Prediction of the excitation energies of the 2_1^+ states for superheavy nuclei based on the microscopically derived Grodzins relation

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Background: As the result of synthesis of nuclei with large proton numbers a new region of investigations of the structure of nuclei has been discovered. Due to the recent significant increase in the yield of superheavy nuclei their gamma-spectroscopic studies became possible.
Purpose: To predict the excitation energies of the 2_1^+ states of nuclei with $Z \geqslant 100$.
Method: The microscopic variant of the Grodzins relation derived based on the geometrical collective model and a microscopic approach to description of the low-energy nuclear structure is applied.
Results: The excitation energies of the 2_1^+ states of the even-even nuclei from ^{256}Fm to $^{296}_{120}$X which differ from each other in the number of α particles are predicted.
Conclusion: It is shown that at the beginning of the chain of the studied nuclei the excitation energies of the 2_1^+ states do not exceed 100 keV. Then $E(2_1^+)$ sharply increases with A and reaches maximum value of 400–500 keV in ^{284}Fl or ^{292}Og.

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I. INTRODUCTION

The synthesis of nuclei with large proton numbers up to $Z = 118$ [1–7] has led to the discovery of a new region for investigations of the structure of nuclei, namely, the investigation of the structure of the superheavy nuclei. A number of interesting experimental results have already been obtained [8–11] and calculations that provide information on the single particle spectra and evolution of the shape of these nuclei with increasing Z have been performed [12–41]. A number of calculations of the excited states spectra of superheavy nuclei were made in Refs. [42–50]. Currently, the main source of experimental information on excitation spectra of superheavy nuclei is their α decay. With the start of work of the factory of superheavy elements in Dubna and due to a significant increase in the yield of such nuclei in fusion reactions, gamma spectroscopic studies became possible in this area of the nuclide chart.

One of the most interesting questions related to the study of the properties of superheavy nuclei is the question of the next magic number of protons after $Z = 82$. It is well known that an accurate indicator of what numbers of protons and neutrons are magic is the behavior of the excitation energy of the 2_1^+ states of even-even nuclei. When the values of Z and N approach the magic numbers, the value of $E(2_1^+)$ increases sharply and reaches a maximum at double magic nuclei. This makes information about the excitation energies of the 2_1^+ states of the even-even superheavy nuclei important for the understanding of their structure. It should be noted that the excitation energy of the 2_1^+ state also gives, in principle, information about the shape of these nuclei.

For the experiments planned to measure $E(2_1^+)$ it could be useful to know theoretical predictions of the values of $E(2_1^+)$ in the region of the nuclide chart under investigation. The well known Grodzins relation formulated in 1962 [51], which established that the product of the energy of the 2_1^+ state per probability of the E2 transition from the ground state of the nucleus to the 2_1^+ state, is a smooth function of A and Z. This property does not depend on whether the nucleus is spherical or deformed, although both $E(2_1^+)$ and $B(E2; 0_1^+ \to 2_1^+)$ vary through a large factor. This is especially important when analyzing the properties of nuclei from those parts of the nuclide chart where the transition from deformed to spherical nuclei occurs. Later on Raman and co-workers [52,53], by analyzing a larger set of the experimental data, where the literature has been covered to November 2000, have shown that the Grodzins relation can be presented in the following form:

$$E(2_1^+) \times B(E2; 0_1^+ \to 2_1^+) = 2.57(\pm 45)Z^2A^{-2/3}, \qquad (1)$$

where $E(2_1^+)$ is given in keV and $B(E2; 0_1^+ \to 2_1^+)$ in e^2b^2. This relation has been often used to estimate the unknown $B(E2; 0_1^+ \to 2_1^+)$ values from the known $E(2_1^+)$ in different nuclei, especially in nuclei close to the nuclear drip line, since the measuring of $B(E2)$ is a much more demanding task than measuring excitation energies. In the case of superheavy nuclei both quantities presented in the Grodzins relation are unknown. However, the value of $B(E2; 0_1^+ \to 2_1^+)$ is directly related to quadrupole deformation of nuclei β_2. But this quantity was the object of the numerous theoretical calculations, whose results are quite close to each other. This circumstance gives us a possibility to use the results of calculations of β_2 in order to determine the corresponding values of $B(E2;0_1^+\rightarrow 2_1^+)$, and then using the Grodzins relation to predict $E(2_1^+)$.

The value of the proportionality coefficient in the relation (1) has been considered in detail in [54] using the latest set of the experimental data. The analysis indicates a strong reason for individual fit of the proportionality coefficient in (1) for separate groups of nuclei.

In our previous paper [55] we have derived the Grodzins relation based on the collective quadrupole Bohr Hamiltonian and reproduced the A dependence of the Grodzins product. At the same time, in [55] was proposed a method for calculating the proportionality coefficient in the Grodzins relation, based on the microscopic model of nuclear structure.

The purpose of this work is to calculate the proportionality coefficient in the Grodzins relation for a group of nuclei with $Z \geqslant 100$, based on a microscopic nuclear model, and to predict on this basis the energies of 2_1^+ states of even-even superheavy nuclei.

II. BRIEF DERIVATION OF THE GRODZINS RELATION

Let us repeat shortly a derivation of the Grodzins relation, suggested in [55]. It was noted in [55] that the form of the Grodzins relation indicates that it can be derived using the technique of the energy-weighted sum rule. Therefore, the relation can be derived by analyzing the double commutator of the quadrupole operator $Q_{2\mu}$ with the collective Bohr Hamiltonian which has the form

$$H=-\frac{\hbar^2}{2}\sum_{\mu,\mu'}\frac{\partial}{\partial\alpha_{2\mu}}(B^{-1})_{\mu\mu'}\frac{\partial}{\alpha_{2\mu'}}+V(\alpha_{2\mu}), \tag{2}$$

where $(B^{-1})_{\mu\mu'}$ is an inverted inertia tensor, $\alpha_{2\mu}$ are the collective variables, and V is the potential. It is convenient to present the inertia tensor in terms of the components having fixed values of the angular momentum L,

$$(B^{-1})_{\mu\mu'}=\sqrt{5}\sum_{LM}C^{LM}_{2\mu 2\mu'}(B^{-1})_{LM}, \tag{3}$$

where $C^{LM}_{2\mu 2\mu'}$ is a Clebsch Gordan coefficient. For a double commutator we obtain

$$[[H,Q_{2\mu}],Q_{2\mu'}]=-\hbar^2 q^2\sqrt{5}\sum_{LM}C^{LM}_{2\mu 2\mu'}(B^{-1})_{LM}, \tag{4}$$

where $q=3/4\pi eZr_0^2A^{2/3}$. Taking the average of (4) over the ground state $|0_1^+\rangle$ we obtain

$$\sum_n E(2_n^+)\times B(E2;0_1^+\rightarrow 2_n^+)=\frac{5}{2}\hbar^2q^2\langle 0_1^+|(B^{-1})_{00}|0_1^+\rangle, \tag{5}$$

where summation takes place over all collective quadrupole 2^+ states related to the surface mode treated by the Bohr Hamiltonian. Only one term in (5) containing the 2_1^+ state is included in the Grodzins relation. Therefore, it is necessary to evaluate the contribution of the remaining terms in the total sum. In the limit of harmonic quadrupole oscillations $E2$ transition from the ground state is possible only to the 2_1^+ state. In this case, leaving on the left in (5) only the transition to the 2_1^+ state, we get on the right the proportionality factor equal to 5/2. Let us consider the experimental data on spherical nuclei. The probabilities of the $E2$ transitions from the ground to the first, second, and third 2^+ states are experimentally known in some cases. We transfer the contributions corresponding to the last two transitions to the right part of Eq. (5). We get that the proportionality factor on the right side in (5) is equal for ^{106}Pd 4.7/2, for ^{108}Pd 4.8/2, and for ^{112}Cd 4.4/2. Thus, the experimental data for spherical nuclei are close to the values for the harmonic limit. Consider another limiting case, namely rigid rotational motion. In [56], it was shown that nonzero contributions to the sum of (5) are also given by $E2$ transitions from the ground state to the 2^+ states of the beta- and gamma-rotational bands. Moving the corresponding terms to the right side of the relation (5), and leaving on the left only the term corresponding to the transition $0_1^+\rightarrow 2_1^+$, we get the proportionality coefficient on the right equal to 2/2. The experimental data for deformed nuclei are as follows. In the case of ^{164}Dy 3.9/2, in the case of ^{158}Gd 3.6/2. The same consideration of experimental data for nuclei transitional between spherical and deformed gives the following results: ^{154}Gd 1.9/2, ^{152}Sm 3.5/2, ^{152}Gd 4.4/2, ^{148}Sm 2.9/2, ^{196}Pt 4.0/2, ^{194}Pt 4.9/2, ^{192}Pt 4.9/2. We see that the values of this coefficient show a large variation. In our calculations below, we use a proportionality factor of 2/2 as it follows theoretically for the limiting case of the deformed nuclei, since according to the numerous calculations, nuclei with $Z = 100$–110 considered below are well deformed very heavy nuclei. This is just the value of the proportionality factor that makes it possible to reproduce below the only experimentally known value of $E(2_1^+)$ for one of the nuclei considered below, namely, for ^{256}Fm. At the same time our predictions for nuclei with smaller deformation will underestimate the values of $E(2_1^+)$ for this choice of the proportionality factor. Thus, below, the following relation will be used to calculate the value of $E(2_1^+)$:

$$E(2_1^+)\times B(E2;0_1^+\rightarrow 2_1^+)=\tfrac{2}{2}\hbar^2q^2\langle 0_1^+|(B^{-1})_{00}|0_1^+\rangle. \tag{6}$$

The components of the inertia tensor given in the laboratory frame can be expressed through their components in the intrinsic frame [57]:

$$(B^{-1})_{LM}=D^L_{M0}(B^{-1})^{\rm in}_{L0}+\frac{1}{\sqrt{2}}\left(D^L_{M2}+D^L_{M-2}\right)(B^{-1})^{\rm in}_{L2}+\frac{1}{\sqrt{2}}\left(D^L_{M4}+D^L_{M-4}\right)(B^{-1})^{\rm in}_{L4}, \tag{7}$$

where $(B^{-1})^{\rm in}_{LK}$ in general case depends on β and γ. We see that only $(B^{-1})^{\rm in}_{00}$ contributes to (5). In the case of axial symmetry, when we put $\gamma=0$ the components $(B^{-1})^{\rm in}_{L0}$ can be expressed through the inertia coefficients for β and γ motion, and the rotational inertia coefficient [57]:

$$\frac{1}{B_\beta}=(B^{-1})^{\rm in}_{00}-\sqrt{\frac{10}{7}}(B^{-1})^{\rm in}_{20}+3\sqrt{\frac{2}{7}}(B^{-1})^{\rm in}_{40}, \tag{8}$$

$$\frac{1}{B_\gamma}=(B^{-1})^{\rm in}_{00}+\sqrt{\frac{10}{7}}(B^{-1})^{\rm in}_{20}+\frac{1}{2}\sqrt{\frac{2}{7}}(B^{-1})^{\rm in}_{40}, \tag{9}$$

$$\frac{1}{B_{\rm rot}}=(B^{-1})^{\rm in}_{00}-\frac{1}{2}\sqrt{\frac{10}{7}}(B^{-1})^{\rm in}_{20}-2\sqrt{\frac{2}{7}}(B^{-1})^{\rm in}_{40}. \tag{10}$$

We obtain from (8)–(10) that

$$(B^{-1})^{\rm in}_{00} = \frac{2}{5}\frac{1}{B_{\rm rot}} + \frac{2}{5}\frac{1}{B_\gamma} + \frac{1}{5}\frac{1}{B_\beta}. \quad (11)$$

Substituting (11) and the relation $B(E2; 0_1^+ \to 2_1^+) = q^2\beta_2^2$, which is, in fact, an experimental definition of β_2, into (6) we obtain

$$E(2_1^+) = \hbar^2 \frac{1}{\beta_2^2}\left(\frac{2}{5}\frac{1}{B_{\rm rot}} + \frac{2}{5}\frac{1}{B_\gamma} + \frac{1}{5}\frac{1}{B_\beta}\right). \quad (12)$$

The cranking model expression for the inertia coefficients B_β, B_γ, and $B_{\rm rot}$ in the case of the single particle Hamiltonian with Woods-Saxon potential are

$$B_{\rm rot} = 2\hbar^2 R_0^2 \sum_{s,t} \frac{\left|\langle s|\frac{dV}{dr}\frac{1}{\sqrt{2}}(Y_{21}+Y_{2-1})|t\rangle\right|^2[\varepsilon_s\varepsilon_t - (E_s-\lambda)(E_t-\lambda) - \Delta_s\Delta_t]}{2\varepsilon_s\varepsilon_t(\varepsilon_s+\varepsilon_t)^3}, \quad (13)$$

$$B_\gamma = 2\hbar^2 R_0^2 \sum_{s,t} \frac{\left|\langle s|\frac{dV}{dr}\frac{1}{\sqrt{2}}(Y_{22}+Y_{2-2})|t\rangle\right|^2[\varepsilon_s\varepsilon_t - (E_s-\lambda)(E_t-\lambda) + \Delta_s\Delta_t](\varepsilon_s+\varepsilon_t)}{2\varepsilon_s\varepsilon_t\left((\varepsilon_s+\varepsilon_t)^2-\omega_\gamma^2\right)^2}, \quad (14)$$

$$B_\beta = 2\hbar^2 R_0^2 \sum_{s,t} \frac{\left|\langle s|\frac{dV}{dr}Y_{20}|t\rangle\right|^2[\varepsilon_s\varepsilon_t - (E_s-\lambda)(E_t-\lambda) + \Delta_s\Delta_t](\varepsilon_s+\varepsilon_t)}{2\varepsilon_s\varepsilon_t\left[(\varepsilon_s+\varepsilon_t)^2-\omega_\beta^2\right]^2}, \quad (15)$$

where E_s is the single particle energy, λ is the Fermi energy, ε_s is the single quasiparticle energy, Δ_s is the energy gap parameter depending on the single particle quantum number, and $\omega_\beta, \omega_\gamma$ are the energies of the β and γ phonons. By entering definitions

$$B_x \equiv 2\hbar^2 R_0^2 \Sigma_x \quad (16)$$

where $x = {\rm rot}, \beta, \gamma$ and substituting (16) into (12) we obtain

$$E(2_1^+) = \frac{1}{2\beta_2^2 R_0^2}\left(\frac{2}{5}\frac{1}{\Sigma_{\rm rot}} + \frac{2}{5}\frac{1}{\Sigma_\gamma} + \frac{1}{5}\frac{1}{\Sigma_\beta}\right), \quad (17)$$

where Σ_β, Σ_γ, and $\Sigma_{\rm rot}$ are the sums in Eqs. (13)–(15).

III. MODEL AND RESULTS

As it is seen from (13)–(15) in order to calculate the quantities $\Sigma_{\rm rot}$, Σ_γ, and Σ_β presented in the expression for $E(2_1^+)$ we need in the single particle and single quasiparticle energies matrix elements of the single particle operators and the energies of β and γ vibrations. All these quantities can be calculated in the framework of the quasiparticle phonon model (QPM) [58–63]. Although this method is not self-consistent it provides a sufficiently powerful tool for extensive calculations and predictions.

The Hamiltonian of QPM used below has the following structure:

$$H = H_{\rm sp} + H_{\rm pair} + H_M. \quad (18)$$

The mean field potential $V_{\rm sp}$ in $H_{\rm sp}$ contains the central potential $V_{\rm WS}$ in the Woods-Saxon form for the neutrons and protons, the spin-orbit part $V_{\rm so}$, and the Coulomb field $V_{\rm C}$ for protons:

$$V_{\rm sp} = V_{\rm WS} + V_{\rm so} + V_{\rm C}, \quad (19)$$

where

$$V_{\rm WS} = -V_0(1+\exp[(r-R(\theta,\varphi))/a])^{-1}. \quad (20)$$

Here the axially deformed form of the Woods-Saxon potential is assumed:

$$R(\theta,\varphi) = R_0\left(1+\beta_0+\sum_{\lambda=2,4}\beta_\lambda Y_{\lambda,0}(\theta,\varphi)\right), \quad (21)$$

where $R_0 = r_0 A^{1/3}$. The parameters of the potential are given in [64].

The term $H_{\rm pair}$ describes the monopole pairing forces with the strength set to reproduce the odd-even mass differences. After Bogoliubov transformation, we obtain the Hamiltonian in terms of the quasiparticle creation and annihilation operators.

The term H_M in (18) describes the multipole interaction of quasiparticles. The separable forces expressed through the operators of the multipole moments are used as the residual interaction,

$$H_M = -\frac{1}{2}\sum_{l,\mu}\sum_{\tau,\rho_\tau=\pm1}\left(\kappa_0^{(l\mu)} + \rho_\tau\kappa_1^{(l\mu)}\right)M^+_{l\mu}(\tau)M_{l\mu}(\tau). \quad (22)$$

Here τ denotes neutrons or protons. The isoscalar $\kappa_0^{(l\mu)}$ and isovector $\kappa_1^{(l\mu)}$ constants depend on angular momentum and projection μ on the symmetry axis. The choice of their values was justified in [49,59,65]. We have used the set of interaction constants suggested for the region of heavy nuclei [65]. H_M generates phonon excitations in nuclei.

Using single particle wave functions and single particle energies of the Hamiltonian $H_{\rm SP}$ with Woods-Saxon potential, u-v coefficients of the Bogoliubov transformation, the values of Δ_ν and the single quasiparticle energies calculated taking into account $H_{\rm pair}$, as well as the energies of the β and γ vibrations obtained using H_M, we can calculate $\Sigma_{\rm rot}$, Σ_γ, and Σ_β necessary to find $E(2_1^+)$ using the relation (17).

Below, we use the relation (17) to predict the energies of 2_1^+ states of a series of superheavy nuclei with proton numbers from 100 to 120. As an example, we take a chain of even-even nuclei from $^{256}_{100}$Fm to $^{296}_{120}$X, which differ from each

TABLE I. The predicted energies of the 2_1^+ states. Calculations are based on the microscopic variant of the Grodzins relation (17). The variants [A] and [B] are calculated with the parameters obtained using Strutinsky procedure and the single particle level scheme described in the text. These variants differ in the values of parameters of the spin-orbit part of the single particle potential. The variants [Kowal] and [Möller] are calculated with deformation parameters taken from [68] and [69], correspondingly.

Nucleus	β_2 [A]	$E(2_1^+)$ (keV)	β_2 [B]	$E(2_1^+)$ (keV)	β_2 [Kowal]	$E(2_1^+)$ (keV)	β_2 [Möller]	$E(2_1^+)$ (keV)
^{256}Fm	0.279	44	0.266	49	0.25	58	0.240	66
^{260}No	0.287	42	0.267	49	0.25	53	0.242	57
^{264}Rf	0.275	43	0.249	51	0.24	61	0.232	70
^{268}Sb	0.263	34	0.252	37	0.23	39	0.232	38
^{272}Hs	0.231	75	0.235	72	0.23	73	0.221	76
^{276}Ds	0.232	89	0.224	95	0.21	100	0.210	101
^{280}Cn	0.181	86	0.180	87	0.19	83	0.086	507
^{284}Fl	0.139	217	0.173	141	0.15	140	0.064	934
^{288}Lv	−0.137	202	−0.137	185	−0.12	256	0.075	433
^{292}Og	0.083	532	0.074	523	0.08	433	0.075	480
^{296}120	−0.102	176	−0.102	168	0.09	324	0.075	384

other in the number of α particles. According to numerous calculations, these nuclei include both highly deformed nuclei and spherical (or close to spherical) nuclei. Due to this reason, for our purpose it is convenient to use the Grodzins relation, since its use is not limited to any particular shape of nuclei. The practice of using it in the case of well studied nuclei has confirmed it.

Table I shows the results of calculations of the energies of the first 2_1^+ states of nuclei from the selected chain.

Columns 2–5 show the results of calculations based on the Hamiltonian QPM with Woods-Saxon potential described above and quadrupole deformations obtained using the Strutinsky method [66,67]. Thus, these deformations correspond to a minimum of the potential energy surface. The two variants of the calculations indicated in Table I as [A] and [B] differ in the values of the parameters of the spin-orbital part of the Woods-Saxon potential. The results presented in columns 6–9 are obtained using the same single particle level scheme as above, however, with the values of the quadrupole deformation β_2 taken from [68] (denoted as [Kowal]) and from [69] (denoted as [Möller]). Thus, in these two cases equilibrium deformations are not determined self-consistently with the single particle level scheme used for calculations of the inertia coefficient. However, this gives us a possibility to check a sensitivity of the obtained results to variations in deformation parameters. In addition to the quadrupole deformation each nucleus in Table I is also characterized by the value of the hexadecopole deformation which is not indicated. This can lead to different values of $E(2_1^+)$ even if the value of β_2 and the parameters of the microscopic Hamiltonian are the same.

The results of calculations are illustrated also in Fig. 1. We see that qualitatively all four variants given in Table I are similar in the nature of the change with Z. At the beginning of the studied region at $Z = 100$–110, where quadrupole deformation is large, the energies of 2_1^+ states do not exceed 100 keV, i.e., correspond to rotational states. Then, with decrease in deformation, $E(2_1^+)$ rises sharply and reaches a maximum value of 400–900 keV in ^{284}Fl ([Möller]) or in ^{292}Og ([A], [B], [Kowal]), i.e., in nuclei with a minimal value of β_2. Clearly, this reflects the characteristics of the underlying single particle level scheme. As noted above, our predictions for nuclei with small deformation underestimate the values of $E(2_1^+)$. Thus, values of 400–900 keV should be considered as the lower boundary. Note that even in nuclei with $Z = 114$–120 the number of neutrons is far from the magic one $N = 184$. Note also that the use of the above microscopic model to calculate the characteristics of nuclei with a very small deformation requires justification. This applies especially to calculation for ^{284}Fl performed at $\beta_2 = 0.064$. This work, however, does not consider this issue.

In Fig. 2 are shown the results of the calculations obtained using Eq. (17), as well as the results obtained using the phenomenological formula (1). Since in (1) the coefficient on the right side of the equation also contains information

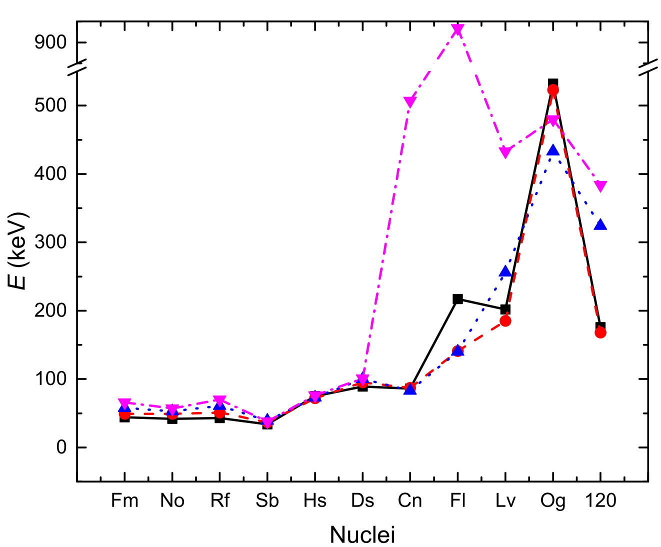

FIG. 1. The predicted energies of the 2_1^+ states for different nuclei. Calculations are based on the microscopic variant of the Grodzins relation (17) with different sets of quadrupole deformation. Solid line with squares (black): variant [A]; dashed line with circles (red): variant [B]; dot line with triangles (blue): variant [Kowal]; dash-dot line with inverted triangles (magenta): variant [Möller].

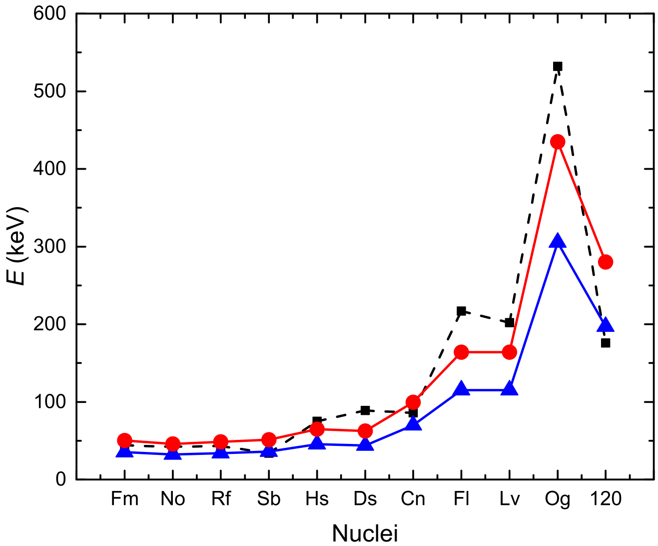

FIG. 2. The predicted energies of the 2_1^+ states for different nuclei. Calculations are performed for the microscopic variant of the Grodzins relation (17) (variant [A]) and the phenomenological Grodzins relation (1) [$E(2_1^+)_{\max}$ and $E(2_1^+)_{\min}$ with the proportionality coefficient 3.02 and 2.12, respectively]. Solid line with circles (red): $E(2_1^+)_{\max}$; solid line with triangles (blue): $E(2_1^+)_{\min}$; dashed line with squares (black): variant [A].

about the error of its definition, in Fig. 2 are shown two lines corresponding to the maximum $E(2_1^+)_{\max}$ and minimum $E(2_1^+)_{\min}$ values of this coefficient. In the calculations a set of deformation parameters β_2 given in the second column of Table I is used. It is seen from Fig. 2 that the results of calculations based on (17) go beyond the limits bounded by the lines corresponding to $E(2_1^+)_{\max}$ and $E(2_1^+)_{\min}$ in more than half of the cases.

IV. CONCLUSION

Based on the Grodzins relation derived using the Bohr collective Hamiltonian and the microscopical model of nuclear structure, the excitation energy of the first 2^+ states of the chain of even-even superheavy nuclei with Z from 100 to 120 are predicted. Calculations are performed for several sets of deformation parameter β_2 calculated by us or taken from the other publications. We see that for all sets of deformation parameters, at the beginning of the studied region of nuclei at $Z = 100$–110, where quadrupole deformation is large, the energies of the 2_1^+ states do not exceed 100 keV, i.e., correspond to rotational states. Then, with decrease in deformation, $E(2_1^+)$ rises sharply and reaches a maximum value in ^{284}Fl or in ^{292}Og, i.e., in nuclei with minimal values of β_2.

We note that our predictions for nuclei with small deformation underestimate the value of $E(2_1^+)$ because the proportionality coefficient in Grodzins relation should increase with deformation decrease. At the same time using the present microscopic model to calculate the characteristics of nuclei with very small deformation requires justification. This is important for nuclei around the magic or double magic ones for which mean square fluctuations of β_2 should be used instead of their equilibrium values.

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