COLLECTIVE QUADRUPOLE EXCITATIONS OF TRANSACTINIDE NUCLEI

K. Zając, L. Próchniak, K. Pomorski

Institute of Physics, Maria Curie-Skłodowska University
Pl. M. Curie-Skłodowskiej 1, 20-031 Lublin, Poland

S.G. Rohoziński and J. Srebrny

Faculty of Physics, Warsaw University, Hoża 69, 00-681 Warsaw, Poland

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Dedicated to Adam Sobiczewski in honour of his 70th birthday

The quadrupole excitations of transuranic nuclei are described in the frame of the microscopic Bohr Hamiltonian modified by adding the coupling with the collective pairing vibrations. The energies of the states from the ground-state bands in U to No even–even isotopes as well as the B(E2) transition probabilities are reproduced within the model containing no adjustable parameters.

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1. Introduction

The evidence of excited states of transuranic, or even transfermium $Z > 100$ nuclei has significantly enriched in last years due to the enormous progress in the experimental techniques. These nuclei are especially interesting with regard to their nearness to the super-heavy mass region, for instance the spectroscopic measurements performed for ^{252}No and ^{254}No Ref. [1–4] gave us an insight into the structure of $Z = 102$ isotopes.

The nuclei from this region are axially deformed and their ground state bands are well described by the rotational model as was already shown *e.g.* in Ref. [5] on basis of the HFB calculations. However, the proper description of higher states from the ground state band as well as of other excited collective states can be only achieved when one adds at least the coupling of the rotational motion with the quadrupole shape vibrations. Also, the influence of the pairing correlations is not negligible and the corresponding collective modes [6] should be taken into account.

Recently we have developed [7] a microscopic quadrupole plus pairing collective Hamiltonian which describes well the low-lying nuclear excitations. Our model, which is essentially a generalization of the collective Bohr Hamiltonian [8–10], was successfully applied in the wide range of transitional nuclei from neutron-rich Ru isotopes up to rare earth nuclei [11–13]. The aim of the present study is to check how our model works in the region of the heaviest nuclei.

2. Description of the model

Following the idea of the generalized Bohr Hamiltonian we construct a similar collective Hamiltonian but in a more extensive space of collective variables. To the five usual quadrupole degrees of freedom, namely the two Bohr deformation parameters, β and γ, describing the nuclear shape in the intrinsic frame of reference and the three Euler angles denoted as Ω, which determine the orientation of the principal axes of nucleus with respect to the laboratory axes, we add the next four variables describing the pairing correlations of protons and neutrons in the nucleus. These are: the proton and neutron pairing gap parameters, Δ^p and Δ^n, which describe the pairing vibrations, and the proton and neutron gauge angles, Φ^p and Φ^n parameterizing rotations in the gauge space *i.e.* changes in numbers of protons and neutrons in the system.

The full Bohr Hamiltonian in the "quadrupole plus pairing" collective space is the sum of kinetic and potential collective energies. The former is the second order differential operator in all the nine collective variables and contains various second order mixed derivatives. The latter consists of the deformation and pairing potentials. It is rather difficult to solve the nine-dimensional eigenvalue problem for such a Hamiltonian in its most general form. We have not solved this complicated problem as yet. Up to now we usually assume that a coupling between the quadrupole and the pairing degrees of freedom in the kinetic energy is weak and neglect all mixed derivatives over a quadrupole and a pairing variable. Then, the collective Hamiltonian is separated into the quadrupole and the pairing parts, namely

$$\hat{\mathcal{H}}_{\mathrm{CQP}} = \hat{\mathcal{H}}_{\mathrm{CQ}}(\beta,\gamma,\Omega;\Delta^p,\Delta^n) + \hat{\mathcal{H}}_{\mathrm{CP}}(\Delta^p,\Phi^p,\Delta^n,\Phi^n;\beta,\gamma)\,. \qquad (1)$$

However, this does not mean at all that the quadrupole and pairing degrees of freedom are decoupled completely from each other. We are going to take approximately the quadrupole-pairing coupling into account in the following.

The operator $\hat{\mathcal{H}}_{\mathrm{CQ}}$ describes the quadrupole excitations (vibrations and rotations) of nucleus and takes the form of the usual generalized Bohr Hamiltonian [8,9]

$$\hat{\mathcal{H}}_{\mathrm{CQ}} = \hat{\mathcal{T}}_{\mathrm{vib}}(\beta,\gamma;\Delta^p,\Delta^n) + \hat{\mathcal{T}}_{\mathrm{rot}}(\beta,\gamma,\Omega;\Delta^p,\Delta^n) + V_{\mathrm{coll}}(\beta,\gamma;\Delta^p,\Delta^n)\,. \quad (2)$$

Here $V_{\rm coll}$ is the collective potential, the kinetic vibrational energy reads

$$\hat{\mathcal{T}}_{\rm vib} = -\frac{\hbar^2}{2\sqrt{wr}}\left\{\frac{1}{\beta^4}\left[\partial_\beta\left(\beta^4\sqrt{\frac{r}{w}}B_{\gamma\gamma}\partial_\beta\right)-\partial_\beta\left(\beta^3\sqrt{\frac{r}{w}}B_{\beta\gamma}\partial_\gamma\right)\right]+\frac{1}{\beta\sin 3\gamma}\right.$$
$$\left.\times\left[-\partial_\gamma\left(\sqrt{\frac{r}{w}}\sin 3\gamma B_{\beta\gamma}\partial_\beta\right)+\frac{1}{\beta}\partial_\gamma\left(\sqrt{\frac{r}{w}}\sin 3\gamma B_{\beta\beta}\right)\partial_\gamma\right]\right\}, \qquad (3)$$

and the rotational energy is

$$\hat{\mathcal{T}}_{\rm rot} = \frac{1}{2}\sum_{k=1}^{3}\frac{\hat{I}_k^2}{\mathcal{J}_k}\,. \qquad (4)$$

The intrinsic components of the total angular momentum are denoted as $\hat{I}_k$, $(k=1,2,3)$, while w and r are the determinants of the vibrational and rotational mass tensors. The mass parameters $B_{\beta\beta}$, $B_{\beta\gamma}$ and $B_{\gamma\gamma}$ and three principal moments of inertia $\mathcal{J}_k$, $(k=1,2,3)$ depend on intrinsic variables β,γ and pairing gap values Δ^p,Δ^n. All inertial functions are determined from a microscopic theory. We apply the standard cranking method to evaluate the inertial functions assuming that the nucleus is a system of nucleons moving in the deformed mean field (Nilsson potential) and interacting through monopole pairing forces. One has to stress that for Δ corresponding to the minimum of the BCS energy the operator $\hat{\mathcal{H}}_{\rm CQ}$ is exactly the same as the Bohr Hamiltonian used in Ref. [9].

For a given nucleus (no pairing rotation) the second term in Eq. (1) describes collective pairing vibrations of systems of Z protons and $A-Z$ neutrons

$$\hat{\mathcal{H}}_{\rm CP} = \hat{\mathcal{H}}_{\rm CP}^{Z} + \hat{\mathcal{H}}_{\rm CP}^{A-Z}\,, \qquad (5)$$

and it can be expressed in the following form [6,18]:

$$\hat{\mathcal{H}}_{\rm CP}^{\mathcal{N}} = -\frac{\hbar^2}{2\sqrt{g(\Delta)}}\frac{\partial}{\partial\Delta}\frac{\sqrt{g(\Delta)}}{B_{\Delta\Delta}(\Delta)}\frac{\partial}{\partial\Delta} + V_{\rm pair}(\Delta)\,, \qquad (6)$$

where $\mathcal{N}=Z$, $\Delta=\Delta^p$ for protons and, respectively, $\mathcal{N}=A-Z$, $\Delta=\Delta^n$ for neutrons. The functions appearing in the Hamiltonian (6), namely the pairing mass parameter $B_{\Delta\Delta}(\Delta)$, the determinant of the metric tensor $g(\Delta)$ and the collective pairing potential $V_{\rm pair}(\Delta)$ are obtained microscopically.

We are interested in taking approximately an effect of the pairing vibrations on the quadrupole excitations into account. Therefore, we solve the eigenvalue problem for the Hamiltonian of Eq. (1) in two steps. First, we find the pairing collective excitations at given deformations and next, we modify the Schrödinger equation for the quadrupole motion allowing

for the zero-point pairing vibrations. This is an approach similar to the Born–Oppenheimer approximation for molecules where one first finds the electronic motion at given positions of nuclei and next takes an effect of the electronic binding on the molecular vibrational and rotational excitations into account.

Solving the eigenproblem of the collective pairing Hamiltonian (6) one can find the pairing vibrational ground-state wave function Ψ_0 and the ground-energy E_0 at each (β,γ) deformation point. The most probable value of the energy gap $\Delta_{\max}$ corresponds to the maximum of the probability of finding a given gap value in the collective pairing ground-state (namely the maximum of the function $g(\Delta)|\Psi_0(\Delta)|^2$). The value of $\Delta_{\max}$ is shifted towards smaller gaps from the equilibrium point $\Delta_{\rm eq}$ determined by the minimum of $V_{\rm pair}$ or simply by the BCS formalism. Such a behavior of the pairing ground state function Ψ_0 is due to the rapid increase of pairing mass parameter $B_{\Delta\Delta}$. In general the ratio of $\Delta_{\max}$ to $\Delta_{\rm eq}$ is of about 0.7.

All collective functions appearing in Eqs. (3), (4) are calculated using the most probable pairing gap values for protons and for neutrons instead the equilibrium ones. The collective potential corresponds to the ground state of the $\hat{\mathcal{H}}_{\rm CP}$ Hamiltonian (5) and it is very close to the BCS energy in each β,γ point. The approximation described above is rather crude but it includes the main effect of the coupling with the pairing vibrational mode. This procedure improves significantly the accuracy in reproducing the experimental data and it introduces no additional parameters into the model.

The nucleon single particle motion is described by the Nilsson (modified harmonic oscillator) potential with the correction terms

$$V_{\rm corr} = -\hbar\omega_0\,\kappa\left[2\,\boldsymbol{l}\boldsymbol{s} - \mu(\boldsymbol{l}^2 - \langle\boldsymbol{l}^2\rangle_N)\right]\,. \tag{7}$$

Parameters κ, μ are equal $\kappa_n = 0.0635$, $\kappa_p = 0.0570$, $\mu_n = 0.32$ and $\mu_p = 0.66$ are taken from [14] for the mass $A = 250$.

The dependence of the strengths of the pairing forces on the nucleon number is assumed as $G_\tau = g_{0,\tau}/N_\tau^{2/3}$, where τ denotes protons or neutrons. The parameters $g_{0,\tau}$ are taken from [15], where they have been estimated from mass differences and they are equal $g_{0,\rm n} = 0.267\,\hbar\omega_0$ and $g_{0,\rm p} = 0.284\,\hbar\omega_0$ for the pairing window (*i.e.* levels taken into account) includes the same number of levels equal to $\sqrt{15N_\tau}$ below and above the Fermi level. Moreover, we use an approximate projection of the BCS wave function on a good particle number, which modifies formula for the BCS energy [16].

The collective energy is calculated by Strutinsky microscopic–macroscopic method. The moments of inertia and mass parameters are determined within the cranking model. We have used a new parameterization of the macroscopic (liquid drop) energy which contains the dependence on the curvature of a surface of a nucleus (LSD) from [17].

The potential energy, mass parameters and electric moments have been computed in 188 points in the (β, γ) sextant $(0, 0.75) \times (0°, 60°)$.

The collective quadrupole motion is described by the generalized Bohr Hamiltonian, the method of solving its eigenproblem is the same as in [7]. There are two parameters that determine the basis we use in the collective space: μ_2 and n. The former enters in the common exponential factor $\mathrm{e}^{-(\mu_2\beta)^2/2}$ of the basis functions while the latter (n) determines the truncation of the basis and is equal to the highest order of the polynomial in β. All calculations have been made with the choice $\mu_2 = 12$ and $n = 36$. The consequence of such rather large value of n is that the results are insensitive against the changes of μ_2 in a quite big range $10 < \mu_2 < 15$.

3. Results

The results presented here are rather preliminary because our model does not contain the deformations of multi-polarities higher than 2. Nevertheless, the theoretical energies of the ground-state bands for U, Pu, Cm, Cf, Fm, and No isotopes are close to the experimental data as it can be seen in Fig. 1.

The calculated values for 2^+ states are connected in Fig. 1 by full lines while corresponding experimental points taken from Refs. [1,2,4] are marked with diamonds. For 4^+ states we have used the dashed lines and triangles, for 6^+ states — the dotted lines and circles and for 8^+ states — the dot-dashed lines and crosses. The agreement of the theoretical estimates of the energies

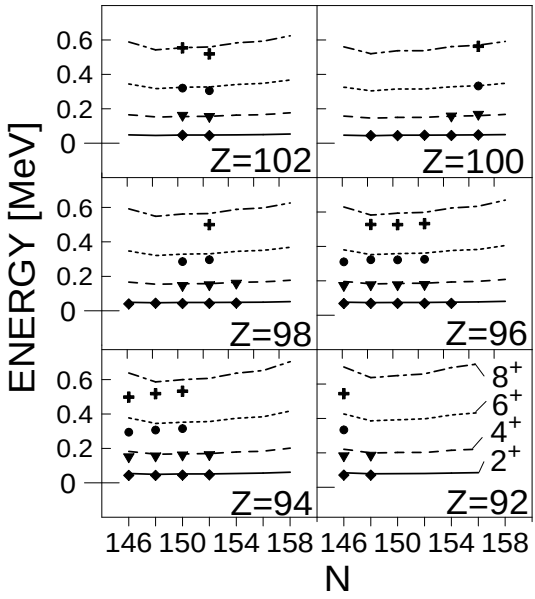

Fig. 1. The ground state band energies of in even–even transuranic isotopes.

of the 2^+ and 4^+ states is good. The energies of the 6^+ and 8^+ states are overestimated for the isotopes with $Z < 100$ while for Fm and No isotopes the calculated energies of these states are very close to the experimental data.

The reduced B(E2) transition probabilities within the members of the ground-state band are shown in Fig. 2 for the considered transactinide nuclei. The theoretical values of the $2^+ \to 0^+$ transitions are connected by the full lines while corresponding experimental [4] points are marked with the diamonds. For $4^+ \to 2^+$ transitions we have used the dashed lines and triangles, for $6^+ \to 4^+$ transitions the dotted lines and circles and for $8^+ \to 6^+$ transitions the dot-dashed lines (no experimental evidence). The empty points for No isotopes represent some estimations found in Ref. [3] for the $2^+ \to 0^+$ transitions. It is seen in Fig. 2 that the theoretical values of B(E2) are too small by approximately 20% with respect to the measured data.

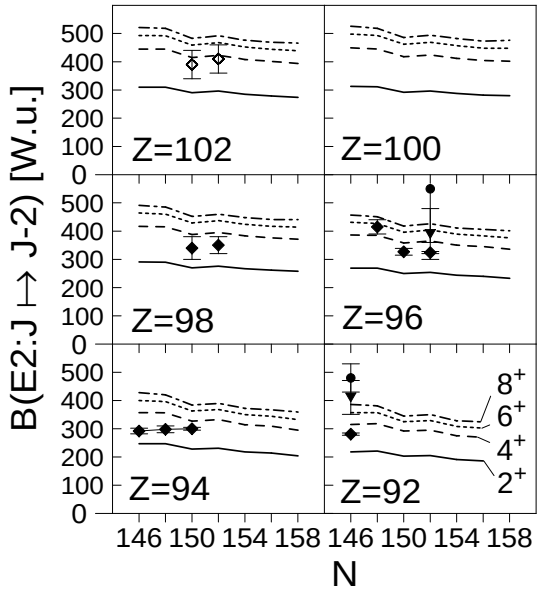

Fig. 2. The reduced E2 transition probabilities in the ground-state bands of transuranic nuclei.

The calculated reduced matrix elements of the electric quadrupole operator in the states from the ground-state band are presented in Fig. 3 for nuclei from the same region. As previously the full, dashed, dotted and dot-dashed lines correspond to the 2^+, 4^+, 6^+ and 8^+ states, respectively. All values remain nearly constant when the number of neutron grows.

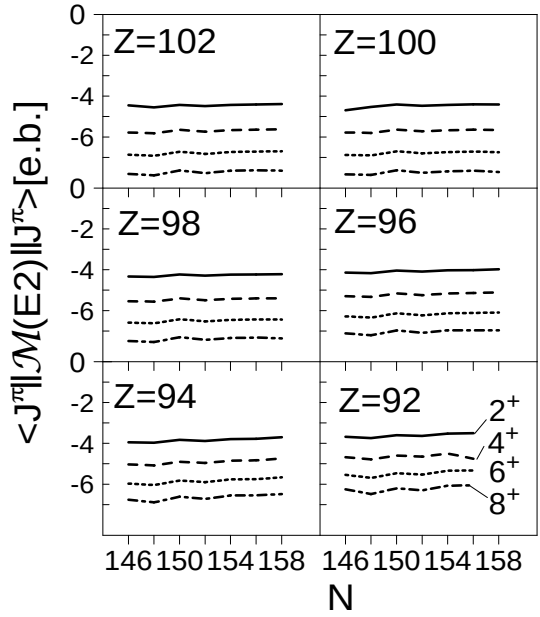

Fig. 3. The reduced matrix elements of the electric quadrupole operator in the ground-state band.

In Fig. 4 the dependences of the theoretical energies of the first 2_1^+ (l.h.s. map) and of the second 2_2^+ (r.h.s. map) excited states are plotted as a function of N and Z. The smallest energy of the 2^+ state is predicted for ^{248}Fm isotope which has the largest quadrupole deformation as it will be seen later. The energy of the 2_2^+ state in ^{252}Fm is the largest one and it is twice as large as the corresponding energy in the ^{238}U isotope.

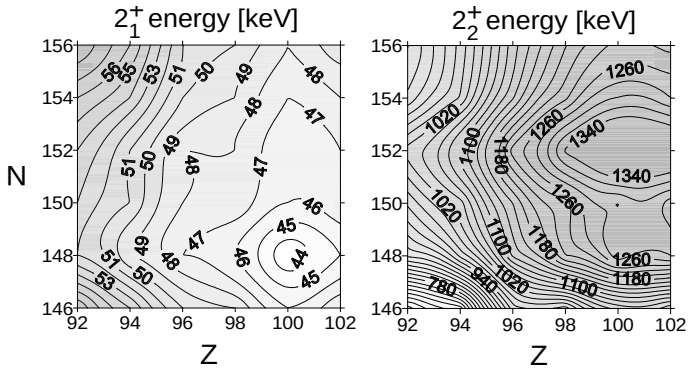

Fig. 4. The contour plot of the energy of the first 2_1^+ (the left map) and of the second 2_2^+ excited state (the right map) on (Z, N) plane.

A similar dependence of the energy of the second 0^+ state on the number of protons and neutrons is shown in Fig. 5. For all nuclei from the considered mass region the energy of the 0^+ state is approximately 30% larger than the energy of the 2^+ state and it shows similar shell structure, maximum for ^{252}Fm.

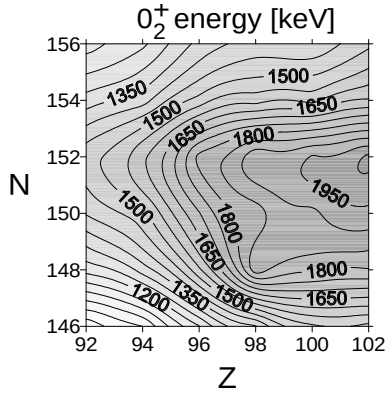

Fig. 5. The same as Fig. 4 but for the 0_2^+ state.

The expectation values of the quadrupole axial β (the left map) and non-axial γ (the right map) deformation in the ground-state wave function is plotted in Fig. 6 on the (Z, N) plane. The corresponding average deformations in the ground state bands are growing very slowly with angular momentum, for example for 2^+ state the average β appears of at most 0.001 and the average γ of at most 0.05° greater than the expectation ground-state value. The average value of β is the largest one in ^{246}Cm isotope while the nucleus ^{248}Fm has the smallest mean value of the nonaxial deformation ($\gamma \approx 10^\circ$).

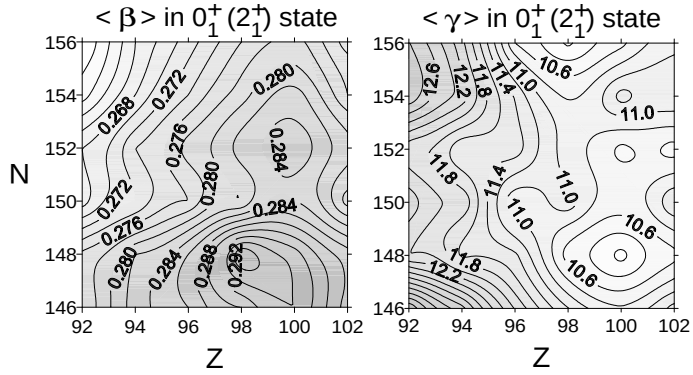

Fig. 6. The average value of β (the left map) and γ (the right map) deformation in the ground-state wave function as a function of the number of protons Z and neutrons N.

Similar data as in Fig. 6 but for the second 2^+ and 0^+ excited states are shown in Fig. 7 and in Fig. 8, respectively. It is seen that the change of the average deformation of the system is strictly correlated with the variance of the energy of the 2_2^+ and 0_2^+ states as it was seen in Figs. 4 and 5.

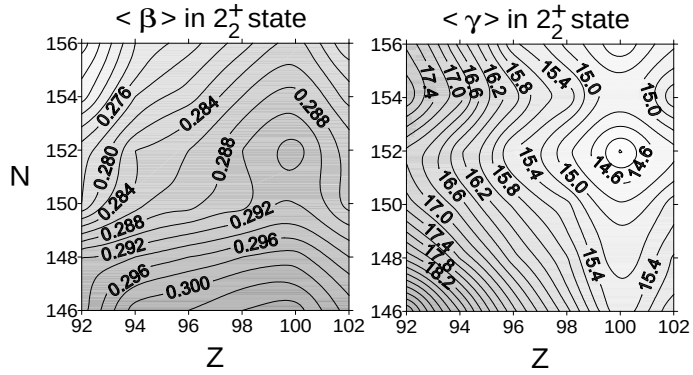

Fig. 7. The same as in Fig. 6 but for the 2_2^+ state.

The relative differences between the first 2^+ state energy obtained with the generalized Bohr Hamiltonian $E_{\rm th}$ and similar energy evaluated in the minimum of the collective nuclear potential within the pure rotational model with the cranking moment of inertia $E_{\rm rot}$ are plotted in Fig. 9 as function of proton and neutron number. The l.h.s. plot corresponds to the cranking moment of inertia evaluated in the BCS minimum of the total energy while the r.h.s. one to the rotational energy obtained with the moment of inertia calculated with the most probable pairing gaps ($E_{\rm rot}^{\Delta}$). The 2^+ state energies obtained with the standard pairing strength in the pure rotational model are on average by 20% larger than those evaluated in our model and around 15%

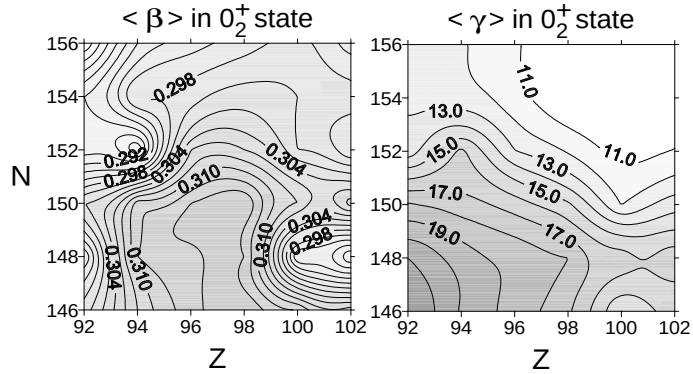

Fig. 8. The same as in Fig. 6 but for the 0_2^+ state.

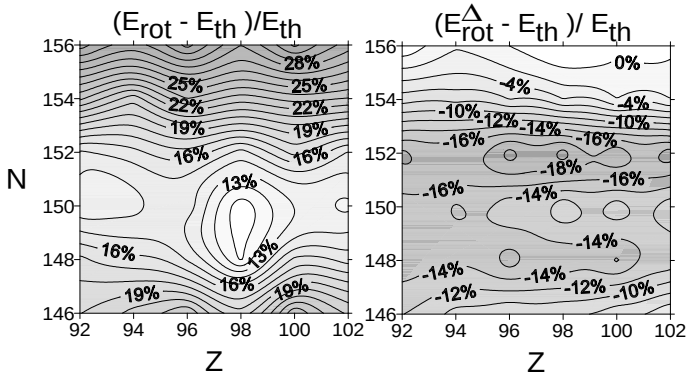

Fig. 9. The relative differences between the energies of the first 2^+ state obtained in our theory ($E_{\rm th}$) and in the pure rotational model ($E_{\rm rot}$).

smaller when one uses the most probable Δ in the microscopic calculations of the cranking moments of inertia. This result shows that the rotational model can not describe propely the energies of the ground state band members when the standard pairing correlations are used.

4. Conclusions

Concluding, we may say that adding of the coupling with the pairing vibrations to the generalized Bohr Hamiltonian improves significantly the quality of theoretical estimates for the even–even heaviest nuclei. We have shown that the coupling between quadrupole and pairing collective degrees of freedom brings the energy levels down to the scale comparable with that characteristic for the experimental levels.

In spite of some simplicity of the Nilsson single-particle potential our approximation works good in this rather extreme mass region and a reasonable agreement with the experimental data is obtained without any adjustment of the parameters. It confirms that our model takes into account the main features of the collective nuclear excitations of the transactinide nuclei. Also we would like to point out that the rotational character of the ground-state bands in Pu and No isotopes was manifested in our model.

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