form:

$$\left[ -\frac{\hbar^2}{2M} \Delta + V(\beta, \gamma, \vec{r}) - E \right] \Psi = 0. \quad (3)$$

We make the identity transformation. Adding and subtracting the spherically symmetrical part of the potential  $V(0, 0, r)$  we have:

$$\left[ -\frac{\hbar^2}{2M} \Delta + V(0, 0, r) + \tilde{V}(\beta, \gamma, \vec{r}) - E \right] \Psi = 0 \quad (4)$$

where

$$\tilde{V}(\beta, \gamma, \vec{r}) = V(\beta, \gamma, \vec{r}) - V(0, 0, r).$$

Following paper <sup>5</sup> we expand  $\tilde{V}(\beta, \gamma, \vec{r})$  in a series in spherical functions:

$$\tilde{V}(\beta, \gamma, \vec{r}) = \sum_{\lambda, \mu} C_{\lambda}^{\mu}(\beta, \gamma, r) Y_{\lambda}^{\mu}(\theta, \phi). \quad (5)$$

Here

$$V(\beta, \gamma, \vec{r}) = -V_0 \left\{ 1 + \exp \left[ \frac{r - R(\beta, \gamma, \theta, \phi)}{a} \right] \right\}^{-1} + V_{s.o.}(\beta, \gamma, r, \theta, \phi) \quad (6)$$

The term  $V_{s.o.}$  in eq. (6) correspond to the spin-orbital interaction. It was shown earlier <sup>11</sup> that the account of the change in the interaction

$V_{s.o.}$  with nucleus deforming leads to rather small corrections. Therefore we put that  $\tilde{V}_{s.o.}(\beta, \gamma, \vec{r}) = 0$ . Thus

$$\tilde{V}(\beta, \gamma, r, \theta, \phi) = -V_0 \left\{ \left[ 1 + \exp \left( \frac{r - R(\beta, \gamma, \theta, \phi)}{a} \right) \right]^{-1} - \left[ 1 + \exp \left( \frac{r - R_0}{a} \right) \right]^{-1} \right\} \quad (7)$$

From eqs. (1) and (7) it follows that the expression  $\tilde{V}(\beta, \gamma, r, \theta, \phi)$  is invariant with respect to the transformations:

$$\phi \rightarrow -\phi; \quad \phi \rightarrow \pi + \phi; \quad \theta \rightarrow \pi - \theta \quad (8)$$

Therefore the expansion coefficients (5) possess the following property

$$C_{\lambda}^{\mu} = C_{\lambda}^{-\mu} \quad \text{and} \quad \lambda, \mu \quad \text{are even.} \quad (9)$$

As before <sup>5</sup>, we find the solution for eq. (4) in the form of a superposition:

$$\Psi = \sum_{n\ell j m} a_{n\ell j}^m \psi_{n\ell j}^m \quad (10)$$

where  $\psi_{n\ell j}^m$  are the eigenfunctions of the states obtained from the Schrodinger equation with spherically symmetrical potential:

$$\left[ -\frac{\hbar^2}{2M} \Delta + V(0,0,r) - \epsilon_{n\ell j} \right] \psi_{n\ell j}^m = 0 \quad (11)$$

in this case  $\psi_{n\ell j}^m = R_{n\ell j}(r) y_{\ell j}^m$ ,  $y_{\ell j}^m$  is the spherical spinor. As is shown in ref. 12 the radial part of the wave function (12) can be well represented in the form

$$R_{n\ell j}(r) = N r^{-1} H_n [S(r)] \exp \left[ -S^2(r)/2 \right] \quad (13)$$

(for the definition of the function  $S(r)$  see ref. 12).

Inserting the expansion (10) into eq. (4), multiplying the l.h.s. by  $(\psi_{n'\ell'j'}^{m'})^*$  and integrating we get

$$(\epsilon_{n'\ell'j'} - E) a_{n'\ell'j'}^{m'} + \sum_{n\ell j m} a_{n\ell j}^m \langle \psi_{n'\ell'j'}^{m'} | \sum_{\lambda} C_{\lambda}^{\mu} Y_{\lambda}^{\mu} | \psi_{n\ell j}^m \rangle = 0 \quad (14)$$

in this case:

$$\begin{aligned} & \langle \psi_{n'\ell'j'}^{m'} | \sum_{\lambda\mu} C_{\lambda}^{\mu} Y_{\lambda}^{\mu} | \psi_{n\ell j}^m \rangle = \\ & = \sum_{\lambda\mu} \langle R_{n'\ell'j'} | C_{\lambda}^{\mu} | R_{n\ell j} \rangle \langle y_{\ell'j'}^{m'} | Y_{\lambda}^{\mu} | y_{\ell j}^m \rangle = \\ & = (4\pi)^{-1/2} \sum_{\lambda\mu} \langle R_{n'\ell'j'} | C_{\lambda} | R_{n\ell j} \rangle (-1)^{\ell'+\ell'-m-m'} x \end{aligned} \quad (15)$$

$$\times [(2\lambda + 1)(2\ell + 1)(2j' + 1)]^{1/2} (\ell\lambda 00 | \ell'0)(\lambda j' \mu - m' | j - m) W(\ell\lambda' 1/2 j'; \ell' j)$$

By solving the system of equations (14) we may determine the energy  $E$  and the coefficients  $a_{n\ell j}^m$  of (10), i.e. the wave functions of the states.

Since the expansion (5) for  $\bar{V}(\beta, \gamma, \vec{r})$  includes the terms only with even  $\lambda$  then the contribution to (10) will be given by the functi-

ons  $\psi_{nl}^m$  which have the definite parity, i.e. the summation in (10) is made only either over the even or over the odd values of "l".

### 3. Expansion of the potential $V(\beta, \gamma, r, \theta, \phi)$ in a series in spherical functions

To solve the system of equations (14) it is necessary to calculate the functions  $C_{\lambda}^{\mu}(\beta, \gamma, r)$  :

$$C_{\lambda}^{\mu}(\beta, \gamma, r) = \int_0^{2\pi} \int_0^{\pi} V(\beta, \gamma, r, \theta, \phi) Y_{\lambda}^{\mu}(\theta, \phi) \sin \theta d\theta d\phi. \quad (16)$$

These functions were obtained by numerical integration. Fig.(1) ( $\beta$  is 0.16 and  $\gamma$  is 0.32) gives the curves corresponding to the functions  $[\frac{2\lambda+1}{4\pi} \frac{(\lambda-\mu)!}{(\lambda+\mu)!}]^{1/2} = C(\beta, \gamma, r)$  depending on  $r$  for different values of the parameter  $\gamma$ .

It is seen from Fig.1 that with increasing parameter  $\gamma$  the components of the expansion (5) with different  $\lambda$  but for  $\mu = 0$  have the shape of the corresponding curves for  $\gamma = 0$ . However, their values decrease. On the contrary, with increasing  $\gamma$  the components with  $\mu \neq 0$  become more important. Among the components with nonzero  $\mu$  the most important is  $C_2^2(\beta, \gamma, r)$ . This is due to the fact firstly that the function  $C_2^2$  has no zeros. Therefore the radial part of the matrix elements entering equations (14) for this component is the largest one. Secondly, the function  $C_2^2$  exceeds all other functions and rapidly increases with increasing  $\gamma$  :

$$C_2^2(0, 32; \pi/12; R_0) / C_2^0(0, 32; \pi/12; R_0) = 0,04.$$

$$C_2^2(0, 32; \pi/3; R_0) / C_2^0(0, 32; \pi/3; R_0) = 0,25.$$

A similar picture occurs at  $\beta = 0.16$  with the only difference that the absolute value of the functions  $C_{\lambda}^{\mu}$  is twice as small.

#### 4. Neutron levels

It may be expected that the violation of the axial nuclear symmetry occurs in the transition regions between the spherical and strongly deformed nuclei<sup>13</sup>. One of such regions is formed by nuclei near Nd<sup>143</sup>. Therefore the calculation were made for the nuclei of this group.

The one-particle wave functions and the energies of the spherical N<sup>143</sup> state should naturally be chosen as the basic ones<sup>12</sup>.

Using the expansion (5) we solve the system in a numerical way.

In the expansion (10) it is necessary to restrict oneself only to those  $\psi_{n\ell}^m$  states of the spherically symmetrical nucleus the account of which is very essential. Such are the bound and the lowest states of the continuous spectrum. The problem of the account the continuous spectrum states is rather complicated. However, approximately this problem can be solved in just the same way as in ref.<sup>5</sup>, especially as the used approximation is satisfactory enough<sup>6</sup>.

This approximation is based on the fact the most contribution should be given by those states of the continuous spectrum which correspond to the quasistationary levels. The wave functions of these levels are maximum inside the nucleus, the effective barrier penetrability being small. Such states possess low energies and large angular momenta. Taking into consideration the character of the problem they can be well described by the stationary wave functions. The difference of these functions from the real ones outside the barrier is of no importance since the matrix elements of (14) contain the quantity  $\sqrt{V}$ , which rapidly tends to zero for large  $r$ . It is necessary to take into account several lowest quasistationary states because they noticeably affect the behaviour the highest bound states of the deformed nucleus. The wave functions and the energies of the quasistationary states are calculated by the method presented in ref.<sup>12</sup>.

We have used the following values of the Saxon-Woods potential parameters:

$$V_0 = 48,8 \text{ MeV}; \quad r_0 = 1,24 \text{ f}; \quad a = 0,65 \text{ f}$$



$\kappa = 0,28$  is the constant of the spin-orbital interaction.

Fig.2 gives the space diagram-fragment showing the behaviour of the neutron states of the even shell at beta and gamma nucleus deformations.

Fig.3 and 4 give the systems of upper neutron levels for different  $\gamma$  at  $\beta = 0,16$  and  $\beta = 0,32$  respectively.

For the sake of convenience, the even and odd states are presented separately.

The basic wave functions and the energies are given in Tables I and II (the parameters defining these functions have the same meaning as in ref.<sup>12</sup>). The asteriks denote the quasistationary states of the continuous spectrum which are taken into account. The rank of the energy matrix for even states is -49, and that for odd states is 42,.

In the calculations we have restricted ourselves to the account of the components with  $\lambda < 4$  in (5) since the contribution of the components with  $\lambda \geq 6$  is very small (see ref.<sup>5</sup>).

As is seen from the above considerations we have taken into account a large number of basis states of equal parity. The necessity of such an approach follows from the comparison of the data obtained by the described approach with these obtained with the aid of the "independent shell" model which was used by Nilsson<sup>3</sup> and Newton<sup>9</sup>. A fragment of the neutron level system ( $\beta = 0,32$ ) is given in Fig.5 as an example of such an approach. The continuous lines show the behaviour of the levels in our approximation the dotted line is the same levels calculated by the "independent shell" model (only states belonging to a given shell interact, the rank of the energy matrix being sharply decreased). We see that both cases essentially differ from one another. When the interaction is switched on between the shells there appear noticeable displacements of levels, the behaviour of the curve often changes. Fig.5 shows that the interaction between the shells should be taken into account.

## 5. Proton level system

In order to calculate the proton one-particle levels we have to expand the Coulomb potential of a deformed nucleus in a series in spherical functions. The Coulomb potential is determined by the formula

$$V_{\text{coul}} = \frac{3(Z-1)e^2}{4\pi R_0^3} \int \frac{n(\beta, \gamma, r', \theta', \phi') d\vec{r}'}{|\vec{r} - \vec{r}'|} \quad (17)$$

Putting

$$n(\beta, \gamma, r', \theta', \phi') = n_0(r') + \bar{n}(\beta, \gamma, r', \theta', \phi') \quad (18)$$

where  $n_0(r')$  is the radial density of the charge of a spherical nucleus of the same volume and assuming that it is described by the Fermi-type function, in just the same way as in section 3 we get:

$$\bar{n}(\beta, \gamma, r', \theta', \phi') = \sum_{\lambda, \mu} C_{\lambda}^{\mu}(\beta, \gamma, r') Y_{\lambda}^{\mu}(\theta', \phi'). \quad (19)$$

Using then the formulas

$$\frac{1}{|\vec{r} - \vec{r}'|} = \begin{cases} \frac{1}{r} \sum_k \left(\frac{r'}{r}\right)^k P_k(\cos H), & r' < r \\ \frac{1}{r'} \sum_k \left(\frac{r}{r'}\right)^k P_k(\cos H), & r' > r \end{cases} \quad (20)$$

and

$$P_k(\cos H) = \frac{4\pi}{2k+1} \sum Y_k^{\nu*}(\theta', \phi') Y_k^{\nu}(\theta, \phi) \quad (21)$$

for  $\bar{V}_{\text{coul}}(\beta, \gamma, r, \theta, \phi)$  we get:

$$(22)$$

$$\bar{V}_{\text{coul}}(\beta, \gamma, r, \theta, \phi) = \sum_{\lambda, \mu} D_{\lambda}^{\mu}(\beta, \gamma, r) Y_{\lambda}^{\mu}(\theta, \phi)$$

where

$$D_{\lambda}^{\mu}(\beta, \gamma, r) = \frac{3(Z-1)e^2}{4\pi R_0^3} \frac{4\pi}{2\lambda+1} \left[ \int_0^r C_{\lambda}^{\mu}(\beta, \gamma, r) \frac{r'^2}{r} \left(\frac{r'}{r}\right)^{\lambda} dr' + \int_r^{\infty} C_{\lambda}^{\mu}(\beta, \gamma, r') r' \left(\frac{r}{r'}\right)^{\lambda} dr' \right] \quad (23)$$

Thus, in calculating the proton level system the radial matrix elements include the sum

$$C_{\lambda}^{\mu}(\beta, \gamma, \tau) + D_{\lambda}^{\mu}(\beta, \gamma, \tau). \quad (24)$$

The proton level system for nuclei close to  $Nd^{143}$  is given in Fig.6 and 7.

In Fig.8 the part of the level scheme calculated with the account of (24) (continuous lines) and for  $D_{\lambda}^{\mu}(\beta, \gamma, \tau) = 0$  (dotted line) is given to show the effect of the term  $V_{\text{cool}}^{\mu}(\beta, \gamma, \tau, \theta, \phi)$  on the position of the levels. Different levels react to a different extent to the Coulomb field distortion. This should have been expected since the radial matrix elements essentially depend on the behaviour of the radial wave functions which, in the case of different states, have different form and value in the region where  $D_{\lambda}^{\mu}(\beta, \gamma, \tau)$  noticeably differ from zero.

## 6. Conclusion

This paper is of a methodical character. The main aim of it is the construction of the method for calculating the one-particle states of deformed nuclei using the realistic diffuse potential.

It is established that in calculating the levels it is necessary to take into account the effect of at least neighbouring shells of the same parity.

The method allows one to take into account in a consistent way the deformation of the Coulomb potential. The results can be used for a more correct solution of the problem of the existence of nonaxial deformed nuclei in the transition regions.

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Table 1

Basic neutron functions

	State	$E_{nlj}$	a	$b_1$	c	b	N
1	1K 17/2 *	15.26	6.092	4.715	4.707	4.308	0.564
2	1j 15/2 *	6.42	5.857	4.494	4.602	4.644	0.589
3	1i 11/2 *	4.79	5.352	4.019	4.117	4.177	0.578
4	2g 9/2 *	1.87	5.226	3.131	3.713	3.755	0.392
5	1i 13/2	-2.29	5.623	4.193	4.386	4.264	0.576
6	3p 1/2	-3.05	4.091	1.855	2.696	3.039	0.168
7	2f 5/2	-3.13	4.699	2.739	3.327	3.424	0.360
8	3p 3/2	-3.98	4.129	1.853	2.702	3.148	0.169
9	1h 9/2	-5.32	5.112	3.736	3.924	3.987	0.570
10	2f 7/2	-5.85	4.824	2.746	3.376	3.690	0.364
11	1h 11/2	-10.71	5.375	3.834	4.093	4.382	0.573
12	3s	-12.08	3.494	1.323	2.169	3.178	0.176
13	2d 3/2	-12.18	4.298	2.313	2.936	3.621	0.371
14	2d 5/2	-14.05	4.399	2.313	2.955	3.745	0.368
15	1g 7/2	-14.94	4.866	3.383	3.630	4.114	0.570
16	1g 9/2	-18.72	5.100	3.434	3.733	4.375	0.563
17	2p 1/2	-21.31	3.833	1.816	2.444	3.535	0.367
18	2p 3/2	-22.29	3.898	1.815	2.452	3.591	0.363
19	1f 5/2	-23.82	4.589	2.957	3.249	4.088	0.555
20	1f 7/2	-26.23	4.783	2.985	3.311	4.260	0.545
21	2s	-30.34	3.202	1.202	1.826	3.204	0.353
22	1d 3/2	-31.82	4.252	2.456	2.778	3.920	0.527
23	1d 5/2	-33.13	4.395	2.467	2.809	4.024	0.517
24	1p 1/2	-38.77	3.785	1.860	2.191	3.565	0.484
25	1p 3/2	-39.32	3.873	1.861	2.203	3.619	0.476
26	1s	-44.65	3.011	1.081	1.407	2.880	0.415

Table 2

## Basic proton functions

State	$E_{nlj}$	a	$b_1$	c	b	N
1j 15/2*	14.63	5.830	4.588	4.711	4.817	0.608
1i 11/2*	14.19	5.315	4.093	4.195	4.295	0.594
2g 9/2*	11.18	5.221	3.185	3.786	3.857	0.399
3p 1/2*	6.86	4.114	1.867	2.730	3.275	0.174
2f 5/2*	6.61	4.702	2.777	3.382	3.789	0.379
1i 13/2*	5.91	5.614	4.290	4.488	4.856	0.610
3p 3/2*	5.77	4.159	1.867	2.741	3.389	0.175
1h 9/2*	3.86	5.097	3.806	3.977	4.404	0.601
2f 7/2*	3.40	4.845	2.792	3.444	4.043	0.380
3s	-2.37	3.543	1.210	2.032	3.164	0.167
1h 11/2	-2.44	5.384	5.078	5.384	4.222	0.683
2d 3/2	-2.56	4.327	2.608	3.111	3.427	0.376
2d 5/2	-4.73	4.444	2.583	3.137	3.969	0.389
1g 7/2	-5.86	4.870	4.412	4.796	3.902	0.676
1g 9/2	-10.31	5.130	4.323	4.880	4.676	0.685
2p 1/2	-11.71	3.894	2.086	2.868	3.596	0.385
2p 3/2	-12.84	3.970	2.016	2.703	3.637	0.381
1f 5/2	-14.75	4.624	3.629	3.356	4.304	0.593
1f 7/2	-17.61	4.840	3.555	3.384	4.440	0.572
2s	-20.74	3.326	1.354	2.175	3.164	0.373
1d 3/2	-22.64	4.326	2.821	2.863	4.049	0.546
1d 5/2	-24.23	4.491	2.774	2.890	4.150	0.530
1p 1/2	-29.36	3.930	1.980	2.326	3.703	0.491
1p 3/2	-30.04	4.038	1.960	2.349	3.767	0.481
1s	-34.86	3.331	1.050	1.689	3.175	0.419

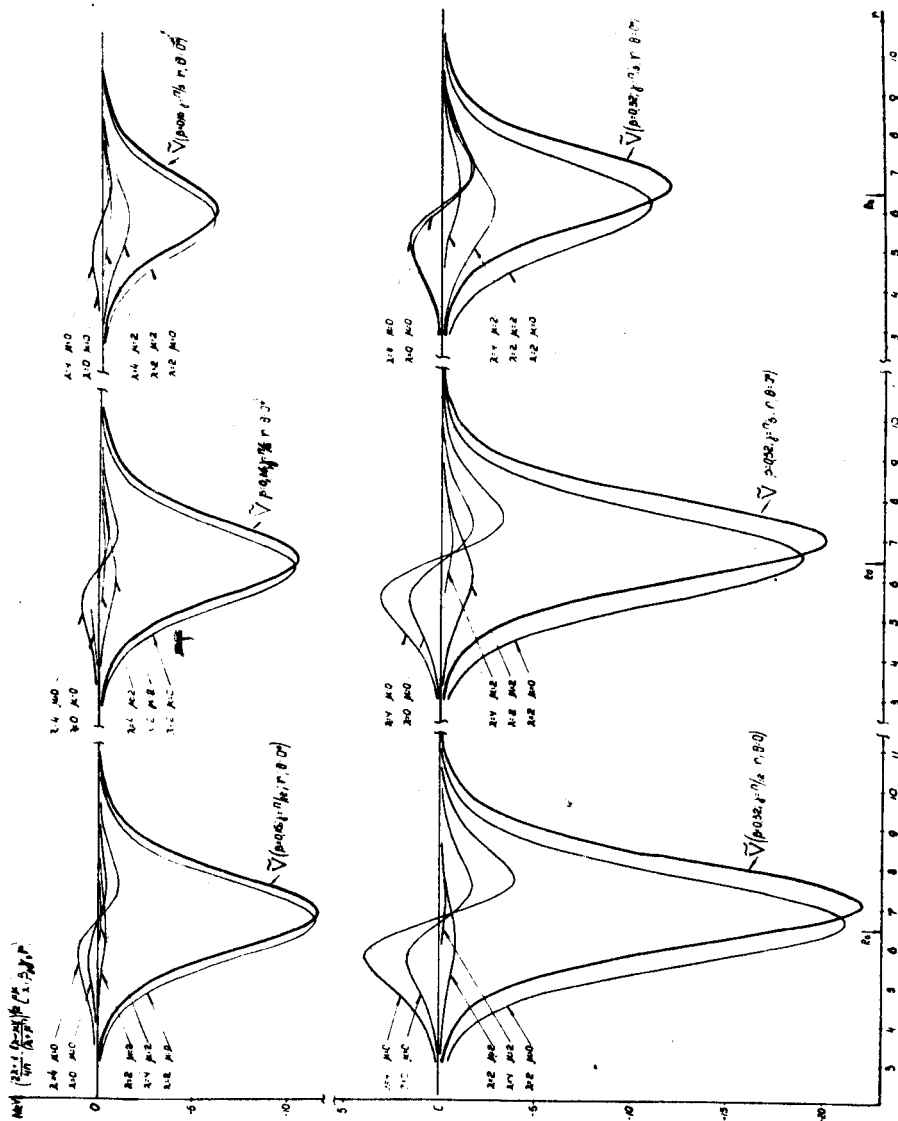


Fig. 1. The functions  $\left[ \frac{2\lambda+1}{4\pi} \frac{(\lambda-\mu)!}{(\lambda+\mu)!} \right]^{1/2} C_\lambda^\mu(\beta, \gamma, r); \lambda = 1/2, 1$ .

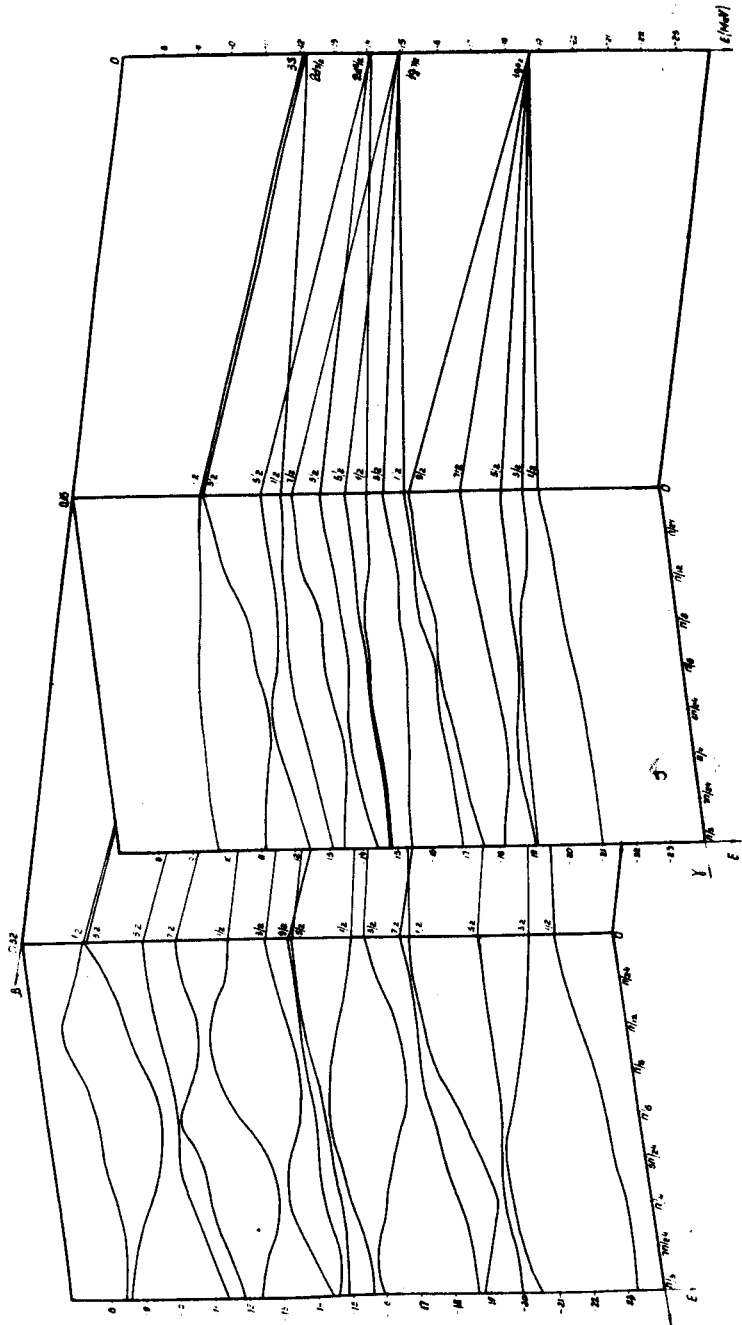


Fig.2. A part of the neutron level system ( shell  $N = 4$  ) at the beta and gamma nuclear deformations.







$$\beta = 0,32 \quad N = 4$$

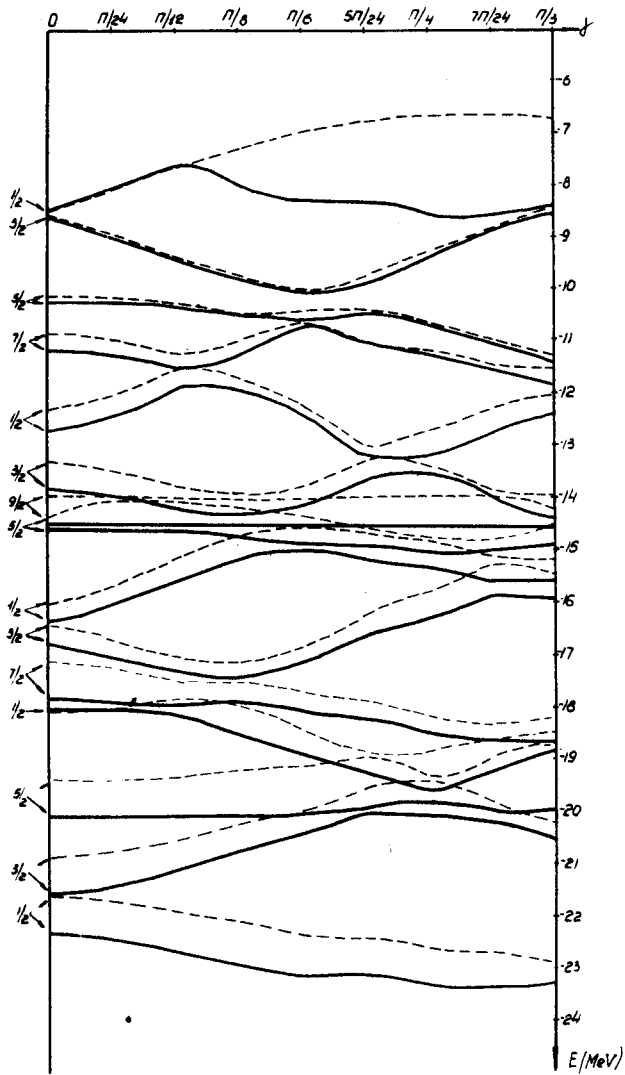


Fig.5. The effect of the interaction of states belonging to different (of the same parity) shells.



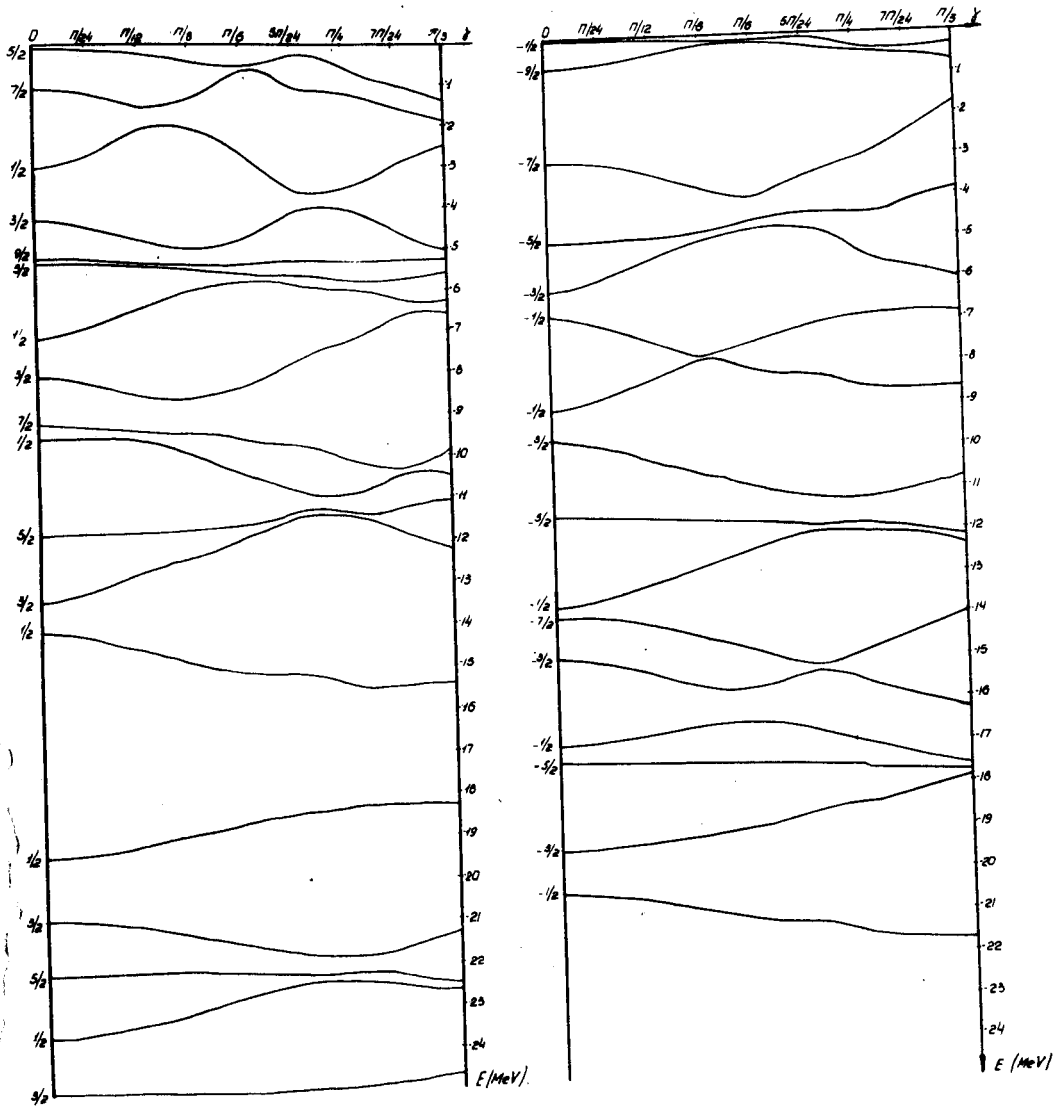


Fig.7. Upper proton levels as a function of  $\gamma$  ( $\beta = 0.32$ ).

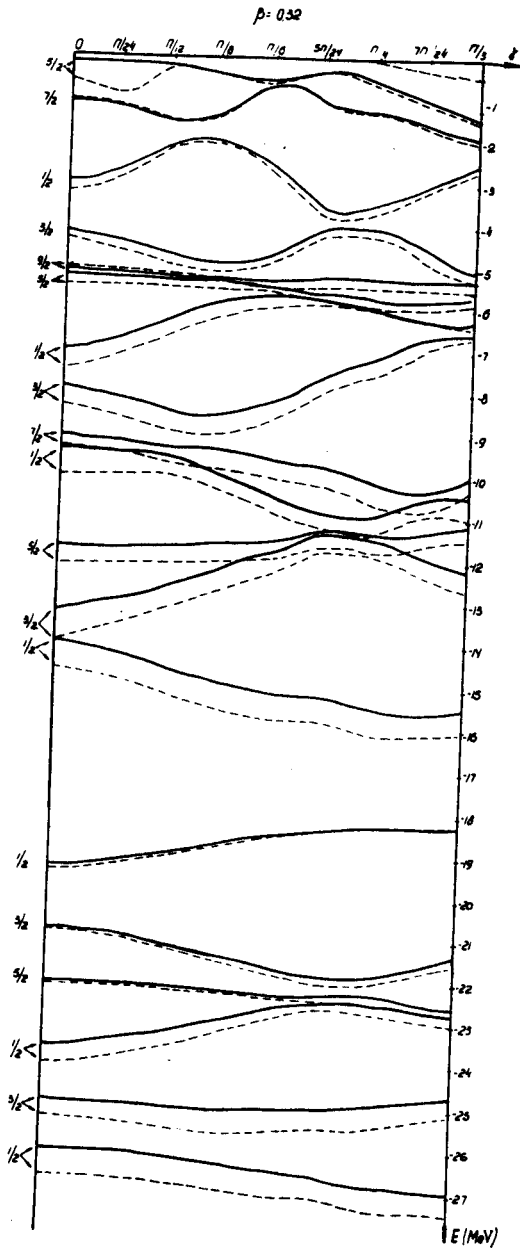


Fig.8. The effect of the Coulomb field distortions due to the nuclear deformations on the position of the one-particle proton levels.