ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

Дубна

E4 - 3629

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ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

ON NUCLEAR OCTUPOLE DEFORMATIONS

1967.

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Submitted to Nuclear Physics

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Introduction

The problem of the dependence of the energy of the nucleus on the deformation parameters of higher mutipole orders ($\lambda > 2$) has attracted much attention[1]. A knowledge of this dependence is important for the interpretation of a very broad class of effects such as the equilibrium deformation , vibrational spectra, fission barriers etc. In this paper we shall investigate the effect of the shell structure on deformations of the quadrupole β_2 and octupole β_3 types.

For nuclei in the $218 \leq A \leq 232$ region octupole $I_\pi = 1^-$ states have very unusual properties. Their energies are very low, momenta of inertia large and hindrance factors for α-decay small[2]. Such behaviour indicates, that for these nuclei the shell structure may strongly change the simple (liquid drop) dependence of the energy on the octupole deformation. Besides, this region of nuclei is also on the boundary between spherical and deformed nuclei. Therefore we have chosen this region for our calculations. Because the projection of the angular momentum on the nuclear symmetry axis in low-lying $I_\pi = 1^-$ states is equal to zero we shall limit ourselves to axially-symmetric nuclei. Preliminary results of our calculations were already published in[3].

The problem of nuclear stability with respect to octupole deformations was investigated in papers[4-7]. The restoring force parameter C_3 was calculated using various approximations (usually perturbation theory). The restoring force consists of two terms, of approximately the same magnitude, but opposite sign. The quantity C_{def} characterizes the repulsion of the filled and unfilled shells which contributes to the deformation, C_{rest} originates from the "inertia of closed shells" or volume conservation which counteracts the deformation. In the mentioned papers the restoring force parameters were small and positive, i.e. the nuclei were "soft" but nondeformed.

The purpose of this paper is to obtain more detailed information about the dependence of the potential energy on the parameters of the quadrupole and octupole deformation.

The method of calculating the $\mathcal{E}(\beta_2, \beta_3)$ function.

To calculate the energy of the nucleus we shall use the method, which has already proved to be successful when considering the equilibrium quadrupole deformation (see e.g.[1] and references mentioned there). According to this method the energy of the nucleus is calculated as the energy of a system of nucleons, interacting via pairing forces and moving in a deformed average field.

Let the equipotential surface have the form

$$r = R_0 k(\beta_2, \beta_3)[1 + \beta_2 Y_{20}(\theta, \phi) + \beta_3 Y_{30}(\theta, \phi) - \frac{9}{2}\sqrt{\frac{3}{35\pi}}\beta_2\beta_3 Y_{10}(\theta, \phi)]. \quad (1)$$

The last term in the square brackets assures the constancy of the centre of mass and the $k(\beta_2, \beta_3)$ function assures the volume conservation. The condition of volume conservation is a consequence of the constancy of the average nuclear density.

The potential, in analogy with Nilsson[8], is of the form

$$V = \frac{1}{2} M \overset{\circ}{\omega}{}_0^2 r^2 [1 + \frac{5}{4\pi}(\beta_2^2 + \beta_3^2)][1 - 2\beta_2 Y_{20}(\theta, \phi) - 2\beta_3 Y_{30}(\theta, \phi) + 18\sqrt{\frac{3}{35\pi}}\beta_2\beta_3 Y_{10}(\theta, \phi)]. \quad (2)$$

In the lowest approximation with respect to β_2 and β_3 the potential (2) has the equipotential surfaces (1) and in the spherical limit is equal to the harmonic oscillator one.

Let us note, that the octupole potential of the $\approx r^3 Y_{30}$ type used in [4,6] does not have surface of the (1) type, moreover, its equipotential surfaces have one branch extending to infinity. Therefore we use the octupole potential $\approx r^2 Y_{30}$ following from (1).

The single-particle hamiltonian has the usual form

$$H(\beta_2, \beta_3) = -\frac{\hbar^2}{2M}\Delta + V(\beta_2, \beta_3) + C\,\vec{\ell}\,\vec{s} + D(\vec{\ell}^{\,2} - \langle \vec{\ell}^{\,2} \rangle_{shell}). \qquad (3)$$

The parameters C,D used in our calculations were taken from [9] $C_N = -0.856$, $C_p = -0.779$, $D_N = -0.139$, $D_p = -0.253$ (In MeV). The total energy, contrary to the individual level order, does not depend critically on these parameters.

The hamiltonian (3) was diagonalized in the spherical oscillator basis, i.e.

$$\Psi_i = \sum_{N\ell\Lambda} a^i_{N\ell\Lambda} |N \ell \Lambda \Sigma\rangle$$

in the Nilsson ϵ- representation [8]. In this representation the only non-zero matrix elements of the quadrupole part of (3) are the diagonal $\Delta N = 0$ ones. However, in the octupole part additional second order terms arise

$$\approx \epsilon_2 \cdot \epsilon_3 \left(\frac{40}{63}\sqrt{\frac{\pi}{11}}\,Y_{50}(\theta,\phi) - \frac{56}{45}\sqrt{\frac{\pi}{7}}\,Y_{30}(\theta,\phi) + \frac{72}{35}\sqrt{\frac{\pi}{3}}\,Y_{10}(\theta,\phi)\right),$$

which were neglected similarly as the change in the vectors $\vec{\ell}$ and $\vec{s}$. The non-zero matrix elements of the octupole part of (3) are the nondiagonal ones with $\Delta N = 1,3,5$ ... . We limit ourselves to elements with $\Delta N = 1$ and 3. The influence of the others is negligible because the energy differences are large and the matrix elements themselves are small. The effect of the octupole part of (3) on the energy of the nucleus is mainly connected with the matrix elements having $\Delta N = 1$ between shells in the vicinity of the Fermi surface. Taking further shells placed symmetrically with respect to the Fermi surface into account, as well as terms with $\Delta N = 3$, increases the effect of the octupole part by about 20%. In our calculations we took 5 oscillator shells for protons and 5 oscillator shells for neutrons and matrix elements with $\Delta N = 1,3$. Note, that filled shells which do not participate in the diagonalization, contribute nevertheless to the stabilization of the spherical form, owing to the volume conservation condition.

The eigenvalues $\mathcal{E}(\beta_2, \beta_3)$ of hamiltonian (3) were used in the equations of the superfluid nuclear model

$$2/G = \sum_s \frac{1}{\sqrt{(\epsilon_s - \lambda)^2 + \Delta^2}} ,$$

$$N = \sum_s \left(1 - \frac{\epsilon - \lambda}{\sqrt{(\epsilon_s - \lambda)^2 + \Delta^2}}\right) \qquad (4)$$

and the quantities Δ, λ for neutrons ($132 \leq N \leq 140$) and protons ($86 \leq Z \leq 92$) were calculated. The following values were used for the pairing interaction constants $G_N = 21/A$, $G_p = 25/A$ (MeV). After solving the system (4) the energy $\mathcal{E}(\beta_2, \beta_3)$ was calculated according to

$$\mathcal{E}_{BCS}(\beta_2, \beta_3) = \sum_s E_s\left(1 - \frac{\epsilon_s - \lambda}{E_s}\right) + \lambda_N N - \Delta_N^2 / G_N +$$

$$+ \sum_t E_t \left(1 - \frac{\epsilon_t - \lambda}{E_t}\right) + \lambda_p Z - \Delta_p^2 / G_p , \qquad (5)$$

where $E = \sqrt{(\epsilon - \lambda)^2 + \Delta^2}$ is the quasiparticle energy. The summation over s contains all the neutron states, over t all the proton ones. For noninteracting particles, which however for each deformation fill the lowest $1/2N$

and 1/2Z levels one obtains

$$\mathcal{E}_{IP}(\beta_2, \beta_8) = \sum_{s=1}^{\frac{1}{2}N} 2\epsilon_s(\beta_2, \beta_8) + \sum_{t=1}^{\frac{1}{2}Z} 2\epsilon_t(\beta_2, \beta_8) . \qquad (6)$$

Let us note that the formulae (5) or (6) contains implicitly various approximations. E.g. the Coulomb energy of the protons was neglected, the states were not projected onto the subspace with definite angular momentum and parity etc. However, for not too large deformations, neither of the mentioned approximations can change the results considerebly.

Discussion

The single particle energies $\mathcal{E}(\beta_2, \beta_8)$, the quantities $\Delta(\beta_2, \beta_8)$ and $\lambda(\beta_2, \beta_8)$ as well as the functions $\mathcal{E}_{BCS}(\beta_2, \beta_8)$ and $\mathcal{E}_{IP}(\beta_2, \beta_8)$ were calculated for nuclei with $218 \leq A \leq 232$, with the step 0.06 in β_2 and β_8. Between these points the parabolical interpolation was used, the control calculation show that errors connected with the interpolation are not substantial. The results are represented in the form of figures and tables and are discussed below.

a) The quadrupole deformation.

Fig.1 gives the dependence of $\mathcal{E}_{BCS}$ on β_2 (for $\beta_8 = 0$) for some selected nuclei. The curves are normalized so that the minimum energy is always equal to zero (this it true for all figures). Besides the expected shift of the minimum with increasing A towards the larger deformations, one can note a change in curvature from nucleus to nucleus. The curvature has a minimum value for nuclei with neutron number N= 136 i.e. these nuclei are "softest" with respect to quadrupole deformations. The equilibtium deformations obtained from our calculations are somewhat smaller than the experimental ones (see also Tab.1).

b) Pairing correlations

On Fig.2 the dependence of the square of the correlation function (energy gap) on the β_2 deformation is shown for systems with various numbers of neutrons. The analogical picture for protons is shown on Fig.3. The increase of Δ^2 with the increase of N or Z for zero deformation is related to the increase of the level density, with the removal from a magic nucleus. The characteristic features of both figures is the existence of a rather narrow region of β_2 values in which the energy gap does not depend on N or Z. In this region of deformations the singte particle spectrum is close to an equidistant one. The periodical change of Δ^2 with β_2 is a consequence of the periodical change of the level density. Since the correlation energy is equal to $-\Delta^2/G$ one can see from the behaviour of Δ^2 that pairing interactions promote the stabilization of the spherical form in spherical nuclei and lead to a decrease of the curvature of the potential energy for the deformed nuclei.

The quantity Δ^2 decreases monotonously as the octupole deformation β_3 increases. This qualitative feature is independent on Z or N and β_2. A typical example of the function $\Delta^2(\beta_3)$ is shown by the dashed lines on Fig.2 (N= 136) and Fig.3 (Z=90). These curves were calculated for $\beta_2=0.2$. One can conclude from the behavior of the $\Delta^2(\beta_3)$ function that pairing correlations counteract the octupole deformation and increase the restoring force with respect to the octupole vibrations.

c) General features of the dependence of the energy on β_3.

The dependence of the energy of the nucleus on the octupole deformation has some general features which do not depend on the atomic number. To demonstrate them we choose the characteristic example of the ^{244}Ra nucleus shown on Fig.4. The curves $\mathcal{E}(\beta_3)$ calculated using formulae (5) and (6) for different values of β_2 are shown. The $\mathcal{E}(\beta_3)$curve is always a flat minimum for $\beta_3=0$ and has no other minima. The curvature of $\mathcal{E}(\beta_3)$ decreases as β_2 increases i.e. the restoring force decreases for larger quadrupole deformations. The inclusion of the pairing interaction increases the restoring force in comparison with $\mathcal{E}_{IP}$ (Note, that the energy surface $\mathcal{E}_{IP}(\beta_2, \beta_3)$ calculated according to (6), corresponds to the envelope of the energy surface obtained for different configurations of independent particles). The bottom of the $\mathcal{E}(\beta_3)$ curve is more flat than one could expect from a simple quadratic dependence on β_3

d) Properties of the $\mathcal{E}(\beta_2, \beta_3)$ surface.

The functions $\mathcal{E}_{BCS}$ calculated for the spherical nucleus ^{218}Rn, for the transition nuclei ^{224}Ra and ^{226}Th and for the deformed nucleus ^{232}U are shown on Fig.5-8. Analogic figures for $\mathcal{E}_{IP}$ were shown in /3/.

In the harmonic approximation for $\mathcal{E}$ one expects

$$\mathcal{E} = E_0 + C_2(\beta_2 - \beta_{eq})^2 + C_3\beta_3^2 \quad , \tag{7}$$

which on figures should give a system of ellipses with axis in the β_2 and β_3 directions. In reality the curves on figs. 5-8 substantially differ from such a prediction. To demonstrate this fact more clearly we show on fig.9 the "valleys" in the β_3 direction, i.e. the curves connecting the minima of $\mathcal{E}$ for each value of β_3 . These lines, particularly for transition nuclei differ considerably from the direct line β_2=Const, obtained from (7).

The quantities β_2 and β_3 will both change during vibrations with the potential energy $\mathcal{E}$ given on figures 5-8. In the phonon language this is equivalent to an interaction of octupole and quadrupole phonons. One can simply see, that such an interaction leads to the lowering of the energy of octupole vibrations and to an increase of their momentra of inertia. Note, that such an interaction is used often, e.g. in /10/.

e) Approximation of the $\mathcal{E}(\beta_2, \beta_3)$ function by a simple formula. We used the least-square method to approximate the $\mathcal{E}(\beta_2, \beta_3)$ function by the formula

$$\mathcal{E} = E_0 + C_2(\beta_2 - \beta_{eq})^2 + C_3\beta_3^2 + C_{23}\cdot\beta_2\cdot\beta_3^2 \quad . \tag{8}$$

The last term in (8) was added to take the phonon interaction into account. The results for $\mathcal{E}_{IP}$ are given in Table 1. All the coefficients are in MeV. The quantity $C_{23}\,\beta_{eq} / C_3$ in the fifth column is the relative shift (according to the first order perturbation theory) of the octupole phonon energy. We have used the $\mathcal{E}_{IP}$ values to construct the table because they are more sensitive to the atomic number. The restoring force coefficients calculated from the $\mathcal{E}_{BCS}$ values are in narrower limits $C_2 \approx 100-110$, $C_3 \approx 280-300$, $-C_{23} \approx 450-500$.

The other function by which we approximate the potential energy of the nucleus is taken from the liquid drop model with the shell structure correction[11]

$$\mathcal{E} = E_0 + G\exp(-\sum_\lambda \beta_\lambda^2/c) + \sum_\lambda C_\lambda \beta_\lambda^2 . \qquad (9)$$

The quantities G_{MS}, C_{2MS} obtained from the experimental masses and quadrupole momenta are tabulated in[11]. The coefficient c in the exponential function is equal to

$$c = A^{2/3} / 4\pi (\frac{a}{r_0})^2 .$$

In[11] the authors take $a/r_0 = 0.27$ which means that the shell structure effect disappears for the deformation $\beta \approx 0.16$. We have used the same value of c. The results of the fit for $\mathcal{E}_{IP}$ together with G_{MS}, C_{2MS} taken from[11], are shown in table 2. The mean deviation was rather large, i.e. the function (9) describes $\mathcal{E}$ only very roughly. The deformations β were obtained from the condition of a minimum of $\mathcal{E}$. The parameters G_1, C_2 have the same order of magnitude as the liquid drop values in[11] but they change much faster from nucleus to nucleus.

Conclusions

Let us recapitulate the main obtained results. There are no nuclei with non-zero equilibrium octupole deformations in the considered region. The potential energy surface differs substantially from a simple harmonic form, terms describing the interaction between octupole and quadrupole vibrations, as well as anharmonic terms containing higher powers of the deformation parameters are essential. The form of the energy surface changes with the atomic number A, the softest are the transition nuclei with neutron number N=136.

In conclusion I would like to express my thanks to Mrs. V. Abbrentova for her help in compiling the machine-code as well as in computer calculations.

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Received by Publishing Department
on December 15, 1967

Table 1

Nucleus	C_2	C_3	C_{23}	$C_{23}\cdot\beta_{eq}/C_3$	β_{eq}
^{218}Rn	204	205	-500	0.12	0.05
^{220}Rn	181	200	-452	0.13	0.05
^{222}Rn	154	201	-443	0.13	0.05
^{220}Ra	202	191	-465	0.17	0.07
^{222}Ra	174	186	-421	0.18	0.08
^{224}Ra	161	186	-406	0.21	0.09
^{226}Ra	188	171	-313	0.24	0.13
^{228}Ra	197	172	-202	0.19	0.16
^{224}Th	162	181	-380	0.21	0.07
^{226}Th	141	180	-371	0.23	0.13
^{230}Th	185	171	-184	0.18	0.21
^{230}U	154	165	-309	0.32	0.17
^{232}U	163	171	-195	0.24	0.21
^{228}Th	170	166	-287	0.26	0.19

Table 2

Nucleus	G_{MS}	G	C'_{2MS}	C_2	C_3	β_{MS}	β
^{218}Rn	-1.12	-1.42	30	91	145	-	-
^{220}Rn	0.20	-0.76	30	72	155	-	-
^{222}Rn	1.38	-0.65	31	58	160	0.13	
^{220}Ra	0.04	-0.08	29	74	155	-	-
^{222}Ra	1.35	0.56	29	59	165	0.12	-
^{224}Ra	2.51	0.67	29	41	170	0.19	-
^{226}Ra	3.52	3.42	29	29	191	0.21	0.20
^{228}Ra	4.40	5.93	29	17	220	0.22	0.25
^{224}Th	2.33	1.11	22	36	172	0.19	-
^{226}Th	3.48	1.21	22	21	177	0.21	-
^{228}Th	4.48	3.95	22	9	198	0.22	0.27
^{230}Th	5.35	7.67	22	6	240	0.23	0.34

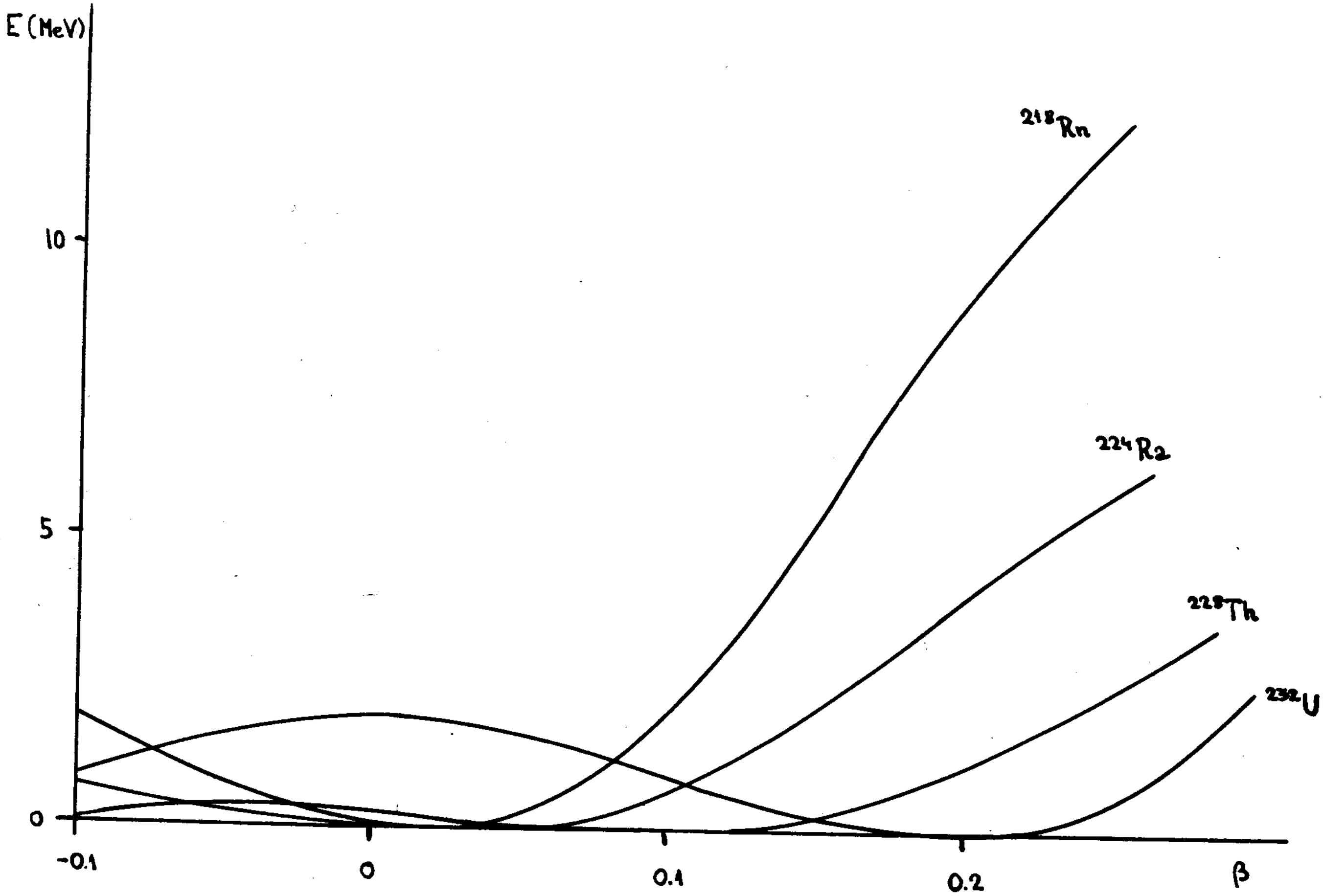

Fig.1. The dependence of $\mathcal{E}_{BCS}$ on β_2

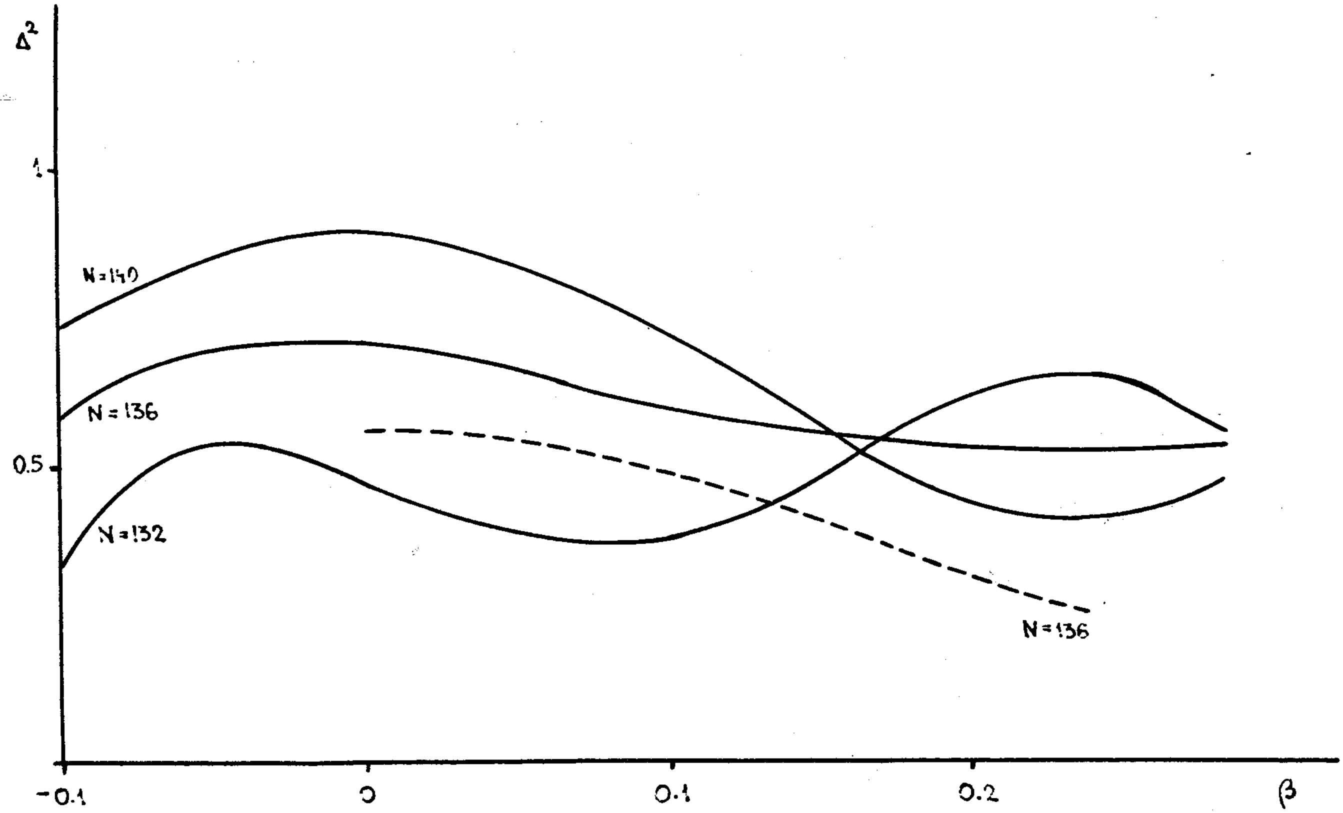

Fig.2. The $\Delta_n^2(\beta_2)$ function (for $\beta_3 = 0$).

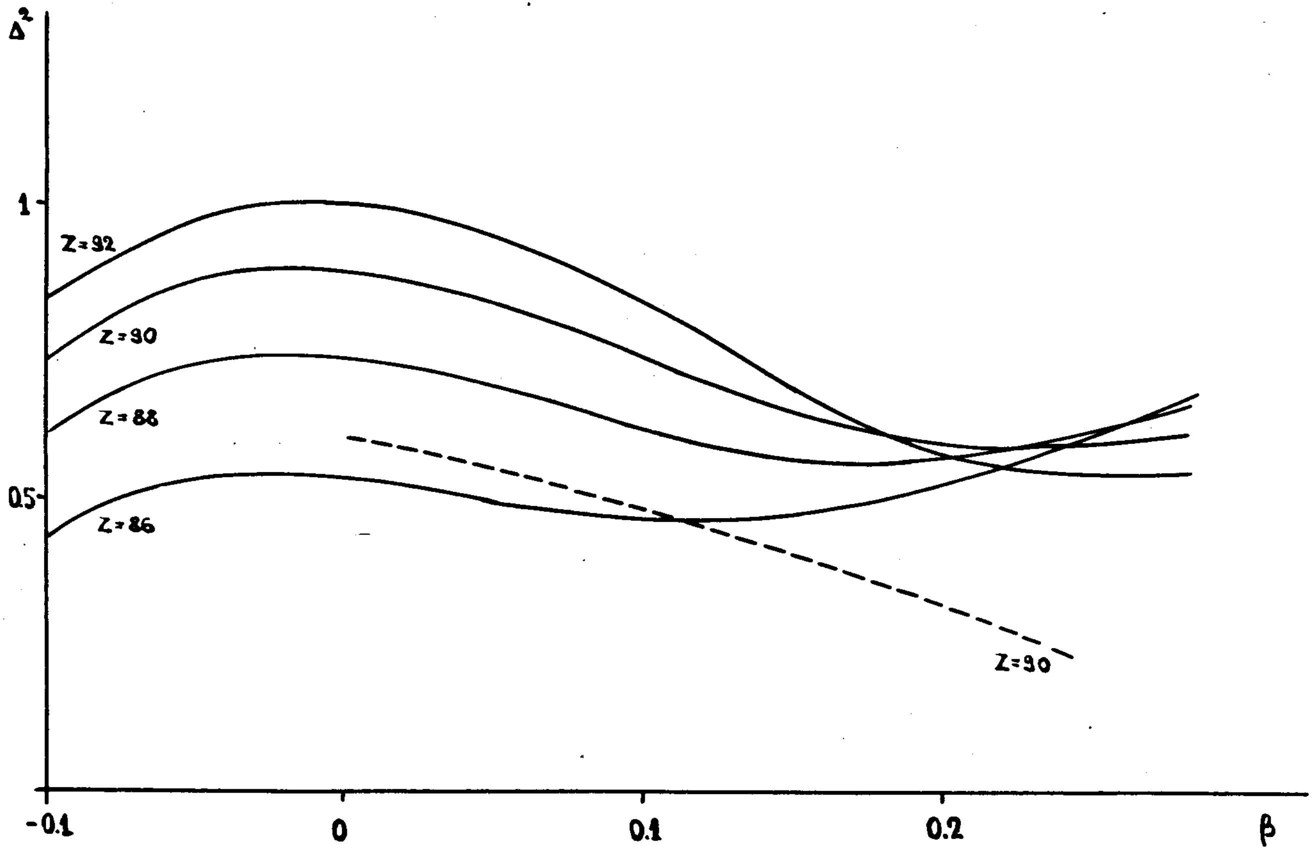

Fig.3. The $\Delta_p^2(\beta_2)$ functions (for $\beta_3 = 0$).

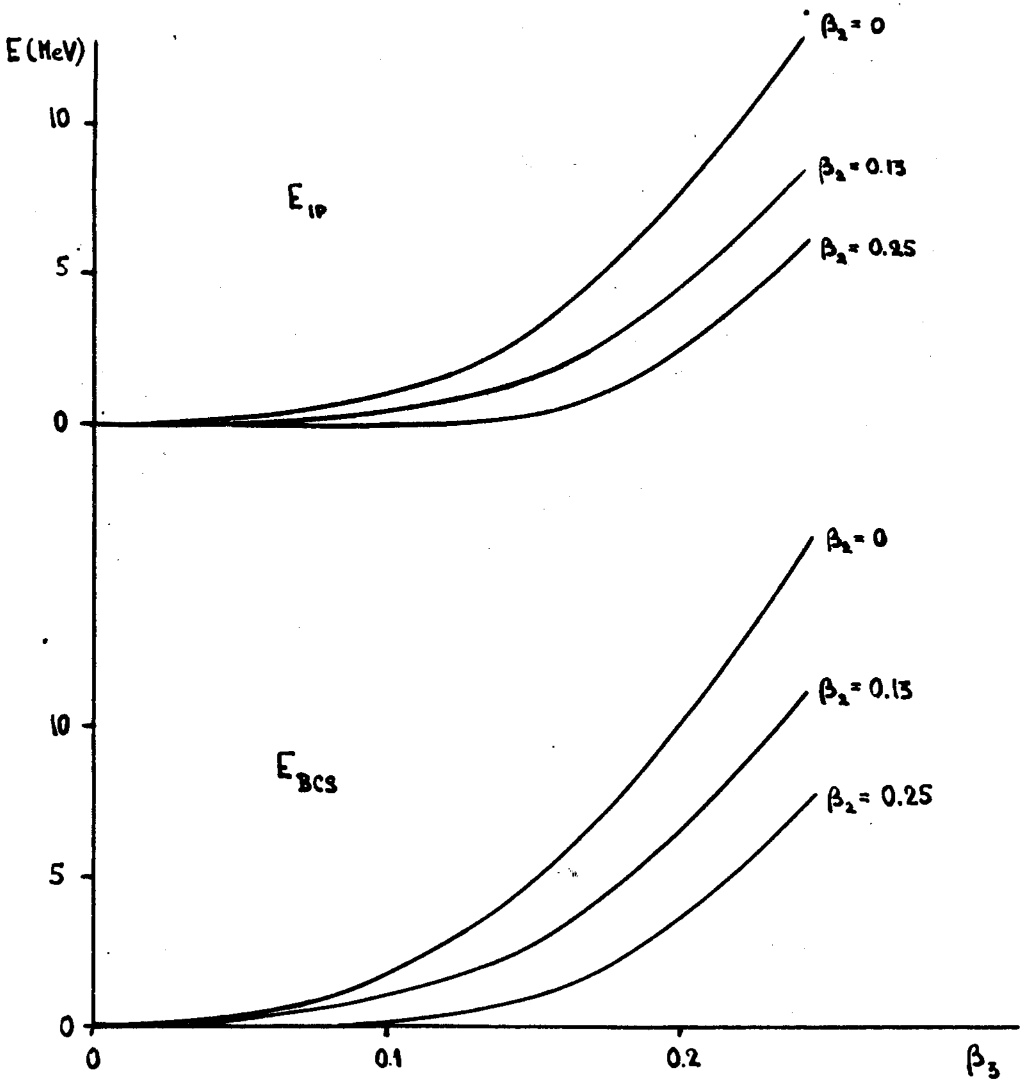

Fig.4. The dependence of $\mathcal{E}_{BCS}$ and $\mathcal{E}_{IP}$ on β_3 for different β_2 values.

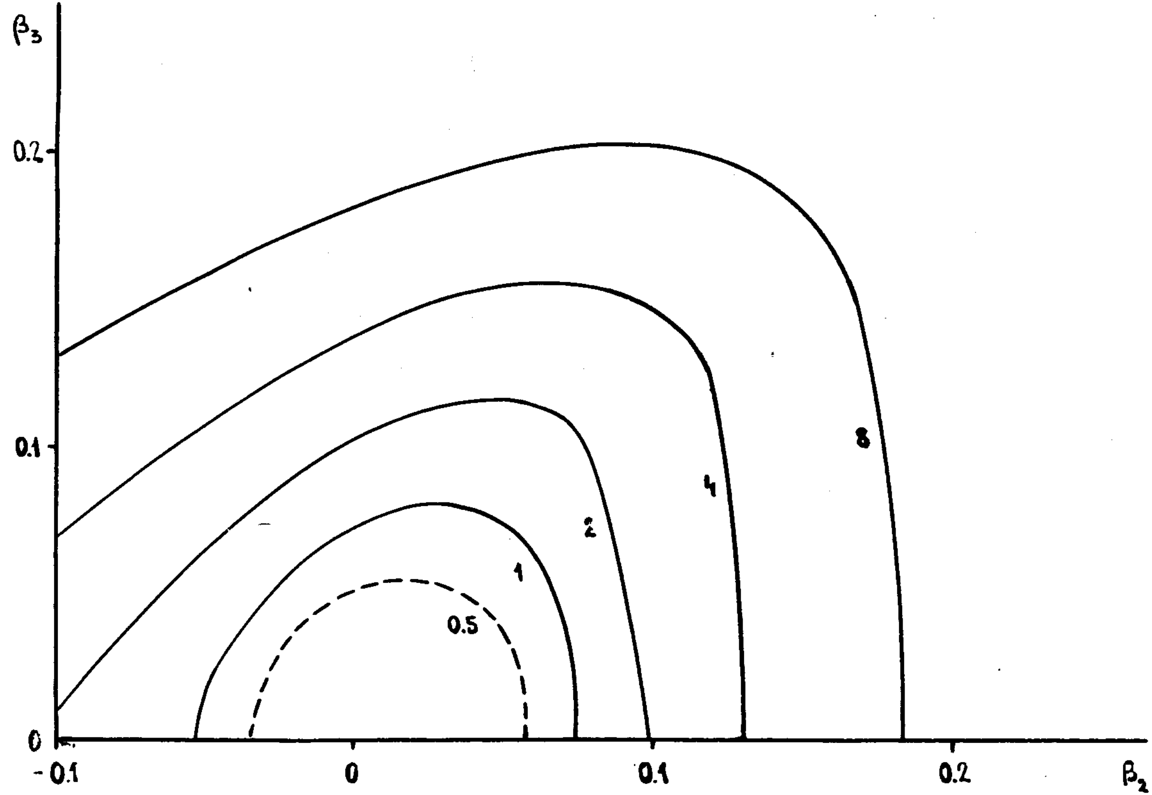

Fig.5. The $\mathcal{E}_{BCS}(\beta_2, \beta_3)$ function for ^{224}Ra.

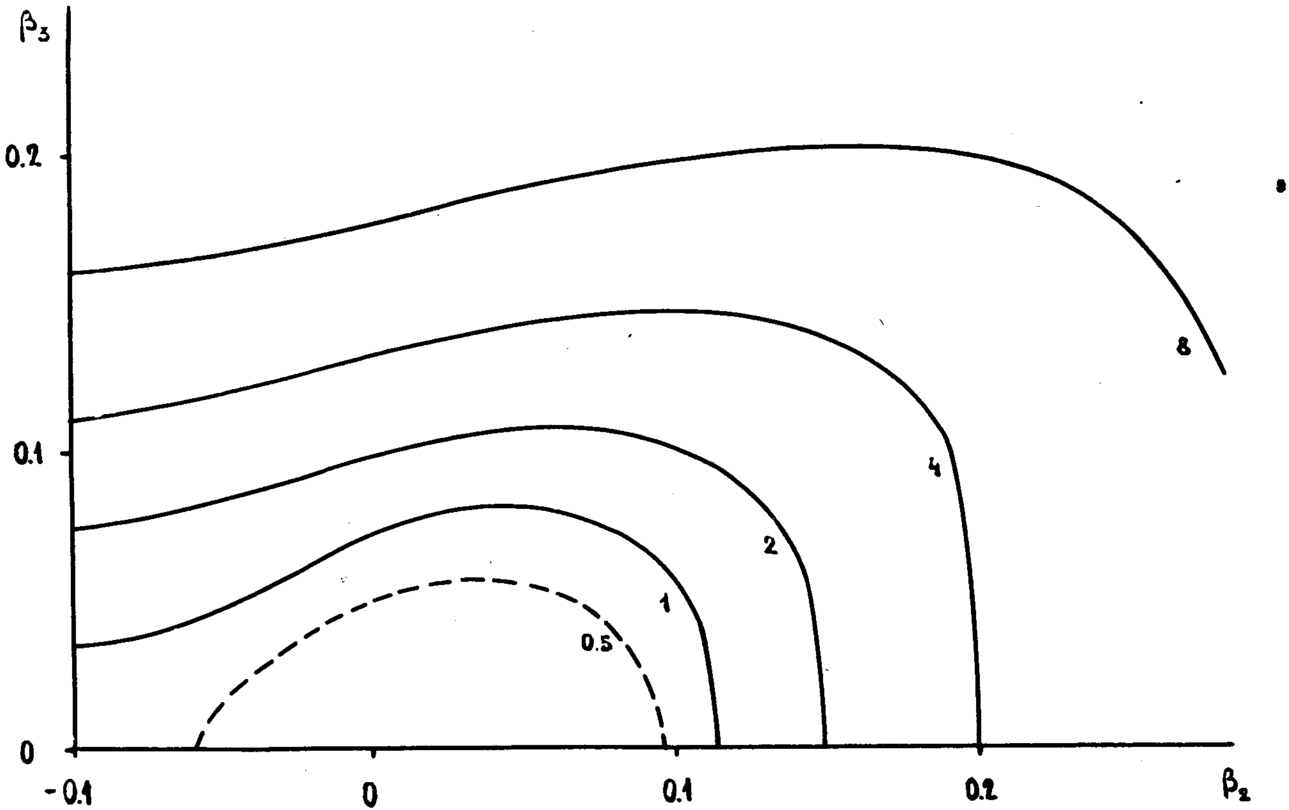

Fig.6. The $\xi_{BCS}(\beta_2\ ,\ \beta_3)$ function for ^{224}Ra.

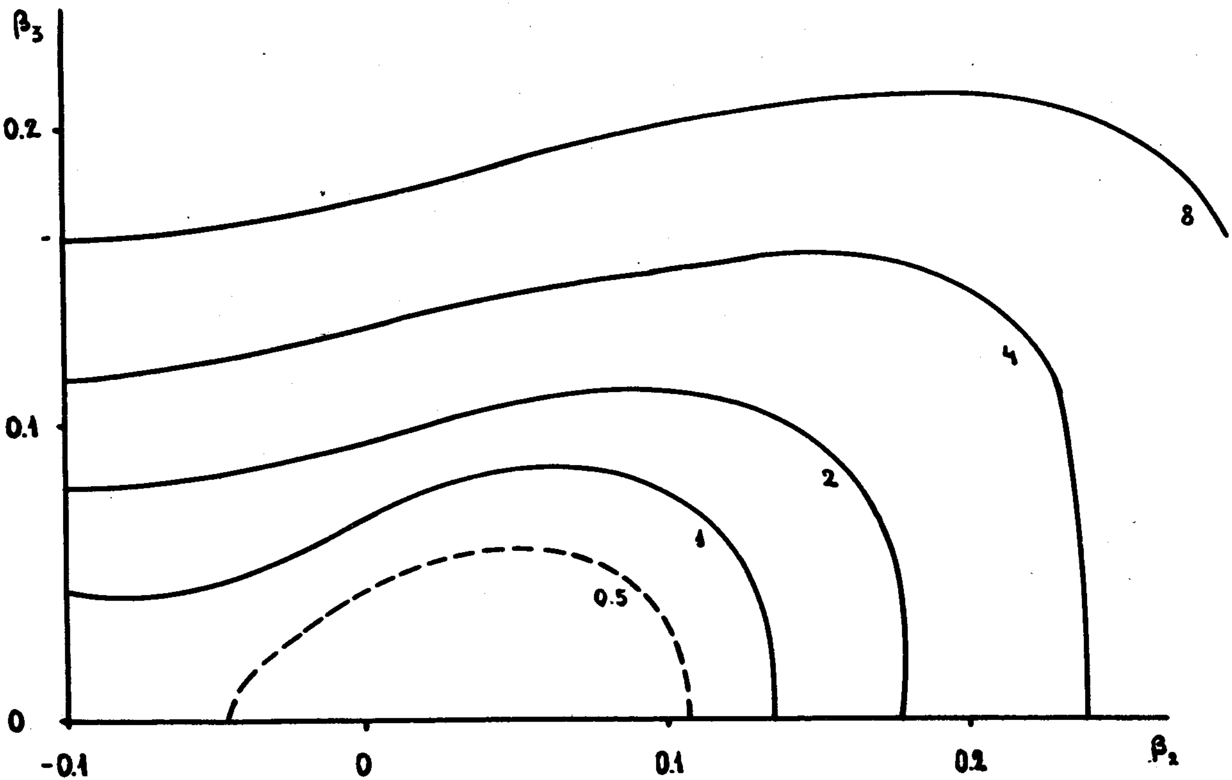

Fig.7. The $\mathcal{E}_{BCS}(\beta_2, \beta_3)$ function for ^{226}Th.

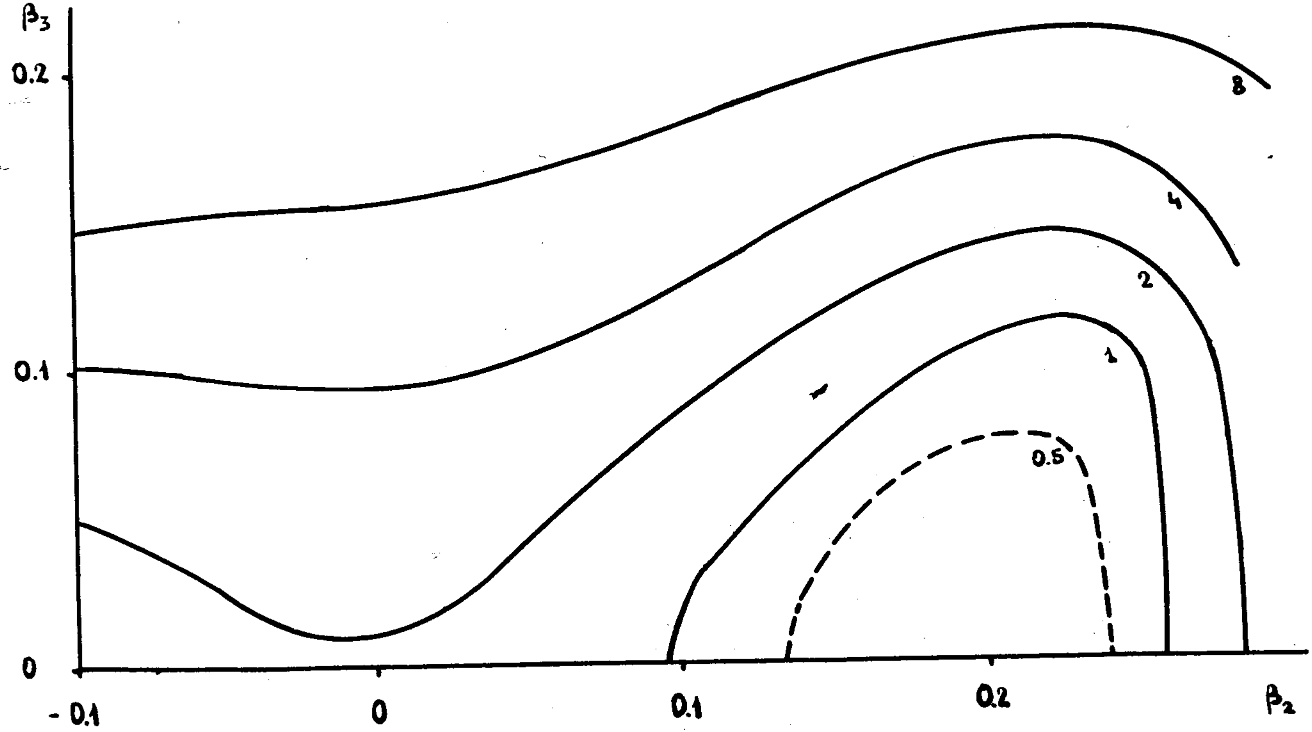

Fig.8. The $\mathcal{E}_{BCS}(\beta_2, \beta_3)$ function for ^{232}U.

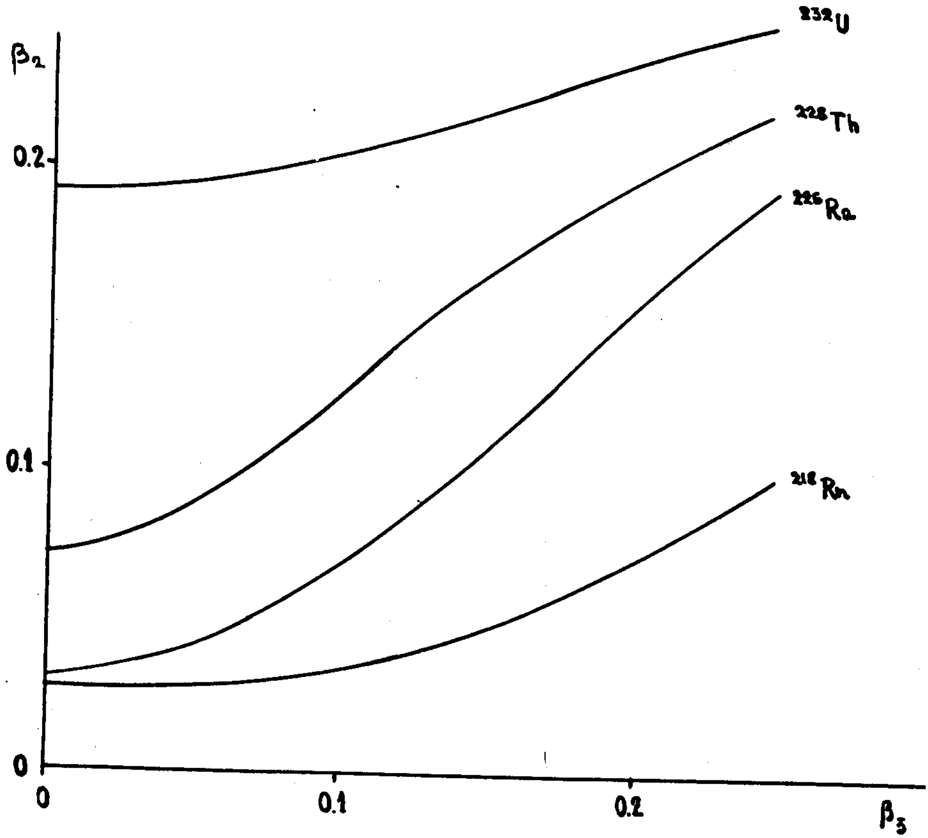

Fig.9. Points along the bottom of the "valley" in the β_3 direction.