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ADVANCED MICROSCOPIC **IBM1** VERSION.  
DESCRIPTION OF THE CROSSING OF BANDS  
IN Xe AND Th ISOTOPES

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Микроскопика расширенной версии IBM1. Описание пересечения полос в изотопах Хе и Тh

Использовано бозонное представление фермионных операторов. Описан метод вычисления параметров бозонных операторов на основе рассмотрения матричных элементов между фононными состояниями с минимальным числом последних. Конфигурационное пространство бозонов расширено вплоть до бозонов с мультипольностью  $J = 14^+$ . В рамках данного метода рассмотрен эффект бэкбендинга в четных изотопах  $^{112-128}\text{Xe}$ , где он ярко проявляется. В четных изотопах  $^{220-236}\text{Th}$ , где бэкбендинг наблюдается только для самого легкого из данных ядер, пересечение полос получено только для двух ядер. Причем для  $^{222}\text{Th}$  оно настолько плавное, что через момент инерции не проявляется. Из свойств рассмотрены энергии ирраст-полос и значения  $B(E2)$ .

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Advanced Microscopic IBM1 Version. Description of the Crossing of Bands in Xe and Th Isotopes

The boson representation of fermion operators is used. A method is described for calculating the parameters of boson operators based on consideration of matrix elements between phonon states with a minimum number of the latter. The configuration space of bosons is expanded up to bosons with multipole  $J = 14^+$ . Within the framework of this method, the effect of backbending in even isotopes  $^{112-128}\text{Xe}$  is considered, where it is clearly manifested. In even  $^{220-236}\text{Th}$  isotopes, where backbending is observed only for the lightest of these nuclei, the intersection of bands is obtained only for two nuclei. Moreover, for  $^{222}\text{Th}$  it is so smooth that it does not appear through the moment of inertia. Among the properties, the energies of the yrast bands and the values of  $B(E2)$  are considered.

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## INTRODUCTION

This paper outlines a theoretical scheme that makes it possible to implement a microscopic method for calculating the parameters of the boson operators of the Hamiltonian and  $E2$  transitions for even-even nuclei. This method is based on the use of elementary excitation modes and the interaction of their combinations with each other. This is one of the ways of boson representation of pair fermion operators. The first works in this field were those of Belyaev and Zelevinsky [1], where the condition was set for the equality of the commutators of fermion pairs on the one hand and the corresponding boson series on the other. This idea was the basis of Sorensen's work [2], the purpose of which consisted in a boson representation of fermion operators and, accordingly, a microscopic calculation of the properties of collective states in even-even nuclei. The next stage was associated with the works of Kishimoto and Tamura [3–6], where it was possible to formulate the requirements for the theory that are necessary for more correct description of the states under consideration. It was found that mapping onto bosons should be carried out not from individual quasiparticle pairs, but from phonons. It also turned out to be fundamental to take into account the connection between collective and non-collective excitation modes. By collective here we mean the quadrupole lowest  $D$  modes or phonons, and by non-collective all other  $B_J$  with  $J$  moments, among which there are giant resonances.

This connection was taken into account using the perturbation theory technique in the Brillouin–Wigner version [7] with separation of state spaces into two types. One consisted only of collective  $D$  phonons, the other contained additionally one of the other  $B_{J=2}$  phonons and only of the quadrupole type. This led to an effective boson Hamiltonian whose parameters are replaced with energy-dependent renormalized values. Using the example of specific calculations, it was shown that taking this connection into account is necessary to obtain a quantitative description of collective states.

The most widely used approach to describing collective states at present is a model derived from a finite representation of phonon operators in terms of boson ones. Such a representation, based on the assumption that the algebra of phonon operators  $D_\mu^+$ ,  $D_\mu$ ,  $[D_{\mu 1}, D_{\mu 2}^+]$  is closed, numbering thirty five elements, was done in the works of Jolos, Janssen, Donau [8–11], which is implemented through  $SU(6)$  algebra. Mapping phonon operators to boson

ones was carried out in such a way that the boson operators formed the same closed  $SU(6)$  algebra. This algebra is characterized by the maximum possible number of lowest quadrupole phonons  $\Omega$ . It was assumed that the use of only the lowest quadrupole phonons could lead to correct values of the parameters of boson operators. In addition to the problem of calculating boson parameters, it turned out that this the model is convenient from a phenomenological point of view, that is, the selection of the parameter values that provide the best description of the energies of collective states and the probabilities of  $E2$  transitions between them. This way of describing collective states in nuclei will be called the IBM phenomenology.

An essentially similar model, but in terms of two types of bosons, quadrupole ( $d$ ) and scalar ( $s$ ), was proposed in the works of Arima and Iachello [12]. The maximum number of quadrupole bosons  $\Omega$  becomes the total number of quadrupole and scalar bosons, and its operator  $\widehat{\Omega} = s^+s + \sum d_\mu^+d_\mu$  commutes with all generators of the  $SU(6)$  algebra of operators  $d_\mu^+s$ ,  $s^+d_\mu$ ,  $d_{\mu 1}^+d_{\mu 2}$ . The emphasis in recent works was on the algebraic properties of the corresponding combinations of boson operators due to the fact that the model described both the vibrational and rotational nature of the spectra. The model has become widely used as a way to describe the properties of collective states, including energies and probability of transitions, demonstrating significant success in doing so. In the work of Arima and Iachello, it received the generally accepted name of the Interacting Boson Model (IBM) or IBM1, which considers the interaction of states constructed from ideal bosons that do not differ in isospin, which were identified with nucleon pairs bound at  $J^\pi = 0^+$  and  $J^\pi = 2^+$  moments.

From an algebraic point of view, the use the operational roots  $\sqrt{\Omega - \widehat{n}_d}$  ( $\widehat{n}_d = \sum d_\mu^+d_\mu$ ) in [8–10] and  $s$  bosons is equivalent. The appearance of roots is associated with the method of obtaining a closed algebra of boson operators, and in addition it can be simultaneously considered as an approximate method of taking into account the Pauli principle. With this interpretation,  $s$  bosons are a formal instrument and do not correspond to pairs of quasiparticles or particles bound at the zero moment. This is what distinguishes the approach presented in [8] and [12].

In accordance with the conclusions of the works of Kishimoto and Tamura, in order to successfully calculate the parameters of the collective boson model describing quadrupole-type states, it is necessary to take into account non-collective excitation modes. Our estimates have shown that, in addition to quadrupole and hexadecapole excitations, it is necessary to consider two-quasiparticle pairs with moments  $J^\pi = 2^+, 4^+, 6^+$ , i.e.,  $B_2$ ,  $B_4$ , and  $B_6$  phonons. Taking these phonons into account provides corrections to the model parameters obtained only taking into account collective  $D$  phonons. These amendments cannot be neglected. We will call this procedure the renormalization of values of IBM1 parameters.

The first attempt to take into account non-collective excitation modes when renormalizing boson parameters was carried out for Se [13] isotopes, as well

as in calculations for  $^{126}\text{Ba}$  [14], isotones with  $N = 70$  [15], isotopes  $\text{Te}$  [16] and  $\text{Xe}$  [17].

Extension of the basis of excitations due to explicit consideration of bosons with spins  $J^\pi \geq 8^+$  leads to the possibility of describing states with higher spins than is possible when using standard versions of IBM1.

There are only a few works that use the boson approach to describe the intersection of a collective band with a band based on a two-quasiparticle high-spin mode. The first of these was the work of Gelberg and Zemel [18] based on IBM1, where the Hamiltonian term responsible for the interaction of the collective and non-collective bands was replaced with a constant and did not depend on either the spin of the pair of quasiparticles  $J$  or the total spin of the  $I$  states. It was naturally assumed that the limiting value is  $J^\pi = 8^+$  for the case of  $\text{Kr}$ ,  $\text{Sr}$  isotopes with a quasiparticle configuration  $g_{9/2}^2$  and  $J^\pi = 10^+$  for the case of isotopes  $\text{Xe}$ ,  $\text{Ba}$ ,  $\text{Ce}$ , etc. with configuration  $h_{11/2}^2$ . In [19], collective states were considered in the IBM2 approximation, and the interaction of collective and quasiparticle excitation modes was considered sequentially through a long chain of matrix elements, in such a way that first the number of collective states, determined by the superposition of  $d$  bosons, is associated with the state containing a pair of quasiparticles with  $J^\pi = 4^+$ . The latter state, in turn, is associated with a state containing a pair of quasiparticles with  $J^\pi = 6^+$  and so on. As a result, to couple a collective mode with a mode containing a pair of quasiparticles with  $J^\pi = 10^+$ , fourth-order perturbation theory will be required. As a result, in such a model, one band is replaced with a quasiparticle one, practically without mixing them, or in the case of a degenerate position of different modes, a strong mixing of 50% is realized with one single spin of the yrast band. This obviously affects the calculated values of  $B(E2)$  along the yrast bands. In this work, the nuclei  $^{126-128}\text{Ba}$  and  $^{130-134}\text{Ce}$  are considered, and the results demonstrate these statements. These studies did not receive further development. In [20], using IBM1, the space was also expanded due to bosons up to  $J^\pi = 10^+$ , but the parameters of the interaction terms of collective states with states including quasiparticle pairs were calculated microscopically. In this case, it was possible to reduce the interaction order to two for communication with states including pairs with  $J^\pi = 10^+$ . However, even in this case, it was not possible to obtain a strong interaction between collective states and states containing non-collective excitation modes, regardless of the energies of the latter. This indicated that the mixing of bands with different excitation modes was insufficient. In this case, the parameters of the purely collective Hamiltonian were selected phenomenologically. This problem was solved in a series of works, the idea of which was outlined in more detail in [21]. It turned out that it is necessary to take into account the connection between high-spin quasiparticle modes and states that also contain quasiparticles, but are used in renormalization of microscopically calculated parameters of the traditional IBM1 Hamiltonian. This is quite a wide range of configurations. A joint consideration of the processes associated with the renormalization of

boson parameters due to non-collective modes and the processes of coupling of various excitation modes with high-spin modes leads to strong mixing of states for several states at once in the region of intersection of bands and large values of  $B(E2)$ , regardless of the position of the energy of the quasiparticle high-spin couples. The exception is nuclei with the number of neutrons close to the closed shell, but this is also confirmed by experimental data for isotopes from Xe to Ce. In moving to heavy and superheavy nuclei, it became necessary to expand the two-quasiparticle basis of phonons and, accordingly, bosons to pairs with  $J^\pi = 12^+$  and  $14^+$ , which is associated with the single-particle levels  $j_{15/2}$  and  $i_{13/2}$ . For the first time such calculations were made in [22]. In this case, the interaction of a collective mode and a mode containing a pair with  $J^\pi = 14^+$  requires a third-order interaction.

The transition in the structure of excitations from the ground state band to a band built on a high-spin quasiparticle pair is experimentally observed by the change in the values of  $B(E2; I \rightarrow I - 2)$  with increasing spin and by the violation of monotonicity in the change in the energies of the yrast states. The most obvious picture illustrating the intersection of bands is the dependence of the effective moment of inertia  $\mathfrak{S} = (2I - 1)\hbar^2/E(I \rightarrow I - 2)$  on the square of the rotation frequency  $\hbar\omega = E(I \rightarrow I - 2)/(\sqrt{I(I + 1)} - \sqrt{(I - 2)(I - 1)})$ . In this case, irregularities in the curve  $\mathfrak{S}$  from  $\omega^2$ , especially the phenomenon of backbending, can indicate how quickly with increasing spin the transition in the yrast band from the collective state to the state including a high-spin phonon mode occurs.

The present work, based on the approach presented in [21] and [22], offers calculation results for Xe isotopes, previously presented in abbreviated form in [23], as well as new calculation results for even Th isotopes in which excitation energies are known. These are nuclei in the  $^{220-236}\text{Th}$  range. The first of them has an almost ideal vibration spectrum and a first excitation energy of 373 keV. The latter, respectively, has an energy of 48 keV. The maximum observed excitation spin  $I^\pi = 30^+$  was obtained for  $^{232}\text{Th}$ , and in the same nucleus the values of  $B(E2)$  were measured almost to the end of the yrast band. A preliminary analysis of the excitation energies showed that it is possible to reproduce well the energies up to the maximum known spins, and these are, respectively,  $22^+$ ,  $26^+$ ,  $18^+$ ,  $20^+$ ,  $22^+$ ,  $24^+$ ,  $30^+$ ,  $24^+$ ,  $10^+$ . In nuclei with  $A = 224, 230, 232$  for the last one or two states with extremely observable spins, the energy values obtained within the phenomenology of IBM1 turn out to be somewhat underestimated. In this regard, the question arises about the role of high-spin quasiparticle modes and their influence on the spectrum of observed states. For this purpose, appropriate calculations were made using the methodology presented in [22]. It turned out that in nuclei with  $A = 220, 222$  the intersection of the bands occurs, but very smoothly, so that for the second of these nuclei this does not affect the dependence of the moment of inertia on the square of the frequency. For heavier thorium isotopes, the band energies are significantly reduced, but the

main component remains collective. The reasons for this are discussed in this paper.

## 1. THEORETICAL CALCULATION OF PARAMETERS IN THE MICROSCOPIC VERSION OF IBM1

**1.1. Construction of the variational functional, determining phonon amplitudes.** Phonons that are not collective, that is, all phonons of arbitrary multipolarity except for  $D$  phonons, are determined through the quasiparticle Tamm–Dankov method:

$$B_{\mu}^{(J)+}(i) = \frac{1}{\sqrt{2}} \sum_{1,2;\tau=n,p} [\psi_{12}^{(J)}(i)a_1^+ a_2^+]_{\tau}(j_1 j_2 m_1 m_2 | 2\mu), \quad (1)$$

using only multipole isoscalar forces.

The elementary excitation mode, corresponding to the lowest quadrupole excitation –  $D$  phonon, is formally defined in the same way as is done within the QRPA (quasiparticle random phase approximation):

$$D_{\mu}^+ = \frac{1}{\sqrt{2}} \sum_{1,2;\tau=n,p} [\psi_{12} a_1^+ a_2^+ + \varphi_{12} a_{\bar{2}} a_{\bar{1}}]_{\tau}(j_1 j_2 m_1 m_2 | 2\mu), \quad (2)$$

where  $a^+(a)$  are operators of creation (annihilation) of quasiparticles; 1, 2 denote the numbers of single-quasiparticle states in the spherical basis; states  $\bar{1}, \bar{2}$  are time-conjugated to 1, 2. Amplitudes  $\psi_{12}$ ,  $\varphi_{12}$  or  $z^{(0)} = \psi + \varphi$ ,  $z^{(1)} = \psi - \varphi$  do not depend on magnetic quantum numbers and are normalized in a standard way,  $\sum_{1,2;\tau=n,p} (\psi_{12}^2 - \varphi_{12}^2) = \sum_{1,2;\tau} (z_{12}^{(0)} z_{12}^{(1)})_{\tau} = 1$ .

However, the amplitudes  $\psi$  and  $\varphi$  are determined from the variational principle using a complex functional that includes additional conditions that are absent in the traditional QRPA.

When justifying the final expansion [8, 9] of phonon operators in terms of boson operators, an assumption is made about the closedness of algebras of phonon operators. Namely, the operators  $D_{\mu}^+$ ,  $D_{\mu}$ ,  $[D_{\mu 1}, D_{\mu 2}^+]$ , thirty-five elements in number, form a closed  $SU(6)$  algebra. This is done provided

$$[[D_{\mu 1}, D_{\mu 2}^+], D_{\mu 3}^+] = -\frac{1}{\Omega} (\delta_{\mu 1, \mu 2} D_{\mu 3}^+ + \delta_{\mu 1, \mu 3} D_{\mu 2}^+), \quad (3)$$

which allows us to obtain an estimate for the value of the maximum number of bosons  $\Omega$ :

$$\begin{aligned} \frac{1}{\Omega} &= -\frac{1}{6} \sum_{\mu} \text{q.p.} \left\langle \left| \left[ D_{\mu 1}, [[D_{\mu}, D_{\mu}^+], D_{\mu 1}^+] \right] \right| \right\rangle_{\text{q.p.}} = \\ &= \frac{5}{3} \sum_{123} \frac{1}{2j_2 + 1} z_{12}^{(0)} z_{12}^{(1)} \left( z_{23}^{(1)2} + z_{23}^{(0)2} \right), \quad (4) \end{aligned}$$

where  $|\rangle_{\text{q.p.}}$  denotes quasiparticle vacuum. Mapping of phonon operators onto ideal boson structures is carried out from the requirement that the

commutators of phonon operators in the vacuum of quasiparticles be equal to the corresponding commutators of boson operators. This leads to a closed algebra with respect to bosons if the correspondence rules are satisfied:

$$D_\mu^+ \longrightarrow \frac{1}{\sqrt{\Omega}} d_\mu^+ s, \quad | \rangle \longrightarrow \frac{1}{\sqrt{\Omega!}} (s^+)^{\Omega} | \rangle, \quad | I \rangle \longrightarrow | I \rangle, \quad (5)$$

where  $| \rangle$  is phonon vacuum,  $| I \rangle$  is phonon state with spin  $I$ ,  $| \rangle$  is boson vacuum,  $| I \rangle$  is boson collective state with spin  $I$ . In this case, the ground state  $| 0 \rangle$  with spin  $0_1^+$  in the boson representation is not a vacuum of bosons, i.e.,  $| 0 \rangle \neq | \rangle$ , and similarly for phonons  $| 0 \rangle \neq | \rangle$ . These compliance rules are adopted in this work.

The used interpretation of  $s$  bosons as formally introduced objects leads to the fact that interaction terms for  $s$  bosons ( $s^+s$  and  $s^+s^+ss$ ) should not be introduced, and the IBM1 Hamiltonian with respect to the vacuum energy of  $d$  bosons in normal order in operators has the form

$$H_{\text{IBM}} = \varepsilon_d \hat{n}_d + k_1 (d^+ \cdot d^+ s s + \text{H.c.}) + k_2 \left( (d^+ d^+)^{(2)} \cdot d s + \text{H.c.} \right) + \frac{1}{2} \sum_L C_L (d^+ d^+)^{(L)} \cdot (d d)^{(L)}, \quad (6)$$

where H.c. means Hermitian conjugation, the point between the operators corresponds to the scalar product, and the quantities  $\varepsilon_d$ ,  $k_1$ ,  $k_2$ ,  $C_0$ ,  $C_2$ ,  $C_4$  are parameters of the IBM1 Hamiltonian.

All parameters of boson operators, which determine both the Hamiltonian and the operator of electric quadrupole transitions, are calculated based on the mapping of fermion operators  $O_F$  to  $O_B$  operators in the ideal boson representation through the Marumori procedure [24]. This is implemented in such a way that the equality

$$\langle I' | O_F | I \rangle = \langle I' | O_B | I \rangle$$

is satisfied. This allows us to find the parameters of each term of any operator separately for both the boson Hamiltonian and the  $E2$ -transition operator. When calculating the parameters, in order to ensure that among the fermion states  $| I \rangle$  there were no nonphysical components, states were considered that would not contain components with more than two  $D$  phonons. Therefore, the parameters of the boson Hamiltonian, taking into account the minimum number of  $D$  phonons only, which corresponds to the index  $(0)$ , are defined as

$$\varepsilon_d^{(0)} = \langle [D_\mu, [h_{\text{RPA}}, D_\mu^+]] \rangle, \\ 2 \left( k_1 \sqrt{\Omega(\Omega-1)} \right)^{(0)} = \frac{1}{5} \sqrt{\frac{2}{N_0}} \sum_\mu \langle [ [h_{\text{RPA}}, D_\mu^+], D_\mu^\pm ] \rangle,$$



$$(k_2\sqrt{\Omega-1})^{(0)} = \frac{1}{\sqrt{2\aleph_2}} \sum_{m_1, m_2} \langle |[[[D_M, H_{20+02} + \widehat{V}_{31+13}], D_{m_1}^+, D_{m_2}^+]] \rangle \times \\ \times (22m_1m_2|2M), \quad (7)$$

$$C_L^{(0)} = \sum_{m_1, m_2, m_3, m_4} \frac{1}{\aleph_L} \langle | [D_{m_2}, [D_{m_1}, [[h_{\text{RPA}}, D_{m_3}^+], D_{m_4}^+]]] \rangle \times \\ \times (22m_1m_2|LM)(22m_3m_4|LM).$$

Here  $\aleph_L = \langle |DD(D^+D^+)^{(L)}| \rangle$  is normalization of the two-phonon state, and the quasiparticle Hamiltonian of the QRPA approximation is defined as  $h_{\text{RPA}} = H_{11} + \widehat{V}_{22} + \widehat{V}_{40+04}$ , where the corresponding indices denote the number of quasiparticle creation and annihilation operators. Expressions for boson parameters in terms of phonon amplitudes using the factorized [25] quasiparticle residual interaction in the particle-hole and partial-particle channels are given in [21] and [26].

One of the elements of the minimized functional is the phonon vacuum energy  $E_0^{(B)}$ , associated with correlations in the ground state. The expression for it, taking into account the forces in the partial-particle and partial-hole channels, is given in [21] (Eq.(26)). When using the standard version of QRPA, taking into account the completeness of phonon functions and up to a constant relative to phonon amplitudes,  $E_0^{(B)}$  in the varied functional can be replaced with  $5/2\varepsilon_d^{(0)}$ , although there is some simplification.

The main part of the minimized functional, oriented to IBM1, is obtained by averaging the boson Hamiltonian (6) with parameters from (7) over arbitrary boson functions  $|I\rangle - (I|H_{\text{IBM}}|I)$ . This functional will depend on internucleon forces, phonon amplitudes  $\psi$ ,  $\varphi$  and boson averages from individual boson operators of the Hamiltonian (6). In particular,

$$n_d(I) = \left( I \left| \sum_{\mu} d_{\mu}^+ d_{\mu} \right| I \right), \quad (8)$$

$$P_1(I) = \frac{1}{2\sqrt{\Omega(\Omega-1)}} (I | (d^+ \cdot d^+ s s + s^+ s^+ d \cdot d) | I).$$

The arbitrary boson wave function in the basis of vibration limit functions to IBM1 –  $SU(5)$  – has the form

$$|I\rangle = \sum_{n_d, v, \omega_{\Delta}} \alpha_d(n_d, v, \omega_{\Delta}, I) \frac{1}{\sqrt{(\Omega - n_d)!}} (s^+)^{\Omega - n_d} |n_d, v, \omega_{\Delta}, I\rangle, \quad (9)$$

where  $|n_d, v, \omega_{\Delta}, I\rangle$  are normalized functions of quadrupole bosons corresponding to the irreducible representation of the  $SU(5)$  group with quantum numbers: number of quadrupole bosons ( $n_d$ ), boson seniority ( $v$ ), i.e., number of quadrupole bosons not bound at zero angular momentum, and number of triplets  $v$  bound at zero angular momentum ( $\omega_{\Delta}$ ). The amplitudes

of this function, in turn, depend on  $(\psi, \varphi)$  and  $(u, v)$  through the parameters  $\varepsilon_d, k_1, k_2, C_0, C_2, C_4$  of the IBM1 Hamiltonian (6). When minimizing the functional (10) in the boson average  $\langle I|H_{\text{IBM}}|I\rangle$ , we will keep two terms, associated with the parameters  $\varepsilon_d$  and  $k_1$ .

The use of the functional  $\langle I|H_{\text{IBM}}|I\rangle$  already implies the presence in the boson Hamiltonian (6) of a term proportional to  $k_1$ , which is absent in the standard QRPA.

If the constructed functional is also used to determine the Bogolyubov parameters of superfluidity  $u$  and  $v$ , then the vacuum energy of quasiparticles  $E_{\text{vac.q.p.}}$  should be added to it, which is clearly independent of the phonon amplitudes. Thus, the energy part of the functional has the form

$$\Phi_E = E_{\text{vac.q.p.}} + E_0^{(B)} + \langle I|H_{\text{IBM}}|I\rangle. \quad (10)$$

Minimization of the functional (10) based on the desired amplitudes is carried out when a number of additional conditions are met. The first of them take into account the presence of normalizations. These include the normalization of  $D$  phonons, normalization of the amplitudes of boson wave functions  $|I\rangle$ , and the condition on the Bogolyubov amplitudes  $u$  and  $v$ .

The following conditions are not related to normalizations of functions. Since the work uses a quasiparticle representation, the conservation of the number of particles on average is realized using chemical potentials  $\lambda_\tau$ , which will depend on both the number of quadrupole bosons and phonon amplitudes. That is, the average number of particles also depends on the presence of phonons. This is a feature of the theory when explicitly considering multiphonon or multiboson states. That is why the corresponding Lagrange term is essential to enter into the phonon problem. Let's look at this statement in more detail.

The mapping of the quasiparticle number operator  $\hat{n}_i$  onto boson operators is also used in calculating the average values of the numbers of protons and neutrons  $\langle I|\hat{N}_\tau|I\rangle = N_{\tau=p,n}$ , fixation of which gives an equation for determining the chemical potentials  $\lambda_\tau$ . The operator of the number of particles when passing to a quasiparticle representation, with a number of simplifications, has the form  $\hat{N}_\tau = \sum_j (2j+1)v_j^2 + \sum_j (u_j^2 - v_j^2)\hat{n}_j$ ;  $\hat{n}_j = \sum_m a_{jm}^\dagger a_{jm}$ . Average over phonon functions from the number operator of quasiparticles  $a_{jm}^\dagger a_{jm}$  is defined as

$$\langle I|a_{jm}^\dagger a_{jm}|I\rangle = \frac{1}{2}(1 - y_j), \quad \langle I|1 - a_{jm}^\dagger a_{jm} - a_{j\bar{m}}^\dagger a_{j\bar{m}}|I\rangle = y_j. \quad (11)$$

Passing to boson averages gives

$$y_j = 1 - 2 \left( n_j^{(1)} n_d(I) + n_j^{(2)} P_1(I) \right), \quad (12)$$

where

$$n_i^{(n)} = \frac{1}{2j_i + 1} \sum_s \left( z_{is}^{(1)2} - (-1)^n z_{is}^{(0)2} \right), \quad n = 1, 2. \quad (13)$$

Thus, the average of the number of particles through boson averages is equal to

$$\begin{aligned} \langle I | \widehat{N}_\tau | I \rangle &\rightarrow (I | \widehat{N}_\tau | I) = N_\tau = \\ &= \sum_j (2j + 1) \left( v_j^2 + (1 - 2v_j^2) \left( n_j^{(1)} n_d(I) + n_j^{(2)} P_1(I) \right) \right) = \\ &= \sum_j (2j + 1) \left( y_j v_j^2 + \frac{1 - y_j}{2} \right), \quad (14) \end{aligned}$$

where  $n_d(I)$  and  $P_1(I)$  are defined in (8); in particular,  $n_d(I)$  is the average number of quadrupole bosons in the boson state  $|I\rangle$ . The factor  $y_j$  can be interpreted as a measure of the occupancy of a single-particle level by quasiparticles. For a level completely free of quasiparticles,  $y_j = 1$ ; for a completely occupied level,  $y_j = 0$ . Otherwise,  $y_j$  is considered as the probability that the level  $jlm$  is free from quasiparticles and through the number of latter ( $n_j$ ) at the level of the spherical field  $j$  is determined as follows:

$$y_j = (j + 1/2 - n_j) / (j + 1/2). \quad (15)$$

As the single-particle level is filled with quasiparticles, which happens as  $n_d$  increases, the values of  $y_j$  will decrease, but should not be negative, which is a condition for the Pauli principle to be satisfied on average. In this case, it lies in the fact that the number of quasiparticles at each single-particle level  $jl$  should not exceed the value  $j + 1/2$ . This is consistent with Eq. (15), since the value of  $y_j$  (12) will be positive. The Pauli principle is also fulfilled on average because the number of quasiparticles is calculated from those components that form the structure of the  $D$  phonon and corresponds to their average number  $n_d(I)$ , as well as the boson average  $P_1(I)$ .

If, as a result of the calculation, the values of  $y_j$  turn out to be negative, then it is necessary to reduce the correlations in the ground state, which will be discussed below. In this case, the phonon amplitudes  $\psi$  and  $\varphi$  will be distributed over a larger number of single-particle levels, increasing the role of extravalent shells. The expression for  $N_\tau$  (14) can be interpreted in such a way that at the  $j$  level, taking into account blocking, there will be  $(2j + 1)y_j v_j^2$  nucleons forming Cooper pairs and  $(2j + 1)(1 - y_j)/2$  unpaired nucleons. This leads to some change in the interpretation of the  $v_j^2$  values, but a similar situation occurs when a level is blocked by one or more nucleons.

With increasing excitation energy and spin, the boson averages change, which leads to a change in the average numbers of particles, determined by

the expression (14). Their invariance can be achieved by varying the values of the chemical potentials  $\lambda_\tau$ . As a result, chemical potentials change during the transition from one collective state to another. This circumstance should be taken into account when calculating excitation energies if self-consistent calculations are performed separately for each collective state.

Another condition reflecting the specificity of IBM1 is the fixation of  $\Omega$ , the maximum number of quadrupole bosons. The condition of invariance of  $\Omega$  when calculating the phonon amplitudes ( $\psi$ ,  $\varphi$ ) for each collective state leads to a slight decrease in the number of quasiparticles at the valence shell levels. This is important, since the maximum number of quasiparticles at each single-particle level cannot exceed the value  $(2j_i + 1)/2$ . The Lagrange term, which allows us to fix the integer value of  $\Omega$ , is taken in the form

$$\delta\Phi'(\omega') = \frac{6}{5} \frac{1}{\Omega(z^{(n)})} \omega'(n_d + 5/2),$$

where  $\Omega(z^{(n)})$  is a function (4) of phonon amplitudes,  $\omega'$  is the Lagrange multiplier, and the value  $(n_d + 5/2)$  is introduced for convenience.

When using the minimized functional (10), one can set the task of achieving self-consistency of all three amplitudes ( $z^{(n)}$ ,  $u(v)$ ,  $\{\alpha_d\}$ ). However, as it turned out, this is impossible when using the designed functionality, as well as when using the standard QRPA version, or the TD approximation. For self-consistency to become possible, it is necessary to set a condition for the regulation of correlations in the ground state. The fulfillment of this condition for fixed values of the force constants is carried out by introducing into the minimized functional an additional term that regulates the value of the sum of squares  $\varphi$ :

$$\Phi_\varphi = 2\chi \left( n_d(I) + \frac{5}{2} \right) \left( \sum_{\tau 12} \varphi_{12\tau}^2 + \frac{1}{2} \right) = \frac{1}{2} \chi \left( n_d(I) + \frac{5}{2} \right) \left( \sum_{\tau 12} (z_{12}^{(1)2} + z_{12}^{(0)2})_\tau \right), \quad (16)$$

where, as before, the factor  $(n_d + 5/2)$  is introduced for convenience. This term for the parameter  $\chi > 0$  leads to a decrease in correlations, as well as a decrease in the contribution of phonon amplitudes in the valence shell, automatically increasing their contribution from two-quasiparticle components outside the valence shell.

Thus, the functional  $\Phi'$  for the phonon problem, defined by all additional conditions, has the form

$$\begin{aligned} \Phi' = & -\omega \left( n_d(I) + 5/2 \right) \sum_{\tau 12} (z_{12}^{(1)} z_{12}^{(0)})_\tau - \sum_{\tau} \lambda_\tau N_\tau - \sum_{\tau, j} e_{\tau j} (u_j^2 + v_j^2)_\tau - \\ & - E_I \sum_{n_d, v, \omega_\Delta} \alpha_d^2(n_d, v, \omega_\Delta, I) + 2\omega' \sum_{\tau 12} (z_{12}^{(1)} z_{12}^{(0)} n_2^{(1)})_\tau \left( n_d(I) + 5/2 \right) + \\ & + \frac{1}{2} \chi \left( n_d(I) + 5/2 \right) \sum_{\tau 12} (z_{12}^{(1)2} + z_{12}^{(0)2})_\tau, \quad (17) \end{aligned}$$

where  $E_I$  is the eigenvalue of the boson Hamiltonian.

It should be kept in mind that, unlike the standard QRPA, the Lagrange multiplier  $\omega$  does not have the meaning of phonon energy. The single-boson energy  $\varepsilon_d^{(0)}$  in Eqs.(7) acts as the phonon energy. In a number of cases, namely, for nuclei that are traditionally considered to be deformed, the single-boson energy becomes negative. Thus, the presented modification of the QRPA allows us to remove the problem of the collapse of the lowest collective mode at a force constant greater than the critical one.

To determine the phonon amplitudes, the minimized functional will have the form

$$\Phi = \langle I | \hat{H} - \sum_{\tau} \lambda_{\tau} \hat{N}_{\tau} | I \rangle + \Phi' = E_0^{(B)} + (I | H_{\text{IBM}} | I) + \Phi', \quad (18)$$

where a simplification is made that instead of the full Hamiltonian  $H_{\text{IBM}}$  in (18) its part is used, determined by the parameters  $\varepsilon_d^{(0)}$  and  $k_1^{(0)}$ , obtained only taking into account  $D$  phonons, and  $E_0^{(B)}$  is replaced with  $5/2\varepsilon_d^{(0)}$ . Thus,

$$E_0^{(B)} + (I | H_{\text{IBM}} | I) \rightarrow \varepsilon_d^{(0)} \left( n_d(I) + \frac{5}{2} \right) + 2 \left( k_1 \sqrt{\Omega(\Omega - 1)} \right)^{(0)} P_1(I) \quad (19)$$

and the minimized functional is taken in the form

$$\Phi = \varepsilon_d^{(0)} \left( n_d(I) + \frac{5}{2} \right) + 2 \left( k_1 \sqrt{\Omega(\Omega - 1)} \right)^{(0)} P_1(I) + \Phi'. \quad (20)$$

The role of the terms  $C_L^{(0)}$ , corrections  $\delta\varepsilon_d, \delta C_L$  to the corresponding parameters due to their renormalization in determining the amplitudes of phonons is reduced to the renormalization of the residual interaction constants and to additions to the two-quasiparticle energies included in equations for amplitudes. This justifies the concept of effective forces. Additions to two-quasiparticle energies turn out to be insignificant. When calculating boson averages, it is necessary to have correct values of boson parameters, and this is achieved after their renormalization by taking into account the connection of collective states constructed from  $D$  phonons with states containing one of the non-collective  $B$  phonons. Let's briefly look at the relevant processes.

**1.2. Renormalization of parameters.** To take into account the connection between collective (consisting only of  $D$  phonons) and non-collective (containing additionally one of the possible  $B_J$  phonons) spaces, the extended wave function

$$\Psi(I) = |\psi_c(I)\rangle + \sum_{i1,c1} \alpha_{i1,c1} |(B_{i1}^+ \psi_{c1})^{(I)}\rangle \quad (21)$$

is considered, where  $|\psi_c\rangle$  is a wave function containing a superposition of only  $D$  phonons and which will be called the collective state function.

The energies of the lowest states of yrast bands with  $I^{\pi} \leq 6^+$  turn out to be significantly lower than the energies of  $B_J$  modes, which are at

least greater than twice the pair gap. This separation of states by energy of two spaces allows us to consider their connection implicitly through the renormalization of boson parameters  $\varepsilon_d$ ,  $k_1$ ,  $k_2$ ,  $C_L$  (7), which was done in [13, 16, 17, 23] using perturbation theory in the Brillouin–Wigner (BW) variant. For this purpose, processes with a minimum number of  $D$  phonons are considered, which include the configurations  $| \rangle$ ,  $D^+ | \rangle$ ,  $D^+ D^+ | \rangle$ . Another set of configurations will additionally contain one of the positive parity  $B_J^+$  phonons with a  $J^\pi$  multipole from  $0^+$  to  $6^+$ .

Taking this interaction into account leads to the polarization of the phonon vacuum, the energy of which  $E_0$  relative to the energy of the quasiparticle-phonon vacuum  $E_0^{\text{(qp-ph)}}$  is found through the solution of the equation

$$-E_0 = R_0(E_0) + R_{01}(E_0),$$

where

$$R_0(E_0) = \sum_i \frac{|\langle H | B_{J=2,i}^+ D^+ \rangle|^2}{\omega_i + \varepsilon_d^{(0)} - E_0},$$

$$R_{01}(E_0) = \sum_{J,i} \frac{|\langle H | B_{J,i}^+ D^+ D^+ \rangle|^2}{\omega_i + 2\varepsilon_d^{(0)} + C_J^{(0)} - E_0},$$

where here and below  $J$  is the multipolarity of the phonon, and  $i$  is the index numbering phonons with a given multipolarity. The first ME denotes the interaction of a zero-phonon state with a state containing simultaneously two phonons —  $D$  and  $B_J$ , the latter phonon being also quadrupole. The presence of polarization of the phonon vacuum in the indicated sense is associated with the modification of the QRPA, which leads to the inequalities

$$\langle H(D^+ D^+)^{(0)} | \rangle \neq 0, \quad \langle H(D^+ B^+)^{(0)} | \rangle \neq 0. \quad (22)$$

The single-phonon energy  $E_1$ , taking into account the considered corrections, is determined from the equation

$$\varepsilon_d^{(0)} - E_1 = R_1(E_1) + R_2(E_1),$$

$$R_1(E_1) = \sum_{J,i} \frac{|\langle D | H | B_{J,i}^+ D^+ \rangle|^2}{\omega_i + \varepsilon_d^{(0)} - E_1},$$

$$R_2(E_1) = \sum_{\lambda,J,i} \frac{|\langle D | H | B_{J,i}^+ (D^+ D^+)_n^{(\lambda)} \rangle|^2}{\omega_i + 2\varepsilon_d^{(0)} + C_\lambda^{(0)} - E_1},$$

where  $\varepsilon_d^{(0)}$  is an estimate for the single-boson energy expressed in terms of the amplitudes of the  $D$  phonon only. In the case when the coherent production is a  $D$  phonon, the major role in the summation over  $B_J$  phonons is played by those phonons whose energies are minimal. If, on the contrary, the  $B_J$  phonon is the coherent production, then the phonons corresponding to the giant quadrupole resonance play a large role in the summation over them.

The equation for the renormalized two-phonon energy  $E_2^{(L)}$ , taking into account that the unperturbed energy is defined as  $2\varepsilon_d^{(0)} + C_L^{(0)}$ , has the form

$$2\varepsilon_d^{(0)} + C_L^{(0)} - E_2^{(L)} = R_3^{(L)}(E_2^{(L)}) + R_4^{(L)}(E_2^{(L)}) + R_5^{(L)}(E_2^{(L)}) + R_6^{(L)}(E_2^{(L)}),$$

$$R_k^{(L)}(E_2^{(L)}) = \sum_{\lambda, J, i} \frac{|\langle (DD)_n^{(L)} | H | B_{J,i}^+ ((D^+)^{k-3})^{(\lambda)} \rangle|^2}{\omega_i + E^{(k-3)} - E_2^{(L)}}, \quad k = 3, 4, 5, 6,$$

where  $E^{(0)} = 0$ ,  $E^{(1)} = \varepsilon_d^{(0)}$  is single-boson energy,  $E^{(2)} = 2\varepsilon_d^{(0)} + C_\lambda^{(0)}$  is two  $d$ -boson energy,  $E^{(3)} = E_{3\lambda}^{(0)}$  is the energy of the three  $d$ -boson state bound at the moment  $\lambda$  and obtained taking into account only the  $D$ -phonon amplitudes, and  $L = 0, 2, 4$  is multipolarity of the two-phonon triplet. When calculating ME  $\langle (DD)_n^{(L)} | H | B_{J,i}^+ ((D^+ D^+ D^+)^{(\lambda)}) \rangle$ , it is necessary to know three  $D$ -phonon normalization, which turned out to be noticeably less than three  $d$ -boson normalization. This is important for subsequent calculations. The index  $n$  for combinations of  $D$  phonons means their normalization.

Non-collective  $B_i$  phonons were considered in the Tamm–Dankov approximation; the technique of summation over them, which does not involve calculating the energies and amplitudes of phonons, was used earlier in [13] and is described in detail in [22].

From the energies found in this way, the values of the renormalized boson parameters of the Hamiltonian are found:

$$\tilde{\varepsilon}_d = E_1 - E_0, \quad C_L = E_2^{(L)} - 2E_1 + E_0. \quad (23)$$

These boson parameters turn out to depend on the spin and energy of the state under consideration. Usually, the renormalizations of the IBM1 parameters are associated with taking into account  $G$  phonons, i.e., quasiparticle pairs with  $J^\pi = 4^+$ . These calculations have shown that the main contribution is made by phonons with a moment equal to  $2^+$ , i.e., again quadrupole phonons, but those that do not belong to the lowest of them. Next in importance are phonons with moments of  $4^+$  and  $6^+$ . For the nuclei under study, the admixture of non-collective states to collective ones (one and two  $D$ -phonon states) turns out to be small. For one  $D$ -phonon state this impurity is  $\sim 9\%$ , for two-phonon states it is somewhat larger: for the state  $(D^+ D^+)^{(0)}$  this impurity is  $\sim 25\%$ , while for  $(D^+ D^+)^{(L=2,4)}$  it is  $\sim 15\%$ .

The found set of admixture amplitudes of non-collective components makes it possible to obtain second-order interaction corrections to the IBM1 parameters  $k_1$  and  $k_2$ . Since these parameters relate states with different numbers of  $d$  bosons, in the  $D$ -phonon space they will accordingly be determined by off-diagonal MEs. This leads to the fact that the resulting corrections for these parameters contain a more complex dependence on the energies of both phonons  $\omega_i$  and the Hamiltonian parameters  $\varepsilon_d^{(0)}$  and  $C_L^{(0)}$  than was the case when determining the parameters  $\varepsilon_d$  and  $C_L$ , which are determined by diagonal MEs.

The IBM1 Hamiltonian term, proportional to the  $k_1$  parameter, ensures the interaction of boson states that differ by two quadrupole bosons coupled at zero angular momentum. This leads to a decrease in correlations in the ground state compared to what the standard version of the QRPA produces. Its renormalization due to non-collective phonons is given by the expression

$$\begin{aligned}
\delta(2\kappa_1\sqrt{\Omega(\Omega-1)}) = & \\
= -\sqrt{\frac{2}{5}} \sum_i & \left\{ \langle |H|(B_{J=2,i}^+ D^+)^{(0)} \rangle \langle (DD)_n^{(0)} |H|(B_{J=2,i}^+ D^+)^{(0)} \rangle \times \right. \\
& \times \frac{x_1 - E_0 - E_2^{(L=0)}}{(x_1 - E_0) (x_1 - E_2^{(L=0)})} + \\
& + \sum_J \langle |H|(B_{J,i}^+ D^+ D^+)^{(0)} \rangle \langle (DD)_n^{(0)} |H|(B_{J,i}^+ D^+ D^+)^{(0)} \rangle \times \\
& \times \left. \frac{x_2 - E_0 - E_2^{(L=0)}}{(x_2 - E_0) (x_2 - E_2^{(L=0)})} \right\}, \\
x_1 = \omega_i + \varepsilon_d^{(0)}, \quad x_2 = \omega_i + 2\varepsilon_d^{(0)} + C_J^{(0)}.
\end{aligned}$$

After this, the parameter  $\kappa_1$  is defined as

$$\tilde{\kappa}_1 = \kappa_1^{(0)} + \delta\kappa_1. \quad (24)$$

The term of the boson Hamiltonian, proportional to the parameter  $\kappa_2$ , carries out the interaction of states that differ by one quadrupole boson. The eigenvalues of the boson Hamiltonian and the transition probabilities between them are invariant with respect to the sign of  $\kappa_2$ , but the signs of the quadrupole moments of the states depend on its sign. Thus, for yrast-band states,  $\text{sign}(Q(I)) = -\text{sign}(\kappa_2)$ . The calculated values of the quadrupole moments depend weakly on the  $e^* \chi_{E2}(d^+ d)^{(2)}$  part of the  $E2$ -transition operator:

$$\hat{T}(E2) = e^* (d^+ s + s^+ d + \chi_{E2} d^+ d)^{(2)} + e_0^* \left( s^+ (d^+ d)^{(0)} d + d^+ (d^+ d)^{(0)} s \right)^{(2)} \quad (25)$$

(a microscopic calculation of its parameters is presented in [27] taking into account  $B_J$  phonons only with  $J^\pi \leq 6^+$ ), without changing the number of  $d$  bosons. This leads to the fact that the values of the quadrupole moments of states are determined by the simultaneous presence in the state of components that differ by one quadrupole boson and the ME operator  $e^*(d^+ s + s^+ d)^{(2)}$ , which also changes the number of quadrupole bosons per unit. Therefore, the magnitudes of the quadrupole moments are, in principle, equally determined by both the proton and neutron structures of the  $D$  phonon. The estimate for  $\kappa_2^{(0)}$  presented in Eq. (7) includes the factor  $(u_1 u_2 - v_1 v_2)$ , which leads to a strong dependence of the resulting value on the details of the location



of the mean-field levels. For this parameter, as well as for others, the terms determined by the next order of interaction were taken into account. There are three such members for it; their origin is clear from the MEs below:

$$\begin{aligned}
\delta(2\kappa_2\sqrt{\Omega-1}) = & \\
= & -\frac{1}{\sqrt{2}} \sum_i \left\{ \sum_J \langle (DD)_n^{(2)} | H | B_{J,i}^+ D^+ \rangle \langle D | H | (B_{J,i}^+ D^+)^{(2)} \rangle \times \right. \\
& \times \frac{x_1 - E_1 - E_2^{(L=2)}}{(x_1 - E_1)(x_1 - E_2^{(L=2)})} + \\
& + \sum_{\lambda,J} \langle (DD)_n^{(2)} | H | B_{J,i}^+ (D^+ D^+)_n^{(\lambda)} \rangle \langle (DD)_n^{(\lambda)} B_{J,i} | H | D^+ \rangle \times \\
& \times \frac{x_2 - E_1 - E_2^{(L=2)}}{(x_2 - E_1)(x_2 - E_2^{(L=2)})} + \\
& + \sum_{\lambda,J} \langle (DD)_n^{(2)} | H | B_{J,i}^+ (D^+ D^+ D^+)_n^{(\lambda)} \rangle \langle (DDD)_n^{(\lambda)} B_{J,i} | H | D^+ \rangle \times \\
& \times \left. \frac{x_3 - E_1 - E_2^{(L=2)}}{(x_3 - E_1)(x_3 - E_2^{(L=2)})} \right\}, \\
x_1 = \omega_i + \varepsilon_d^{(0)}, \quad x_2 = \omega_i + 2\varepsilon_d^{(0)} + C_\lambda^{(0)}, \quad x_3 = \omega_i + E_{3\lambda}^{(0)}.
\end{aligned}$$

After this procedure, the  $\kappa_2$  parameter is determined as

$$\kappa_2 = \kappa_2^{(0)} + \delta\kappa_2. \quad (26)$$

It should be noted that corrections to the parameters  $\kappa_1$  and  $\kappa_2$  are not as significant as to  $\varepsilon_d$  and  $C_L$ , but they are important when one of the parameters, for example  $\kappa_2$ , turns out to be small according to the estimate obtained in first order by interaction.

### 1.3. Total energy and final parameters of the IBM1 Hamiltonian.

After determining all the required amplitudes, including boson ones, which characterize the boson composition of the functions, the numerical values of the energy of the states  $E_I$  are found:

$$E_I = E^{(\text{vac.q.p.})} + E_0^{(B)} + (I | H_{\text{IBM}} | I) + \sum_\tau \lambda_\tau (I | \hat{N}_\tau | I). \quad (27)$$

This approach is not, however, directly related to IBM1. The reason is that, due to the implicit dependence of  $u$ ,  $v$ ,  $z^{(\eta)}$  and  $\lambda$  on the energy and spin of the collective state, the energy of the quasiparticle-phonon vacuum ( $E^{(\text{vac.q.p.})} + E_0^{(B)}$ ) and parameters  $\tilde{\varepsilon}_d$ ,  $\tilde{k}_1$ ,  $k_2$ ,  $C_L$  change from state to state. At the same time, the analysis of the spectra of collective states within the IBM1 is carried out under the assumption that the vacuum energy of bosons and the parameters of the Hamiltonian remain unchanged for all states involved in

this analysis. Therefore, the question arises whether it is possible to rearrange the terms in  $E_I$  in such a way as to isolate a certain background part in the energy of the collective state, which does not change with increasing  $I$ , and an “active” part, similar to the IBM1 Hamiltonian, with slightly changing parameters  $\varepsilon_d$ ,  $k_1$ ,  $k_2$ ,  $C_L$  (all of these parameters now do not have an upper tilde).

To do this, we take the total energy, measured from  $\Sigma\lambda_{0\tau}N_\tau$  ( $\lambda_{0\tau}$  are chemical potentials for the ground state of the nucleus) in the form

$$E_I = \tilde{E}_I + (I|H_{\text{IBM}}(\tilde{\varepsilon}_d, \tilde{k}_1, k_2, C_L)|I), \quad (28)$$

where

$$\begin{aligned} \tilde{E}_I &= E_I^{(\text{q.p.})} + E_0^{(D)} + \sum_{\tau} (\lambda_{\tau} - \lambda_{0\tau})N_{\tau} = \\ &= E_0^{(D)} + \sum_{\tau} \left( \left( \sum_i (2j_i + 1)(\epsilon_i - \lambda_{\tau})v_i^2 \right)_{\tau} - \frac{\Delta_{\tau}^2}{G_{\tau}^{(0)}} + (\lambda_{\tau} - \lambda_{0\tau})N_{\tau} \right), \end{aligned} \quad (29)$$

where  $\epsilon_i$  is the particle energy. Calculations show that the extra-boson energy  $\tilde{E}_I$  increases noticeably with increasing spin, and the single-boson energy  $\tilde{\varepsilon}_d$  (23) decreases on the contrary with the spin of the collective state. These tendencies are especially pronounced for nuclei whose boson structure is close to the vibrational case, when, upon transition to the next spin of the collective state, the average number of quadrupole bosons  $n_d$  increases by one. In cases where the nucleus is more collective, as it turns out to be for deformed nuclei, the values of  $n_d$  change significantly less, and the spin growth is realized due to the angular reconnection of the existing quadrupole bosons. In this case, the changes in  $\tilde{E}_I$  and  $\tilde{\varepsilon}_d$  with changes in spin are less pronounced. In order for the extra-boson energy to remain unchanged and equal to that which occurs for the ground state, the terms included in Eq. (28) must be redistributed. This is done in such a way that, in addition to the extra-boson energy, the parameter  $k_1$  remains unchanged, since  $\tilde{k}_1 = \tilde{k}_1(I^+)$  also changes with spin:

$$\begin{cases} \overline{E}_0 = \tilde{E}_{I=0}; \quad k_1 = \tilde{k}_1(I^{\pi} = 0^+), \\ \tilde{E}_I - \xi_1 n_d - \xi_2 P_1 = \overline{E}_0, \quad I^{\pi} \geq 2^+, \\ 2\tilde{k}_1(I^{\pi})\sqrt{\Omega(\Omega-1)} + \xi_2 = 2k_1\sqrt{\Omega(\Omega-1)}, \quad I^{\pi} \geq 2^+, \\ \varepsilon_d(I^{\pi}) = \tilde{\varepsilon}_d(I^{\pi}) + \xi_1, \quad I^{\pi} \geq 2^+; \end{cases} \quad (30)$$

i.e.,  $\overline{E}_0$  is determined from the extra-boson energy of the ground state and is further assumed to be constant for all other collective states. For states other than the main one, this is one of the conditions for determining two parameters,  $\xi_1$  and  $\xi_2$ . The second condition is the immutability of the parameter  $k_1$ . With the value  $\xi_1$  determined in this way, the one-boson energy  $\varepsilon_d(I^{\pi})$  is found.

This transformation does not change the total energy  $E_I$ . It fulfills its assigned function of achieving the constancy of extrabosonic energy. If  $\tilde{E}_I$  noticeably increases with increasing spin, and  $\tilde{\varepsilon}_d$ , on the contrary, falls, then after the transformation  $\tilde{E}_I$  goes into  $\overline{E}_0$ , and  $\tilde{\varepsilon}_d$  into  $\varepsilon_d$ , which experience only small variations with spin changes. In this transformation for the ground state  $I^\pi = 0_1^+$ , it is assumed that  $\xi_1 = \xi_2 = 0$ . For all others, these parameters are determined from Eqs. (30). With the parameters  $\xi_1$  and  $\xi_2$  defined in this way, the final values of  $\varepsilon_d$  and  $k_1$  are found. In this case, the parameters  $\varepsilon_d$ ,  $k_2$ ,  $C_L$  still differ for different collective states.

After the redefinitions, the total energy, measured from  $\Sigma\lambda_{0\tau}N_\tau$ , is equal to

$$E_I = \overline{E}_0 + (I|H_{\text{IBM}}|I). \quad (31)$$

The energies of excited states relative to the ground state will be determined as

$$\Delta E_I = E_I - E_0. \quad (32)$$

Now we can formulate a variational principle for finding the amplitudes  $u$ ,  $v$ ,  $z^{(n)}$ ,  $\{\alpha_d\}$ . They are found from the minimum energy in relation to their variation under additional conditions. This gives equations for  $(u, v)$  and amplitudes  $z^{(n)}$ . The amplitudes  $\{\alpha_d\}$  of the boson composition  $|I\rangle$  are found from minimization (31) provided that  $\overline{E}_0$  does not change when the spin or collective state number changes.

Varying the functional over phonon amplitudes leads to a system of equations similar to the QRPA equations. Its solution is carried out at fixed values of  $\omega'$  and  $\chi$ . This allows us to determine  $\omega$ . It has been said before that in the context of the usual QRPA the  $\omega$ , being a Lagrange multiplier, at the same time turns out to be a single-phonon energy, which can only be positive, but in the case of the QRPA modification used, the Lagrange multiplier  $\omega$  is not a single-phonon energy and has no physical meaning. The single-phonon energy is the value  $\varepsilon_d^{(0)}$  calculated with the found phonon amplitude, which, for nuclei traditionally considered deformed, is negative. It should be added to this that the renormalization procedure further reduces the single-boson energy  $\varepsilon_d$  relative to  $\varepsilon_d^{(0)}$ .

After determining  $\omega$ , the numerical values of the phonon amplitudes  $z^{(n)}$  are found. The calculation is repeated, and  $\chi$  is selected in such a way that the ratio  $\sum \varphi^2 / \sum \psi^2$  is a strictly defined value, not exceeding 0.05 and the same for all states under consideration. Moreover, the greater the low-energy collectivity, i.e., the lower the energy of the first excitation and the greater the value of  $B(E2; 2_1^+ \rightarrow 0_1^+)$ , the smaller the indicated value is, up to 0.002. The value of the Lagrange multiplier  $\omega'$  is found from the requirement that the maximum number of bosons  $\Omega$  be integer, and such that  $\Omega(\omega') \geq \Omega(\omega' = 0)$ . The presence of a term with  $\omega'$  in the functional makes the system of equations for amplitudes nonlinear, so it is solved iteratively. Once again, it should be noted that the main feature of the MQRPA is the ability to change the level of correlations in the ground state, regardless of the  $D$ -phonon energy. This is implemented in such a way that to any two-quasiparticle energy participating

in the equation for phonon amplitudes, quantities independent of this energy — Lagrange multipliers  $\chi$  and  $\omega'$  — are added:

$$e_{ij} \rightarrow e_{ij} + \omega' n_{ij}^{(3)} + \chi, \quad \text{where} \quad n_{ij}^{(3)} = 2 \sum_1 \left( \frac{z_{i1}^{(1)} z_{i1}^{(0)}}{2j_i + 1} + \frac{z_{j1}^{(1)} z_{j1}^{(0)}}{2j_j + 1} \right).$$

This is especially significant when the single-particle levels  $i$  and  $j$  are states of the valence shell. Such a replacement — modification result — significantly reduces the values of amplitudes  $z_{ij}^{(\eta)}$  for valence shell states, redistributing them over extravalence single-particle states. At the same time, this leads to a significant increase in the maximum number of bosons  $\Omega$ .

Another important feature of the modification considered is the presence of boson averages in the minimized functional, which allows us to pose the problem of self-consistency when the microscopically calculated parameters of the boson Hamiltonian lead to the same bosonic averages that are used in calculating the amplitudes and parameters.

It turned out that such an agreement can be achieved only with the help of an additional condition that makes it possible to reduce the measure of correlations. It was proven that both for  $\chi = 0$  in (17) and for all  $\varphi = 0$ , which corresponds to the TD approximation, this agreement is impossible. It is achieved in a certain corridor of values  $\chi$  within which a stable solution to the problem is realized.

The numerical value of  $\sum \varphi^2 / \sum \psi^2$  in each nucleus naturally depends on the values of the force parameters, boson averages and the  $\chi$  parameter. Moreover, by changing the latter in the calculations, the value of  $\sum \varphi^2$  is regulated. Other things being equal, the excitation energy strongly depends on the measure of correlations; the larger it is, the lower the excitation energy. That is why, when considering a set of states, both excited and ground, it is necessary to remain at the same level of  $\sum \varphi^2$  values. This significantly reduces the corridor of possible values of  $\chi$ . In order to achieve the indicated agreement for the ground and excited states, up to  $I_{\max}$ , it is necessary to increase the values of  $\chi$ , but in such a way that the same value of  $\sum \varphi^2$  is realized for all considered states. In this case, the question remains about the upper limit of the values of  $\chi$ , accordingly, the minimum of  $\sum \varphi^2$ . It can be solved practically, based on specific numerical calculations. The most important of them is the requirement that up to  $I_{\max}$  the number of quasiparticles at each single-particle level does not exceed  $j + 1/2$ .

## 2. BOSON DESCRIPTION OF BAND CROSSING

Renormalization of IBM1 parameters is carried out due to extensions of the wave function of phonon states (21) by inclusion of  $B_J$  phonons with  $J^\pi \leq 6^+$ . At large spins of the yrast-band states, collective and non-collective excitations may turn out to be energetically close. Therefore, the components of these non-collective modes must be explicitly introduced into the basis under consideration, and the values of  $J^\pi$  will already change from  $0^+$  to  $10^+$

in the 50–82 shells and up to  $J^\pi = 14^+$  for the next shell, i.e., for heavy and super-heavy nuclei. This leads not only to additional spectrum compression of collective states, but also to the intersection of bands of different nature.

The class of states under consideration is limited to collective states constructed from  $D$  phonons and non-collective ones, including in addition to  $D$  phonons one non-collective  $B$  phonon. Of the possible interaction channels, those processes that contain coherent sums correspond to the creation or destruction of various phonons in accordance with Figs. 1 and 2. Restricting ourselves to the minimum number of  $D$  phonons, we have five types of matrix elements connecting collective and non-collective states:

$$\begin{aligned} &\langle D|H|B_{J,i}^+D^+\rangle, \langle D|H|B_{J,i}^+(D^+D^+)^{(L)}\rangle, \langle (DD)_n^{(L)}|H|B_{J,i}^+\rangle, \\ &\langle (DD)_n^{(L)}|H|B_{J,i}^+D^+\rangle, \langle ((DD)^{(L)}D)_n|H|B_{J,i}^+\rangle. \end{aligned} \quad (33)$$

Their graphical representation is given in Fig. 1. It is necessary to consider three types of matrix elements connecting various non-collective states:

$$\begin{aligned} &\langle DB_{J_1,i_1}|H|B_{J_2,i_2}^+\rangle, \langle (DD)^{(L)}B_{J_1,i_1}|H|B_{J_2,i_2}^+\rangle, \\ &\langle DB_{J_1,i_1}|H|(B_{J_2,i_2}^+D)^{(I)}\rangle. \end{aligned} \quad (34)$$

Their graphical representation is given in Fig. 2. Thus, the considered basis of states contains an arbitrary number of  $D$  phonons in a purely collective space  $|(D^+)^k\rangle$  and a space containing one non-collective phonon along with an arbitrary number of collective phonons  $|B_{J,i}^+(D^+)^{k'}\rangle$ . Passing from phonons to ideal  $b_{J,i}$  and  $d$  bosons, we obtain the boson Hamiltonian in extended form

$$H_b = H_{\text{IBM1}}^{(0)} + \sum_i (\omega_i' + E_0^{(b)}) b_i^+ b_i + V^{(1)} + V^{(2)} + V^{(3)}, \quad (35)$$

where  $H_{\text{IBM1}}^{(0)}$  (6) is the IBM1 Hamiltonian with parameters defined only in terms of  $D$  phonons, i.e., without taking into account non-collective phonons;

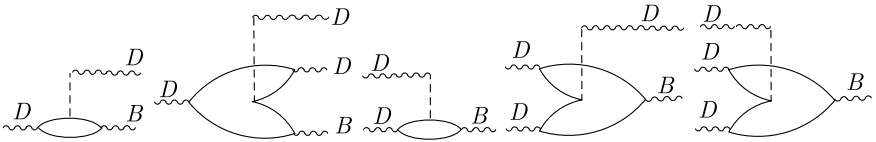


Fig. 1. Graphic representation of the matrix elements of the interaction of  $D$  and  $B$  phonons

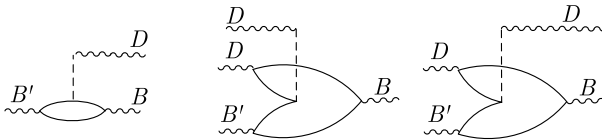


Fig. 2. Graphic representation of the matrix elements of the interaction between various non-collective states

$E_0^{(b)}$  is the energy shift of collective states in the presence of at least one  $b_i$  boson. Here  $\omega'_i$  are the energies of  $b_i$  bosons, and further we will use the notation

$$\omega_i = \omega'_i + E_0^{(b)}. \quad (36)$$

It should be borne in mind that, when solving the problem of eigenvalues and functions, perturbation theory in the Brillouin–Wigner version is used; the second-order interaction terms that lead to renormalization of the standard IBM1 Hamiltonian are discarded. In this case,  $H_{\text{IBM1}}^{(0)}$  is replaced with  $H_{\text{IBM1}}$ ; i.e., the renormalization of parameters is taken into account at the stage preceding the consideration of the connection between collective and non-collective high-spin states.

The interaction of  $V^{(1)}$  and  $V^{(2)}$  expresses the connection between collective states and non-collective ones:

$$\begin{aligned} V^{(1)} = & \sum_i \sqrt{\frac{5}{2J_i + 1}} \nu_1(i) [(d^+ d)^{(J_i)} s^+ \cdot b_i + \text{H.c.}] + \\ & + \sum_{iL} \sqrt{\frac{5}{2J_i + 1}} \nu_2^{(L)}(i) [(d^+ (dd)^{(L)} s^+ s^+)^{(J_i)} \cdot b_i + \text{H.c.}] + \\ & + \sum_i \nu_3(i) [(d^+ d^+)^{(J_i)} s \cdot b_i + \text{H.c.}] + \\ & + \sum_{iL} \sqrt{\frac{2L + 1}{2J_i + 1}} \nu_4^{(L)}(i) [(d^+ d^+)^{(L)} d^{(J_i)} \cdot b_i + \text{H.c.}], \end{aligned} \quad (37)$$

$$V^{(2)} = \sum_{iL} \nu_5^{(L)}(i) [((d^+ d^+)^{(L)} d^+)^{(J_i)} \cdot b_i s s + \text{H.c.}]. \quad (38)$$

The  $V^{(3)}$  operator defines the interaction between states containing different  $b_J$  bosons:

$$\begin{aligned} V^{(3)} = & \sum_{i1 \neq i2} \sqrt{\frac{2J_2 + 1}{5}} (-1)^{J_1 + J_2} u_{i1, i2}^{(1)} [(b_{i1}^+ b_{i2})^{(2)} \cdot d^+ s + \text{H.c.}] + \\ & + \sum_{L, i1 \neq i2} \sqrt{\frac{2J_2 + 1}{2L + 1}} (-1)^{J_1 + J_2} u_{i1, i2}^{(2)}(L) [(b_{i1}^+ b_{i2})^{(L)} \cdot (d^+ d^+)^{(L)} s s + \text{H.c.}] + \\ & + \sum_{L, i1 \neq i2} (-1)^{L + J_2} u_{i1, i2}^{(3)}(L) [(b_{i1}^+ b_{i2})^{(L)} \cdot (d^+ d)^{(L)} + \text{H.c.}]. \end{aligned} \quad (39)$$

The parameters in  $V^{(1)}$  and  $V^{(2)}$  are determined by ME in fermion space using the Marumori procedure:

$$\nu_1(i) = \frac{1}{\sqrt{\Omega - 1}} \langle D | H | (B_i^+ D^+)^{(2)} \rangle,$$

$$\begin{aligned} \nu_2^{(L)}(i) &= \frac{1}{\sqrt{2(\Omega-1)(\Omega-2)}} \langle D|H|(B_i^+(D^+D^+)_n^{(L)})^{(2)}\rangle, \\ \nu_3(i) &= \frac{1}{\sqrt{2(\Omega-1)}} \langle (DD)_n^{(J)}|H|B_i^+\rangle, \\ \nu_4^{(L)}(i) &= \frac{1}{\sqrt{2}} \langle (DD)_n^{(L)}|H|(B_i^+D^+)^{(L)}\rangle, \end{aligned} \quad (40)$$

$$\begin{aligned} \nu_5^{(L)}(i) &= \frac{1}{\sqrt{\aleph_{JL}(\text{bos})(\Omega-1)(\Omega-2)}} \langle [(DD)^{(L)}D]_n^{(J)}|H|B_i^+\rangle, \quad (41) \\ \aleph_{JL}(\text{bos}) &= (|(d(dd)^{(L)})^{(J)}((d^+d^+)^{(L)}d^+)^{(J)}|), \end{aligned}$$

where  $H$  is the quasiparticle Hamiltonian,  $\aleph_{JL}(\text{bos})$  is the value of the three-boson normalization, and the value  $L$  is defined in terms of  $J$  so that  $J(L) = 0(2), 2(0), 3(2), 4(2), 6(4)$ . Combinations of phonon functions are normalized, denoted by the subscript symbol  $n$ .

The parameters in  $V^{(3)}$  are defined as

$$\begin{aligned} u_{i1,i2}^{(1)} &= \frac{1}{\sqrt{\Omega-1}} \langle DB_{i1}|H|B_{i2}^+\rangle, \\ u_{i1,i2}^{(2)}(L) &= \frac{1}{\sqrt{2(\Omega-1)(\Omega-2)}} \langle [(DD)_n^{(L)}B_{i1}]^{(J_2)}|H|B_{i2}^+\rangle, \quad (42) \\ u_{i1,i2}^{(3)}(L) &= \sum_x \langle (DB_{i1})^{(x)}|H|B_{i2}^+D^+\rangle (-1)^x (2x+1) \begin{Bmatrix} 2 & 2 & L \\ J_2 & J_1 & x \end{Bmatrix}. \end{aligned}$$

The boson Hamiltonian (35) and expressions for its parameters were first given in [23], and in the most detailed form they are represented by relations (38)–(44) in [21].

Multipole  $B_i$  phonons in MEs (40) and (41), defining the interactions  $V^{(1)}$ ,  $V^{(2)}$ , vary from  $J^\pi = 0^+$  to  $J^\pi = 6^+$ , and in (42) for interaction  $V^{(3)}$  from  $J^\pi = 2^+$  to  $J^\pi = 14^+$ .

The Hamiltonian (35) contains a large number of bosons  $b_{J,i}$  of each multipole, equal to the number of quasiparticle pairs. Instead of direct diagonalization, the eigenvalues and eigenfunctions of the Hamiltonian (35) are found using perturbation theory in the Wigner variant. Summation over all non-collective phonons of each multipole is carried out using an analytical procedure in the approximation that all non-collective  $B$  phonons are determined in the Tamm–Dankov method using isoscalar type particle–hole forces. The corresponding equations are given in [22].

To implement this procedure, the Hamiltonian (35) is used to highlight the matrix elements in the representation of ideal  $d$  bosons. The matrix elements (33) and (34) remain in the phonon representation in order to explicitly preserve expressions through the amplitudes of  $B$  phonons, and subsequently sum the available expressions over all non-collective phonons. Thus, we get

$$\begin{aligned} \langle \psi_C(I) | H | B_{J,i}^+ \psi_{C_1}(I_1) \rangle &= \\ &= \langle \psi_C(I) | H | B_{J,i}^+ \psi_{C_1}(I_1) \rangle_{V_1} + \langle \psi_C(I) | H | B_{J,i}^+ \psi_{C_1}(I_1) \rangle_{V_2}, \quad (43) \end{aligned}$$

$$\begin{aligned} \langle \psi_C(I) | H | B_{J,i}^+ \psi_{C_1}(I_1) \rangle_{V_1} &= (-1)^{I-I_1+J} \frac{1}{\sqrt{(2I+1)(\Omega-1)}} \times \\ &\times \left\{ \sqrt{\frac{5}{2J+1}} \langle D | H | B_{J,i}^+ D^+ \rangle \langle \psi_C(I) | s^+ (d^+ d)^{(J)} | \psi_{C_1}(I_1) \rangle + \right. \\ &+ \frac{1}{\sqrt{2(\Omega-2)}} \sqrt{\frac{5}{2J+1}} \sum_{L=0,2,4} \langle D | H | B_{J,i}^+ (D^+ D^+)_n^{(L)} \rangle \times \\ &\times \langle \psi_C(I) | s^+ s^+ [d^+ (d^+ d)^{(L)}]^{(J)} | \psi_{C_1}(I_1) \rangle + \\ &+ \frac{1}{\sqrt{2}} \langle (DD)_n^{(J)} | H | B_{J,i}^+ \rangle \langle \psi_C(I) | (d^+ d^+)^{(J)} s | \psi_{C_1}(I_1) \rangle + \\ &+ \left. \sqrt{\frac{\Omega-1}{2(2J+1)}} \sum_{L=0,2,4} \sqrt{2L+1} \langle (DD)_n^{(L)} | H | B_{J,i}^+ D^+ \rangle \times \right. \\ &\left. \times \langle \psi_C(I) | [(d^+ d)^{(L)} d]^{(J)} | \psi_{C_1}(I_1) \rangle \right\}, \quad (44) \end{aligned}$$

$$\begin{aligned} \langle \psi_C(I) | H | B_{J,i}^+ \psi_{C_1}(I_1) \rangle_{V_2} &= (-1)^{I-I_1+J} \frac{1}{\sqrt{(2I+1)(\Omega-1)(\Omega-2)\aleph_{JL}}} \times \\ &\times \langle (DD)^{(L)} D | H | B_{J,i}^+ \rangle \langle \psi_C(I) | [(d^+ d^+)^{(L)} d^+]^{(J)} s s | \psi_{C_1}(I_1) \rangle. \quad (45) \end{aligned}$$

The subscript symbols  $V_1$  and  $V_2$  for matrix elements correspond to boson interaction channels  $V^{(1)}$  and  $V^{(2)}$  in Eqs. (37) and (38);

$$\begin{aligned} \langle (\psi_{C_2}(I_2) B_{J_2, i_2})^{(I)} | H | B_{J_1, i_1}^+ \psi_{C_1}(I_1) \rangle &= \\ &= (-1)^{J_2+I_2+I} \left\{ \begin{matrix} J_2 & I_2 & I \\ I_1 & J_1 & 2 \end{matrix} \right\} \frac{1}{\sqrt{\Omega-1}} \times \\ &\times \left\{ \langle DB_{J_2, i_2} | H | B_{J_1, i_1}^+ \rangle \sqrt{2J_1+1} \langle \psi_{C_2}(I_2) | d^+ s | \psi_{C_1}(I_1) \rangle + \right. \\ &+ \langle DB_{J_1, i_1} | H | B_{J_2, i_2}^+ \rangle \sqrt{2J_2+1} \langle \psi_{C_2}(I_2) | s^+ d | \psi_{C_1}(I_1) \rangle + \\ &+ \frac{1}{\sqrt{2(\Omega-2)}} \sum_L \langle (DD)_n^{(L)} B_{J_2, i_2} | H | B_{J_1, i_1}^+ \rangle \sqrt{2J_1+1} \times \\ &\times \langle \psi_{C_2}(I_2) | (d^+ d^+)^{(L)} s s | \psi_{C_1}(I_1) \rangle + \\ &+ \left. \frac{1}{\sqrt{2(\Omega-2)}} \sum_L \langle (DD)_n^{(L)} B_{J_1, i_1} | H | B_{J_2, i_2}^+ \rangle \sqrt{2J_2+1} \times \right. \end{aligned}$$



$$\begin{aligned}
& \times \langle \psi_{C_2}(I_2) | s^+ s^+ (dd)^{(L)} | \psi_{C_1}(I_1) \rangle + \\
& + (-1)^{J_2} \sum_L \sqrt{(2L+1)(\Omega-1)} \sum_x \left( (-1)^x (2x+1) \left\{ \begin{matrix} 2 & 2 & L \\ J_1 & J_2 & x \end{matrix} \right\} \times \right. \\
& \left. \times \langle (DB_{J_2, i_2})^{(x)} | H | B_{J_1, i_1}^+ D^+ \rangle \langle \psi_{C_2}(I_2) | (d^+ d)^{(L)} | \psi_{C_1}(I_1) \rangle \right), \quad (46)
\end{aligned}$$

where the creation and annihilation operators of non-collective phonons have both moments ( $J$ ) and their numbers ( $i$ );  $\psi_C(I)$  is the collective state on the left of Eqs. (43) and (46) constructed from  $D$  phonons, in the right-hand sides of the same equations from  $d$  bosons. On the left side, all functions are connected in angular momentum  $I$ ; the subsequent summation extends over collective states from three to five pieces (symbol  $C_1$ ) for each of the possible spins  $I_1$ , characterizing these collective states. In addition, the index  $C_1$  means that this is a purely collective state. Additionally, the sums are extended over all phonons ( $i$ ) and their multipolarities ( $J$ ). The presented procedure makes it possible to explicitly isolate the phonon amplitudes in the corresponding matrix elements and then perform summation over all of them.

In the expressions (43)–(46) we can explicitly select amplitudes of non-collective phonons in a uniform way:

$$\langle \psi_C(I) | H | B_{J, i}^+ \psi_{C_1}(I_1) \rangle = \sum_{\tau, 1, 2} \gamma(C, C_1, J, \tau, 1, 2) \psi_{\tau 12}(J, i), \quad (47)$$

$$\begin{aligned}
& \langle (\psi_{C_2}(I_2) B_{J_2, i_2})^{(I)} | H | B_{J_1, i_1}^+ \psi_{C_1}(I_1) \rangle = \\
& = \sum_{\tau, 1, 2} \beta(C, C_2, C_1, J_2, J_1, \tau, 1, 2, 3) \psi_{\tau 12}(J_2, i_2) \psi_{\tau 23}(J_1, i_1), \quad (48)
\end{aligned}$$

where  $\gamma(\dots) = \gamma_1(\dots) + \gamma_2(\dots)$  and each term is determined in accordance with the expressions (44) and (45); the values  $\gamma(\dots)$  and  $\beta(\dots)$  do not depend on the structures of phonons, which are contained only in the amplitudes  $\psi_{\tau 12}(J, i)$  of non-collective phonons; summation over  $\tau$  means summation over neutrons and protons; indices “1”, “2” mean the totality of all quantum numbers of single-particle states except for magnetic ones;  $J$  and  $i$  are the multipolarity of the phonon and its number.

The relations (43)–(48) demonstrate the effectiveness of the boson representation of phonon operators. This representation allows multiphonon states constructed from  $D$  operators to be considered as multibosonic, and at the fermion level the matrix elements with a minimum number of  $D$  phonons are considered as in the presented matrix elements (33) and (34).

In order to take into account in the wave function the components containing both purely collective modes and non-collective modes up to extremely high spins relative to phonons (up to  $J = 14^+$  in nuclei with the number of nucleons of the same type greater than 82), it is convenient to use

matrix elements (43, 46) or (47), (48) divided into three types:

$$(I) \quad \langle B_{J \leq 6} D^k | H | D^{+k'} \rangle, \quad (49)$$

$$(II) \quad \langle B_{J=8,10} D^k | H | B_{J \leq 6}^+ D^{+k'} \rangle, \quad (50)$$

$$(III) \quad \langle B_{J=12,14} D^k | H | B_{J=8,10}^+ D^{+k'} \rangle, \quad (51)$$

where instead of collective functions an arbitrary number of  $D$  phonons is represented.

MEs of type I are used to obtain corrections to boson parameters; joint consideration of matrix elements of types I and II is also for the connection of collective states formed only from  $D$ -phonon components with states containing fermion pairs with  $J^\pi \leq 10^+$ . This is sufficient to describe collective states and the effect of band crossing in nuclei with a number of nucleons less than 82. For heavier nuclei, the nucleons of which are in the range from 84 to 124 or more, it is necessary to consider the set of type-III matrix elements. When renormalizing the parameters of the boson Hamiltonian (6), non-collective phonons are considered implicitly, and when considering the effect of band crossing, all phonons are considered explicitly. Since to describe the intersection of bands it is necessary to use the entire set of matrix elements of type I, ideal bosons  $b_J$  with  $J^\pi \geq 2^+$  are introduced accordingly. In this case, non-collective quadrupole phonons are understood as all phonons except for the lowest one. It should be borne in mind that in the second order of perturbation theory, an interaction of type I is used to renormalize boson parameters and it is necessary to implement the theoretical scheme in such a way that this interaction is not taken into account twice.

The extended wave function with total angular momentum  $I$  in the phonon representation has the following form:

$$|\Psi(I)\rangle = \alpha_0 |\psi_C(I)\rangle + \sum_{J_1=2,4,6,c_1} \alpha_{J_1,c_1} B_{J_1}^+ |\psi_{c_1}\rangle + \\ + \sum_{J_2=8,10,c_2} \alpha_{J_2,c_2} B_{J_2}^+ |\psi_{c_2}\rangle + \sum_{J_3=12,14,c_3} \alpha_{J_3,c_3} B_{J_3}^+ |\psi_{c_3}\rangle, \quad (52)$$

where summation over  $J$  means summation not only over angular momenta, but also over all phonons of the given multipole.

Part of the Hamiltonian, namely,  $V^{(1)}$  (through the ME product  $\langle V^{(1)} \rangle \langle V^{(1)} \rangle$  in the second order according to perturbation theory), is used to renormalize the parameters of the boson Hamiltonian (6) [16, 17]. For the connection of collective states with  $b_{J=8,10}$  and with  $b_{J=12,14}$ , the interaction  $V^{(1)}$  is important along with  $V^{(2)}$  and  $V^{(3)}$  in (35) due to the cross matrix elements  $\langle V^{(1)} \rangle \langle V^{(2)} \rangle$ . Part of the Hamiltonian,  $V^{(2)}$ , through the interaction second order leads to an additional interaction of three  $d$  bosons with each other, which does not reduce to terms of the traditional IBM1 Hamiltonian. The influence of this interaction channel leads to an additional decrease in energies as the spin and excitation energy increase. There is also a direct channel for the additional interaction of three  $d$  bosons with each other, but

its estimate turned out to be significantly less than that given by the second order.

The connection between collective states and configurations containing high-spin bosons  $b_{J=8,10}$  is also carried out through the second order in interaction through the product of ME from  $V^{(1)} + V^{(2)}$  with  $V^{(3)}$ , i.e.,  $\langle V^{(1)} + V^{(2)} \rangle \langle V^{(3)} \rangle$ . In nuclei whose structure is close to the vibrational case, it is the products  $\langle V^{(2)} \rangle \langle V^{(3)} \rangle$  that are important, but in the case when the ground state is already far from the boson vacuum, the product  $\langle V^{(1)} \rangle \langle V^{(3)} \rangle$  will also be important, especially since among the bosons that determine  $V^{(1)}$  there are also those with  $J^\pi = 6^+$ , namely,  $\langle d | V^{(1)} | d^+ d^+ b_{J=6}^+ \rangle$  and  $\langle d^2 | V^{(1)} | d^+ b_{J=6}^+ \rangle$ .

There is a direct channel of interaction between components containing only  $d$  configurations with  $b_{J=8,10}$ , but its estimates turned out to be negligible compared to the values given by the second-order perturbation theory.

Finally, the presence of components in the wave function containing  $B_{J=12,14}$  is carried out through the product of MEs with  $V^{(3)}$ , but differing in values of angular momentum  $J$ .

The equation for the eigenvalues  $E$  of the quasiparticle Hamiltonian in the space of the extended wave function (52) is as follows:

$$H|\Psi(I)\rangle = E|\Psi(I)\rangle. \quad (53)$$

Multiplying this equation from the left by an arbitrary component containing the non-collective phonon  $B_{J_i}^+ |\psi_{c_i}\rangle$ , we obtain  $\langle \psi_{c_i} B_{J_i} | H |\Psi(I)\rangle = E \langle \psi_{c_i} B_{J_i} | \Psi(I)\rangle$ . If in this equation the non-diagonal matrix elements are considered only of three types (49)–(51), then in a more expanded form we have

$$\alpha_0 \langle \psi_{C_i} B_{J_i} | H | \psi_C(I)\rangle + (\omega_i + E_{c_i} - E) \alpha_{J_i, c_i} + \sum'_{J_1, C_1} \alpha_{J_1, C_1} \langle \psi_{C_i} B_{J_i} | H | B_{J_1}^+ \psi_{C_1}\rangle = 0,$$

where the quantity  $\omega_i$  is related to the one-phonon energy and is given in (36); the prime in the sum means that there is no term with ME  $\langle \psi_{C_i} B_{J_i} | H | B_{J_i}^+ \psi_{C_i}\rangle$  in it. This leads to the expression for the amplitudes

$$\alpha_{J_i, C_i} = -\frac{1}{(\omega_i + E_{c_i} - E)} \left( \alpha_0 \langle \psi_{C_i} B_{J_i} | H | \psi_C(I)\rangle + \sum'_{J_1, C_1} \alpha_{J_1, C_1} \langle \psi_{C_i} B_{J_i} | H | B_{J_1}^+ \psi_{C_1}\rangle \right). \quad (54)$$

From this equation we successively obtain all amplitudes according to perturbation theory.

At the first stage for  $J_1^\pi = 2^+, 4^+, 6^+$ ,

$$\alpha_{J_1, C_1} = -\frac{\alpha_0}{(\omega_1 + E_{c_1} - E)} \langle \psi_{c_1} B_{J_1} | H | \psi_C(I)\rangle. \quad (55)$$

At the second stage for  $J_2^\pi = 8^+, 10^+$ ,

$$\alpha_{J_2, C_2} = \frac{\alpha_0}{(\omega_2 + E_{C_2} - E)} \sum_{J_1=4,6,C_1} \frac{\langle \psi_{C_1} B_{J_1} | H | \psi_C \rangle}{(\omega_1 + E_{C_1} - E)} \langle \psi_{C_2} B_{J_2} | H | B_{J_1}^+ \psi_{C_1} \rangle. \quad (56)$$

In this case, the ME  $\langle \psi_{C_1} B_{J_1=8,10} | H | \psi_C \rangle$  was not considered, as mentioned earlier, due to its smallness.

Finally, at the third stage, the connection of the already considered states with phonons with multipole  $J_3^\pi = 12^+, 14^+$  is realized:

$$\begin{aligned} \alpha_{J_3, C_3} &= -\frac{1}{(\omega_3 + E_{C_3} - E)} \sum_{J_2=8,10,C_2} \alpha_{J_2, C_2} \langle \psi_{C_3} B_{J_3} | H | B_{J_2}^+ \psi_{C_2} \rangle = \\ &= -\frac{\alpha_0}{(\omega_3 + E_{C_3} - E)} \sum_{J_2=8,10,C_2} \frac{1}{(\omega_2 + E_{C_2} - E)} \sum_{J_1=4,6,C_1} \frac{\langle \psi_{C_1} B_{J_1} | H | \psi_C \rangle}{(\omega_1 + E_{C_1} - E)} \times \\ &\quad \times \langle \psi_{C_2} B_{J_2} | H | B_{J_1}^+ \psi_{C_1} \rangle \langle \psi_{C_3} B_{J_3} | H | B_{J_2}^+ \psi_{C_2} \rangle. \quad (57) \end{aligned}$$

The eigenvalues of Eq. (53) with the amplitudes (55)–(57) of the wave function (52) and taking into account its normalization are a solution to the equation

$$\begin{aligned} E - \langle \psi_C | H_{\text{IBM}} | \psi_C \rangle &= \\ &= \sum_{C_1, i_1, J_1 \leq 6} \frac{|\langle \psi_C(I) | H | B_{J_1, i_1}^+ \psi_{C_1}(I_1) \rangle|^2 - |\langle \psi_C(I) | H | B_{J_1, i_1}^+ \psi_{C_1}(I_1) \rangle_{V_1}|^2}{E - \omega_{i_1} - E_{C_1}} + \\ &+ \sum_{C_2, i_2, J_2=8,10} \frac{1}{E - \omega_{i_2} - E_{C_2}} \left( \sum_{C_1, i_1, J_1=4,6} \frac{\langle \psi_C(I) | H | B_{J_1, i_1}^+ \psi_{C_1}(I_1) \rangle}{E - \omega_{i_1} - E_{C_1}} \times \right. \\ &\quad \times \langle (\psi_{C_1}(I_1) B_{J_1, i_1})^{(I)} | H | B_{J_2, i_2}^+ \psi_{C_2}(I_2) \rangle \Big)^2 + \\ &\quad + \sum_{C_3, i_3, J_3=12,14} \frac{1}{E - \omega_{i_3} - E_{C_3}} \times \\ &\quad \times \left( \frac{1}{E - \omega_{i_2} - E_{C_2}} \sum_{C_1, i_1, J_1=4,6} \frac{\langle \psi_C(I) | H | B_{J_1, i_1}^+ \psi_{C_1}(I_1) \rangle}{E - \omega_{i_1} - E_{C_1}} \times \right. \\ &\quad \times \langle (\psi_{C_1}(I_1) B_{J_1, i_1})^{(I)} | H | B_{J_2, i_2}^+ \psi_{C_2}(I_2) \rangle \times \\ &\quad \times \langle (\psi_{C_2}(I_2) B_{J_2, i_2})^{(I)} | H | B_{J_3, i_3}^+ \psi_{C_3}(I_3) \rangle \Big)^2, \quad (58) \end{aligned}$$

where  $\langle \psi_C | H_{\text{IBM}} | \psi_C \rangle$  is the energy of IBM1, obtained taking into account the renormalizations of the Hamiltonian parameters (6), determined by  $\langle \psi_C(I) | H | B_{J_1, i_1}^+ \psi_{C_1}(I_1) \rangle_{V_1}$ . The first line of Eq. (58) makes a subtraction so that the same interaction channel is not counted twice.

In [20], the connection between collective and high-spin excitation modes was realized only through the channel  $\langle \psi_C(I) | H | B_{J_1, i_1}^+ \psi_{C_1}(I_1) \rangle_{V_2}$ , which was insufficient. Now, as can be seen from Eq. (52), this is also realized through the interaction channel  $\langle \psi_C(I) | H | B_{J_1, i_1}^+ \psi_{C_1}(I_1) \rangle_{V_1}$ , which turned out to ensure an invariably strong mixing of collective and high-spin modes, at least in the region of the isotopes Xe, Ba, and Ce.

As already mentioned, the method of summing over all solutions of non-collective phonons is given in the Appendix of [22], where Eq. (58) is also given taking into account this summation.

When calculating the ME of the quadrupole electric operator, we will be mainly interested in transitions along the yrast band or transitions with large values of  $B(E2)$ . To do this, it is sufficient to consider transitions between components of the wave function with the same non-collective phonons or bosons, taking into account the action of the  $E2$ -transition operator between  $D$ -phonon or  $d$ -boson states. Matrix elements of the quasiparticle  $E2$  operator between the functions (52) are also given in [22]. Transitions from non-collective components to collective ones are taken into account when renormalizing the effective charges [27], which makes it possible to consider the ME only between collective components expressed in terms of  $d$  bosons, without affecting the  $b_J$  bosons. The boson operator  $\widehat{T}(E2)$  is represented by Eq. (25).

Below is an analysis of two isotopic chains from different mass regions; these are Xe isotopes and Th isotopes, closely adjacent to superheavy nuclei.

### 3. CALCULATION RESULTS FOR $^{112-128}\text{Xe}$

The presented theoretical scheme was applied to a number of nuclei, among which are the  $^{112-128}\text{Xe}$  isotopes, but the results were given only for the  $^{120}\text{Xe}$  and  $^{124}\text{Xe}$  nuclei [23], regarding which there was sufficiently complete experimental information on the values of  $B(E2)$  between the states of the yrast bands. To date, several new works have appeared [28, 29], which indicate that a number of inconsistencies between experimental and theoretical data on transition probabilities can be removed using new data. This provides grounds for presenting here the results of calculations based on all the data considered regarding the properties of yrast bands in even isotopes of Xe. Figure 3 shows the effective moments of inertia as a function of  $(\hbar\omega)^2$  for yrast bands in the isotopes  $^{112-128}\text{Xe}$ . In the figure for  $^{112}\text{Xe}$ , the experimental curve shows a reverse bend at spin  $I^\pi = 10^+$ , and the theoretical data rather indicate “upending”. The difference is due to the fact that the calculated value for this spin exceeds the experimental value by only 34 keV, and for the next level there is no difference in energies. For  $^{114-120}\text{Xe}$  nuclei, backbending, in accordance with experiment and calculation, is essentially not observed. But for nuclei starting with  $^{122}\text{Xe}$  and all subsequent ones it is clearly visible.

In order to reveal the nature of the states as the spin increases, Fig. 4 shows the composition of the wave functions in terms of  $d$  and  $b_J$  bosons, where the collective component and those that correspond to non-collective boson states are indicated with  $J^\pi = 2^+, 6^+, 8^+, 10^+$ .

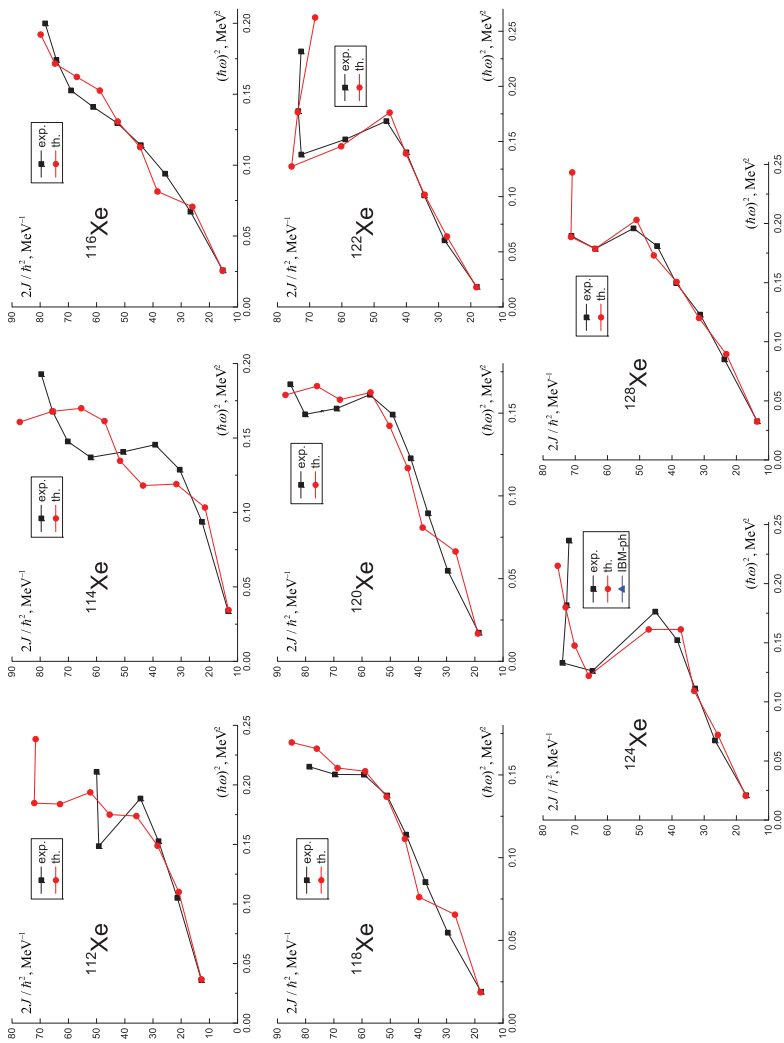


Fig. 3. Dependence of the effective moment of inertia on  $(\hbar\omega)^2$  for yrast bands in  $112\text{--}128\text{Xe}$  isotopes for experimental (exp.) and theoretical (th.) energies

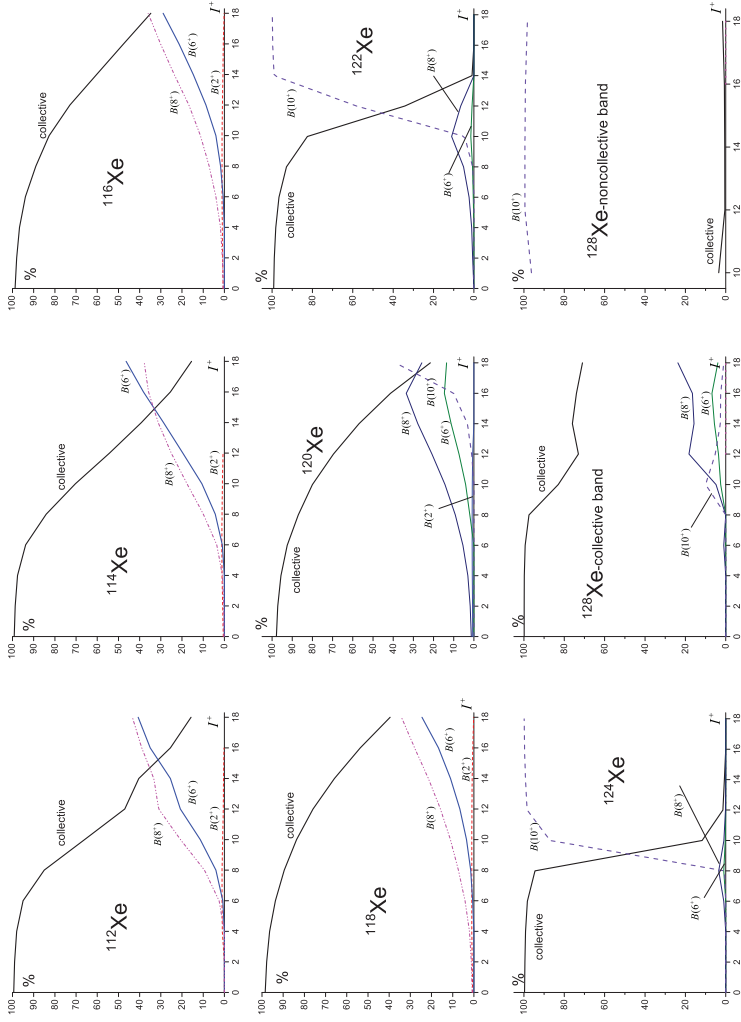


Fig. 4. Boson composition of wave functions of yrast bands in Xe isotopes. By “collective” we mean the contribution to the function (21) of components containing only the  $d$ -boson composition, i.e.,  $|\psi_c(I)^2$ . By  $B(J)$  we mean the contribution from all components containing different bosons  $b_{J,i1}$  with a fixed moment  $J$ , i.e.,  $\sum_{i1,c1} |\alpha_{J,i1,c1}|^2$ . For  $^{128}\text{Xe}$  two figures are given: one corresponds to the collective band, when states starting from  $10^+$  cease to be yrast, and the second corresponds to yrast states

In the  $^{112-120}\text{Xe}$  isotopes, as the spin increases, as can be seen from the figure, the collective component smoothly decreases, leveling off at spin  $I = 16^+$  or  $18^+$  with components containing  $b_6$ ,  $b_8$  and  $b_{10}$  bosons. In  $^{122}\text{Xe}$ , with spin  $I = 12^+$ , the collective component is aligned with the component containing the  $b_{10}$  boson. In  $^{124}\text{Xe}$  this is realized with spin  $I = 10^+$ .

In the  $^{126,128}\text{Xe}$  isotopes, two bands were calculated. The situation for these nuclei is similar; therefore, of the two, information on the composition of the wave functions is given only for  $^{128}\text{Xe}$ . In the last of this series of figures, the information relates to the collective band that, starting from the spin  $I = 10^+$ , ceases to be yrast. The other band is built on the  $b_{10}$  boson and immediately turns out to be yrast with spin  $I = 10^+$ . For the heaviest of the considered  $^{126,128}\text{Xe}$  isotopes, the most rapid transition from a collective state to a non-collective one occurs with very weak interaction between them, which is manifested in the values of  $B(E2)$ .

The  $B(E2)$  values for transitions within the yrast bands in Xe isotopes are shown in Fig. 5. It is clear that for  $^{112-120}\text{Xe}$  isotopes the theoretical values of  $B(E2)$  do not experience a sharp decrease at any spin. As the spin increases, they continue to grow slowly, or experience a slight drop from a certain spin. This is due to the smooth replacement of the collective component by components with high-spin bosons.

In  $^{114}\text{Xe}$ , the correlation of theoretical and experimental data encounters the exotic behavior of the latter depending on the spin, where the inequalities  $B(E2; 6_1 \rightarrow 4_1) < B(E2; 4_1 \rightarrow 2_1) < B(E2; 2_1 \rightarrow 0_1)$  hold [30], although the energy of the first excitation is  $E(2_1^+) = 0.45$  MeV, while the corresponding inequalities take place only for semimagic nuclei, when  $E(2_1^+) > 1$  MeV.

The question of such a relationship for a number of nuclei, including  $^{114}\text{Xe}$ , was discussed in the literature [41], although no satisfactory explanation was given. A similar effect was analyzed in [42] in relation to the  $^{172}\text{Pt}$  and  $^{168}\text{Os}$  nuclei. It was found that, by remaining within the framework of only collective states, but introducing strong nonaxiality, such an effect can be reproduced. In this case, the transition  $6_1 \rightarrow 4_1$  is also greatly suppressed. In the  $^{118}\text{Xe}$  isotope, the  $4_1 \rightarrow 2_1$  transition is also strongly suppressed. In other isotopes of Xe, as well as in all isotopes of Te, Ba and Ce, this phenomenon is not observed. Therefore, the anomaly under discussion still awaits further investigation, both at the level of phenomenology and microscopy, and in the experimental aspect.

It should be noted that already in the nucleus with  $A = 116$  the ratio  $B(4^+ \rightarrow 2^+)/B(2^+ \rightarrow 0^+)$  noticeably exceeds one. The new measurements [28] completely restore the correspondence between theory and experiment. Due to large experimental uncertainty, the next transition does not contradict the calculation result.

A noticeable difference between the experimental and calculated values of  $B(E2)$  in the yrast band is also observed for  $^{118}\text{Xe}$ , where a drop in the value under consideration occurs already at spin  $I = 6^+$ . This behavior is also quite exotic and requires both experimental clarification and a search for a possible theoretical explanation.



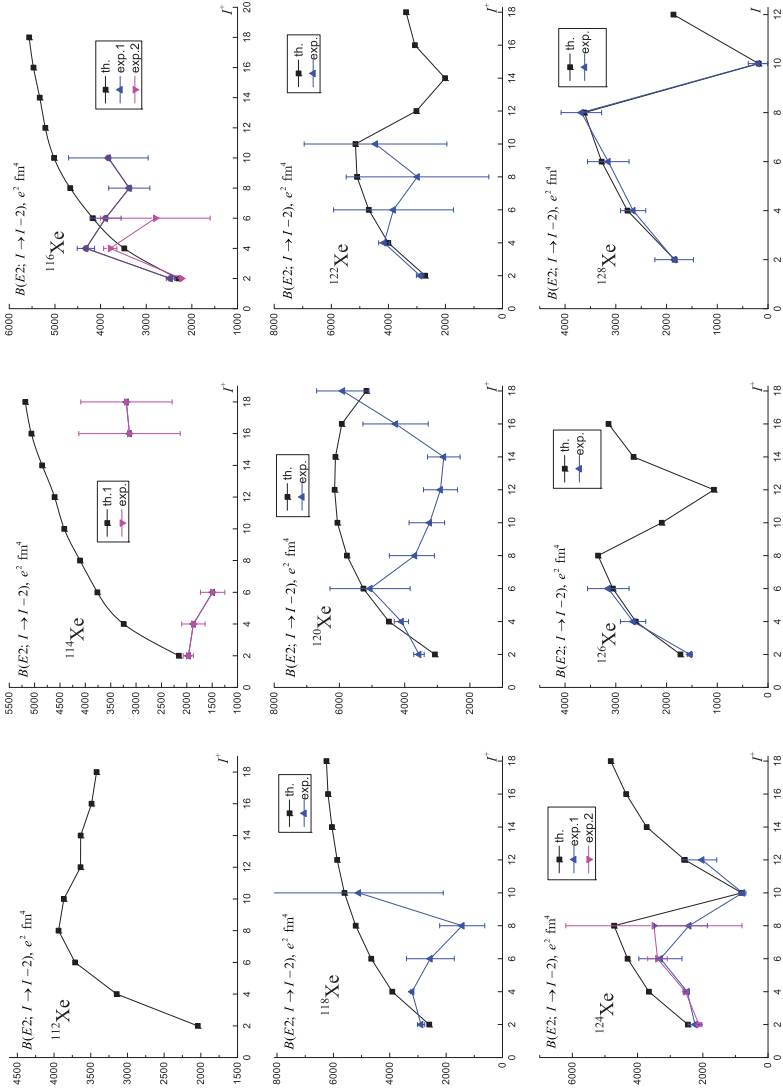


Fig. 5. Values of  $B(E2, I \rightarrow I-2)$  in Xe isotopes, experimental values for  $^{114}\text{Xe}$  from [30], for  $^{116}\text{Xe}$  exp.1 from [31], exp.2 from [28], for  $^{118}\text{Xe}$  from [32, 33], for  $^{120}\text{Xe}$  from [31, 34], for  $^{122}\text{Xe}$  from [31], for  $^{124}\text{Xe}$  exp.1 from [31, 35], exp.2 from [29], for  $^{126}\text{Xe}$  from [36], for  $^{128}\text{Xe}$  links are given in Table 1

In  $^{120}\text{Xe}$ , the description of  $B(E2)$  up to the spin  $I = 6^+$  is satisfactory, but starting from  $I = 8^+$  the experimental values again experience a strong decrease.

In  $^{122}\text{Xe}$ , the description of  $B(E2)$  can be considered acceptable due to large experimental errors. Data are available only up to the spin  $I = 10^+$ , and the predicted theoretical drops in these values begin with the following spins, which is associated with the obvious intersection of the bands as discussed earlier.

In  $^{124}\text{Xe}$ , the value of  $B(E2)$  from the state  $10^+$  is significantly suppressed, and starting from  $12^+$  the values of  $B(E2)$  are again significant, which coincides with the experimental data. As can be seen from Fig. 4, the reason is that, during the transition from the  $8^+$  state to the  $10^+$  state, a significant change occurs in the structure of the wave function. The collective component falls, and the state with  $b_{10}$  becomes the main component, which corresponds to the intersection of bands. At large spins, the transition probabilities become significant again. New experimental estimates, partly due to increased experimental uncertainties, somewhat improve the quality of the description.

For  $^{126}\text{Xe}$ , the values of  $B(E2)$  are described in accordance with the latest experimental data quite accurately, although they extend only to the spin  $I = 6^+$ . But in  $^{128}\text{Xe}$  the values of  $B(E2)$  are described precisely up to the spin  $I = 10^+$ , and its value turns out to be very small. This corresponds to the fact that the yrast band, starting from spin  $I = 10^+$ , is practically exhausted by a component containing the  $b_{10}$  boson and a very small admixture of the collective state, as shown in Fig. 4. Three high-spin bands are observed in  $^{128}\text{Xe}$ ; therefore, Table 1 shows the calculated values of  $B(E2)$  for a number of transitions. The data presented say that the collective band, starting from the spin  $10^+$ , ceases to be yrast; these are the states  $10_2^+$  (3.365),  $12_2^+$  (4.251),  $14_2^+$  (5.097),  $16_3^+$  (5.573),  $18_3^+$ ; the states  $10_1^+$  (3.197),  $12_1^+$  (3.809),  $14_1^+$  (4.618),  $16_2^+$  (5.573),  $18_2^+$  (6.606) are based on two-quasiparticle excitation  $(h_{11/2}^2)^{(10^+)}$ . The band of states  $16_1^+$  (5.288),  $18_1^+$  (6.187),  $20_1^+$  (7.257) can be interpreted as a band built on  $(h_{11/2}^4)^{(16^+)}$ .

We would like to emphasize once again that, when calculating  $B(E2)$ , effective nucleon charges were not introduced. In this case, the probabilities of transitions from the first excited state are reproduced correctly, but the remaining transitions for a number of Xe isotopes give an excess of the theoretical values of  $B(E2)$  over the experimental ones. Similar data were obtained in the Bohr model [43]. It is noteworthy that in the Xe isotopes the increase in the available experimental values of  $B(E2)$  in the yrast bands is noticeably less than in the neighboring Te and Ba isotopes.

The conclusion of the calculations for the properties of the yrast-band states is that in light and heavy isotopes of xenon the bands intersect differently. In light isotopes, the decrease in the contribution of the collective component as the spin increases can occur smoothly, which also corresponds to a smooth change in the values of  $B(E2)$ . This is done in cases where the value of the chemical potential is far in energy from the state of unique

Table 1. Probabilities of  $E2$  transitions in  $^{128}\text{Xe}$ 

$I_i \rightarrow I_f$	$B(E2; I_i \rightarrow I_f)$				
	Exp. [37]	Exp. [38]	Exp. [39]	Exp. [39]	Th.
$2_1^+ (0.443) \rightarrow 0_1$		$1830^{+550}_{-340}$	1760(200)	1540(80)	1840
$4_1^+ (1.033) \rightarrow 2_1$	2430(200)	2370(100)	2390(100)	2260(200)	2770
$6_1^+ (1.737) \rightarrow 4_1$	4060(500)	2360(120)	$2950^{+420}_{-330}$	2970(280)	2380
$8_1^+ (2.513) \rightarrow 6_1$				$3670^{+450}_{-360}$	3620
$10_1^+ (3.197) \rightarrow 8_1$				$> 0.94$	182
$12_1^+ (3.809) \rightarrow 10_1$					1864
$14_1^+ (4.618) \rightarrow 12_1$					2788
$10_2^+ (3.365) \rightarrow 8_1$				$1410^{+700}_{-350}$	3390
$12_2^+ (4.251) \rightarrow 10_2$					3464
$14_2^+ (5.097) \rightarrow 12_2$					3868
$16_3^+ (5.968) \rightarrow 14_2$					4037
$18_3^+ \rightarrow 16_3$					3956
$16_2^+ (5.573) \rightarrow 14_1$					3300
$18_2^+ (6.606) \rightarrow 16_2$					3656

parity (in this case it is  $h_{11/2}$ ). In Xe isotopes, this is the case for  $A \leq 120$ . On the contrary, if the chemical potential turns out to be near the state of unique parity, then the transition in the wave function of the yrast bands from the collective component to that with the  $b_{10}$  boson occurs abruptly at a certain spin  $I_0$ , which is reflected in a significant decrease in the value of  $B(E2; I_0 \rightarrow I_0 - 2)$ . In xenon isotopes this occurs starting from  $^{122}\text{Xe}$ .

Similar studies of the  $^{120-130}\text{Ba}$  isotope chain presented in [44] indicate an obvious intersection of the bands in such a way that in light isotopes the collective component is lost by more than half in states with a spin of  $12^+$ , and in  $^{128,130}\text{Ba}$  with a spin of  $10^+$ . This is confirmed by the consistency of the experimental and theoretical values of  $B(E2)$ .

The properties of the  $^{122-132}\text{Ce}$  isotope chain were considered in [21]. In all these nuclei, the bands invariably intersect. Although backbending is not observed for the  $^{122}\text{Ce}$  nucleus, analysis of the obtained wave function shows that at the spin  $12^+$  in this nucleus the intersection of bands still occurs, which corresponds to a decrease in  $B(E2)$  from this state. In general, all available values of  $B(E2)$  correspond to theoretical values, except for two transitions in  $^{126}\text{Ce}$ .

#### 4. CALCULATION RESULTS FOR $^{220-236}\text{Th}$

A number of works were devoted to the theoretical study of nuclei in the actinide region and the possible reasons for the lack of reverse bending, among them [47], where the properties of a number of nuclei were considered in the context of the HFB method, among which was the  $^{232}\text{Th}$  nucleus. In [48], using the method of pairing self-consistent independent quasiparticles, the

possibility of the occurrence of the reverse bending effect in actinide nuclei was studied. The deformed Woods–Saxon potential was used, followed by pairing. The calculation results explained why there is no reverse bending in most actinide nuclei, and at the same time it was suggested that in some light nuclei, Th and Ra, the backbending effect may occur. Of the thorium isotopes, the  $^{224}\text{Th}$  nucleus was considered. The analysis presented below confirms this assumption.

Among heavy and superheavy nuclei, starting at least from  $Z = 90$ , there are only two nuclei for which backbending is observed. These nuclei include  $^{220}\text{Th}$  and  $^{244}\text{Pu}$ . Indeed, in a number of even isotopes Pu, Cm, Fm, No, the energies of states of the yrast bands are known up to the spin  $32^+$ , as for example in the  $^{248}\text{Cm}$  nucleus, which is demonstrated in Fig. 6, showing the moments of inertia for the  $^{220}\text{Th}$ ,  $^{244}\text{Pu}$  and  $^{248}\text{Cm}$  nuclei.

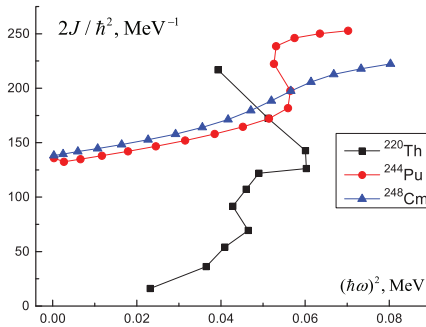


Fig. 6. Effective moments of inertia for  $^{220}\text{Th}$ ,  $^{244}\text{Pu}$ ,  $^{248}\text{Cm}$

For other nuclei with  $Z \geq 90$ , no backbending is observed. To consider the evolution of the nature of states as spin increases, thorium isotopes with  $A$  from 220 to 236 are considered. It should be noted that a preliminary analysis of excitation energies in a number of even thorium isotopes within the IBM phenomenology shows that the calculated energy values at high spins not only do not exceed the experimental ones, but, on the contrary, turn out to be less than the experimental ones. There may be several reasons for this. One is the exhaustion of quasiparticle space in the valence shell as the spin of states increases. This would be automatically taken into account if it were possible to carry out consistent calculations regarding the boson and phonon amplitudes for each collective state considered separately, as was done for the Xe–Ce isotopes. For heavy nuclei, it is possible to achieve matching only based on the ground state. Another possible reason, and this has been realized for a number of nuclei, is the weakening of the connection between collective and non-collective states with increasing spin. This made it possible to satisfactorily reproduce the energies of experimental states at high spins.

The mean-field parameters are taken from [49], the single-particle basis includes 40 levels for both neutrons and protons, and multipole forces are

Table 2. Accepted boson parameters for  $^{220-236}\text{Th}$

Nucleus	$\Omega$	$\varepsilon_d$	$k_1$	$k_2$	$C_0$	$C_2$	$C_4$
$^{220}\text{Th-IBM-ph}$	19	0.42226	-0.0068	0.00456	0	0	0.00341
$^{220}\text{Th-Lp1}$	19	0.4017	0	0	0	0	0.04056
$^{220}\text{Th-Lp2}$	18	0.385	0	0	0	0	0.0271
$^{222}\text{Th-Lp1}$	24	0.5906	-0.0176	0.00944	0.0001	-0.000979	-0.00286
$^{222}\text{Th-Lp2}$	23	0.38555	-0.0067	0.00075	0.0042	0.00074	0.0109
$^{224}\text{Th-Lp1}$	24	0.4871	-0.025	0.0033	0.0045	-0.023	-0.02892
$^{224}\text{Th-Lp2}$	23	0.5447	-0.025	0.01081	0.005	0.0042	-0.00469
$^{226}\text{Th-IBM-ph}$	28	0.36797	-0.031	0.00337	-0.08073	-0.02292	-0.035625
$^{226}\text{Th-Lp1=Lp2}$	28	0.3277	-0.03268	0.00269	-0.08365	-0.02217	-0.04014
$^{228}\text{Th-IBM-ph=Lp}$	30	0.4561	-0.0262	0.00451	-0.09271	-0.01850	-0.03525
$^{228}\text{Th-micr}$	28	0.4127	-0.048	0.0069	0.0011	0.0045	-0.0347
$^{230}\text{Th-IBM-ph=Lp}$	30	0.3172	-0.03393	0.0114	-0.05896	-0.01128	-0.04547
$^{230}\text{Th-micr}$	30	0.0984	-0.0397	0.0193	0.0148	0.0387	-0.042
$^{232}\text{Th-IBM-ph=Lp}$	30	0.440	-0.0293	0.006255	-0.1278	-0.03186	-0.0413
$^{232}\text{Th-micr}$	28	0.03018	-0.04464	0.0164	0.0276	0.0527	-0.0686
$^{234}\text{Th-IBM-ph=Lp}$	28	0.2621	-0.03054	0.00885	-0.09865	-0.03149	-0.0340
$^{234}\text{Th-micr}$	28	0.0570	-0.0409	0.0183	0.0442	0.0482	-0.0728
$^{236}\text{Th-IBM-ph=Lp}$	26	0.3651	-0.02897	0.00901	-0.13094	-0.03698	-0.03874
$^{236}\text{Th-micr}$	26	0.3009	-0.0372	0.0243	0.0916	0.0582	-0.0381

determined with constants close to the estimates given in [25]. With the structure of  $D$  phonons determined in this way, all parameters of the extended Hamiltonian were calculated, which determine the interaction channels of configurations containing  $B_J$  phonons. Since the purpose of this work is to clarify the nature of the states of the yrast band, a calculation method was implemented in which the parameters of the boson Hamiltonian were selected phenomenologically, but close to microscopic estimates in accordance with the matching of boson and phonon amplitudes for the ground state. Unless otherwise stated, two sets of  $H_{\text{IBM}}$  parameters are considered, one for those components of the wave function in which non-collective bosons (Lp1) are not clearly present and a second set where such bosons are present (Lp2). This technique introduces a significant element of phenomenology into the theory used, naturally leading to a better agreement between theoretical and experimental data. The parameters corresponding to the interaction with high-spin excitation modes are found as a result of calculations based on internucleon forces and the average field. It is worth immediately commenting on the notation and data given in Table 2. For each nucleus, sets of Hamiltonian parameters Lp1 and Lp2 are given. For  $^{220,226-236}\text{Th}$  nuclei these are the same. For  $^{228-236}\text{Th}$  nuclei, the values obtained on the basis of microscopic calculations are also given. This was done to compare them with phenomenological values. For any of the nuclei considered in this section, except for  $^{220}\text{Th}$ , due to the large values of the total number of bosons, a large number of configurations with different values of the numbers of quadrupole bosons  $n_d$  are realized already in the ground state, even at a single-boson energy  $\varepsilon_d \simeq 0.4$  MeV.

**4.1. Nucleus  $^{220}\text{Th}$ .** The  $^{220}\text{Th}$  nucleus is one of two  $Z \geq 90$  nuclei for which backbending is observed and the only one in this region where a second backbending is also observed. The  $^{220-230}\text{Th}$  isotopes were previously considered in IBM phenomenology [50]. The total number of bosons corresponded to the number of pairs of valence particles or holes. It changed from 6 to 11 units as the mass number of isotopes increased. In this case, the spin of the calculated states exceeded the permissible value. It can be assumed that the eigenvalues of the Hamiltonian were found not as a result of diagonalization, but based on approximations between various IBM limits. Nevertheless, this stimulated the possibility of describing the energies of the nuclei in question using IBM phenomenology in the present calculations. In particular, this was done for  $^{220}\text{Th}$ . The corresponding energies are given in Table 3. To represent the nature of the spectrum of this nucleus, Fig. 7 shows the energies of the states of the yrast band depending on the spin. It is seen that the nature of the spectrum corresponds to vibration with weak anharmonicity. This is realized using a bosonic Hamiltonian corresponding to the  $SU(5)$  limit of the IBM1 with parameters  $\varepsilon_d$  and  $C_4$ .

The figure does not show any anomaly that leads to the first “backbending”. This is due to a very small anomaly of energies for a given nucleus, and the scale of the figure does not play a role here. When carrying

Table 3. Comparison of experimental [31] and theoretical energy values in keV for  $^{220,222,224}\text{Th}$  nuclei

$I^\pi$	$^{220}\text{Th}$			$^{222}\text{Th}$		$^{224}\text{Th}$	
	Exp.	IBM-ph.	Th.	Exp.	Th.	Exp.	Th.
$2^+$	373.3	373.9	371	183.3	183.1	98.1	97.5
$4^+$	759.8	762.8	762	439.8	450	284.1	283.7
$6^+$	1166	1166	1175	750	763	534.7	533.7
$8^+$	1598.2	1584	1597	1093.5	1102	833.9	834.2
$10^+$	2012.7	2014	2013	1461.1	1468	1173.8	1175.4
$12^+$	2441.9	2456	2433	1850.7	1850	1549.8	1551.3
$14^+$	2885	2908	2887	2259.7	2252	1958.9	1956.9
$16^+$	3376.4	3370	3366	2687.8	2677	2398	2396.5
$18^+$	3867.1	3841	3875	3133.5	3124	2864	2853
$20^+$	4319.6	4319	4416	3596	3599		
$22^+$	4716.1	4804	4977	4077.6	4080		
$24^+$		5294	5586	4577.9	4586		
$26^+$				5097.9	5113		
$28^+$					5655		
$30^+$							
$32^+$							
$34^+$							

out theoretical calculations, it should be borne in mind that it is apparently impossible to implement a self-consistent calculation scheme for a given nucleus, since it assumes non-zero values of the boson Hamiltonian parameter  $k_1$ , which ensures the connection of states that differ by two  $d$  bosons. Therefore, a calculation method was implemented when the parameters of the boson Hamiltonian  $H_{\text{IBM}}$ , determined only by the  $d$  and  $s$  bosons, were selected phenomenologically, and the parameters corresponding to the interaction with high-spin excitation modes were found as a result of calculations based on internucleon forces and the average field, for example, as was carried out in [20]. The parameter  $E_0^{(b)}$  was taken equal to  $-0.25$  MeV. The interaction of collective and quasiparticle modes, which are considered through non-collective bosons, is also additionally suppressed by  $\zeta^2 = 0.7$  (see (59)). The energies of collective states through the parameters of the IBM Hamiltonian that determine them usually differ depending on whether non-collective phonons with multipolarities  $J = 2^+ - 14^+$  are explicitly present in the corresponding components of the wave function. The theoretical energies of the states are given in Table 3, and the corresponding moments of inertia versus the square of the frequency in Fig. 8.

All this leads to a good reproduction of experimental energies and, what is especially interesting, to the reproduction of the moment of inertia at spins of  $10^+$  and  $12^+$ , although the effect is caused by an energy anomaly of only 10 keV. Experimental and calculated energies for  $^{220}\text{Th}$  are shown in Fig. 7 and in Table 3. They also correspond to the moments of inertia shown in

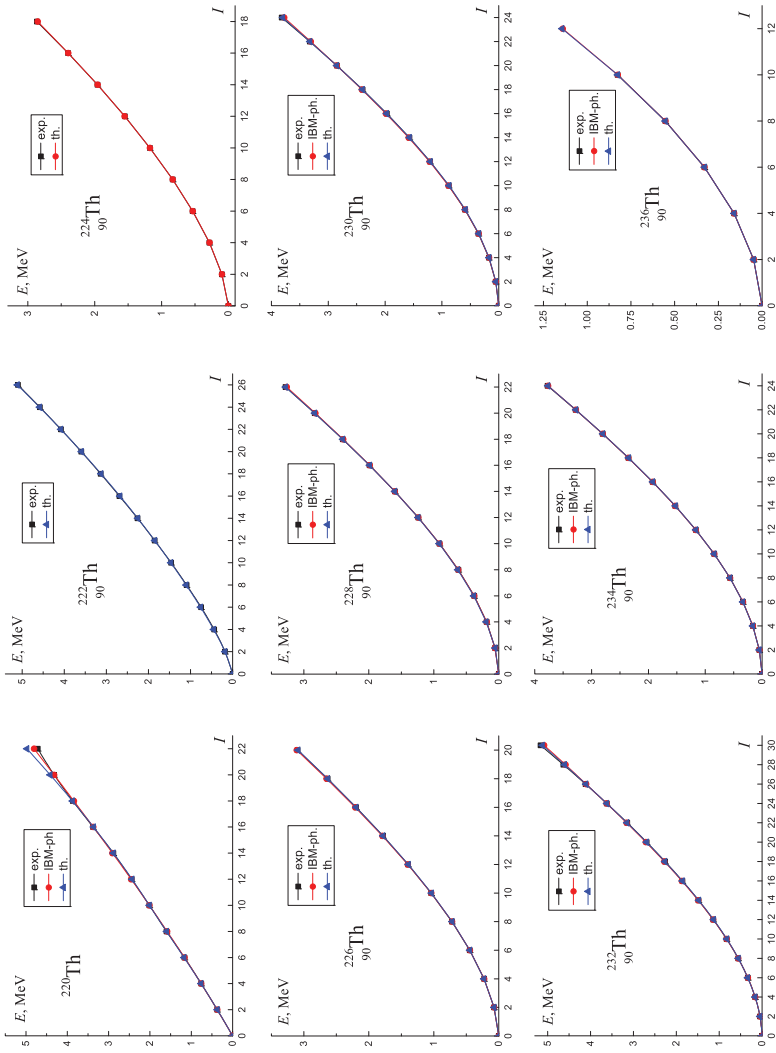


Fig. 7. Experimental, phenomenological and theoretical values of the energies of the yrast bands of Th isotopes depending on the spin



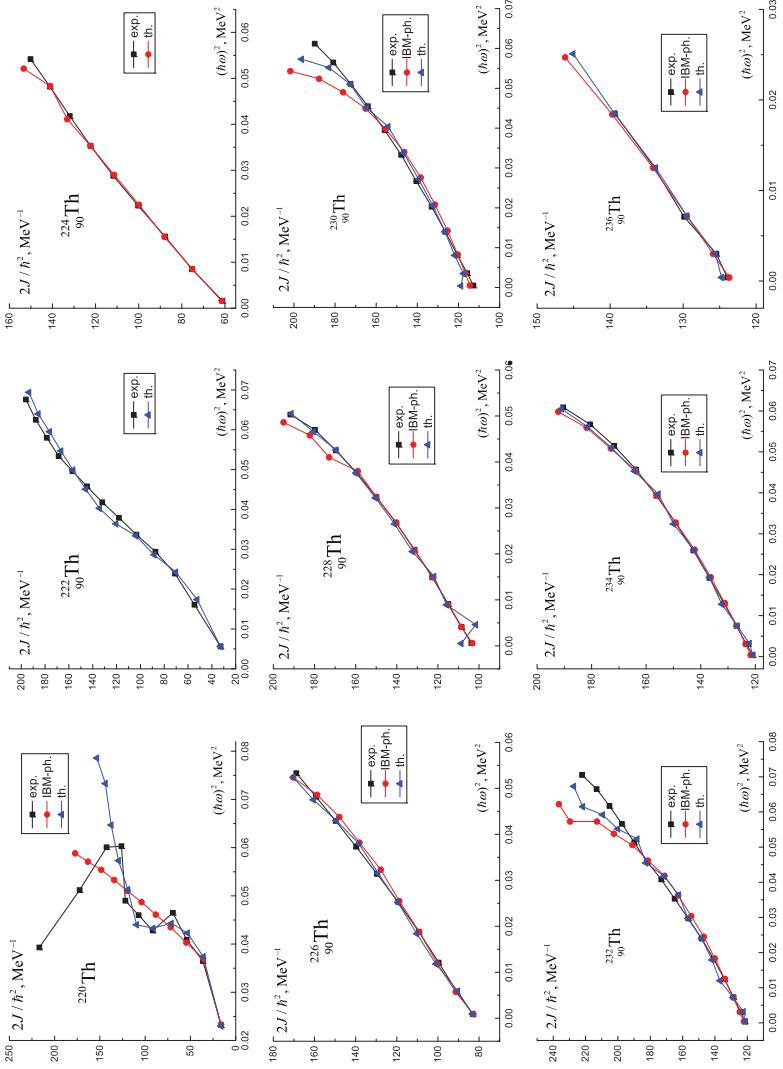


Fig. 8. Effective moments of inertia from experimental and theoretical energy values of yrast bands in Th isotopes

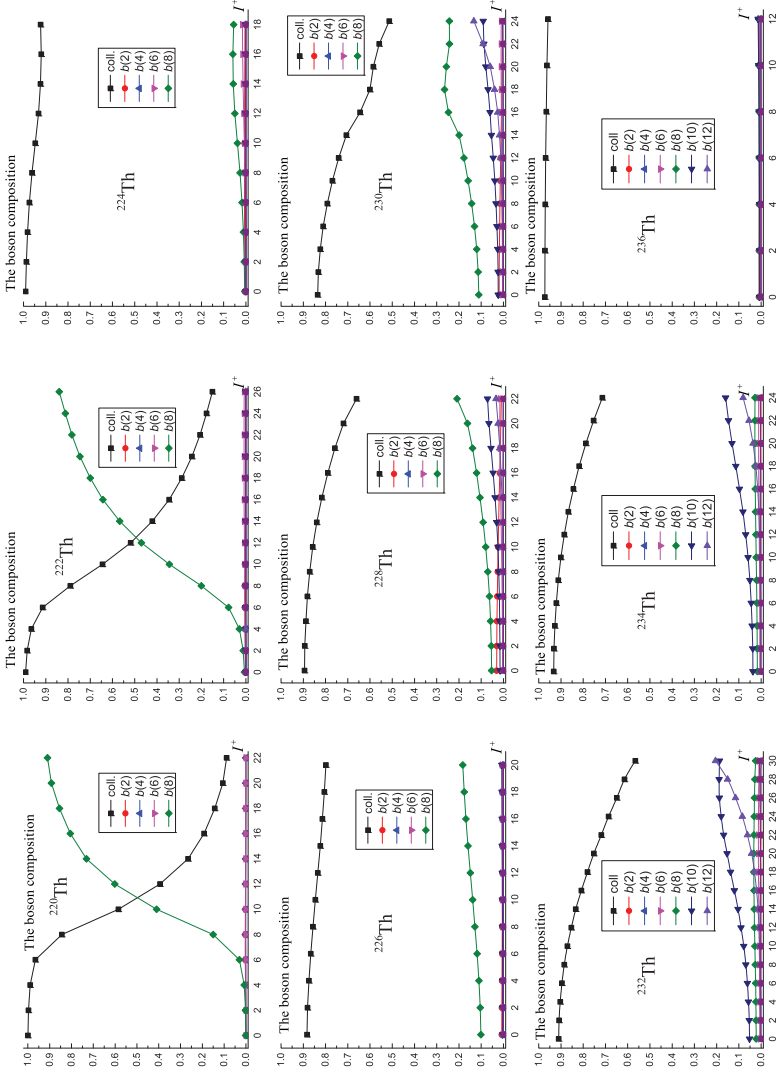


Fig. 9. Composition of wave functions of states of yrast bands in Th isotopes

Fig. 8. From the last figure it is clear that the calculation reproduces the reverse bending of the moment of inertia. The phenomenological calculation, though it gives a seemingly satisfactory quality of description of the energies of states, cannot describe this effect.

Figure 9 shows the boson composition of the wave functions. The component in the wave function with  $B_{J=8}$  becomes the main one at the value of the spin of the yrast band  $I^\pi = 12^+$ ; at  $I^\pi = 10^+$  the corresponding component is significant. In this nucleus, a smooth replacement of the collective component with a quasiparticle component occurs.

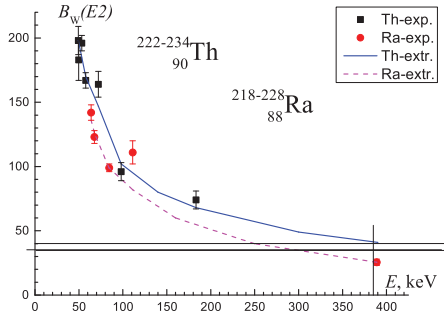


Fig. 10. Values of  $B(E2)$  for the lowest transition in a number of Th and Ra isotopes

There are no experimental estimates of transition probabilities for this nucleus. Therefore, an approximation of the  $B(E2)$  values was carried out depending on the energy using the even isotopes of Th and Ra (Fig. 10). This gives reason to assume that the value of  $B_W(E2; 2_1^+ \rightarrow 0_1^+)$  may be on the order of 40 units. This value was adopted for orientation. A coordinated change in the quadrupole forces in the partial-hole and partial-particle channels makes it possible to leave the phonon energy unchanged, but within a certain limit to change the values of  $B(E2)$ . The paper [51] gives a theoretical estimate for  $B(E2; 2_1^+ \rightarrow 0_1^+)$  equal to 35.6 single-particle units. Figure 11 shows the theoretical values of  $B_W(E2; I \rightarrow I - 2)$ , which implies some decrease for spins  $I^\pi = 10^+$  and  $I^\pi = 12^+$ . Although, based on typical experimental errors, this feature may not be noticed.

Obviously, the second backbending is not described in the theory under consideration. The lowest two-quasiparticle pair in the used quasiparticle basis is the proton pair  $h_{9/2\pi}^2$ . Its maximum angular momentum is  $8^+$ . Accordingly, a four-quasiparticle excitation at this single-particle level will have a spin of  $12^+$ . It is with the admixture of four-quasiparticle states that one can associate the presence of a second backbending in any nucleus. To explain the second backbending by replacing components with one pair of quasiparticles with another in the wave function, for example,  $h_{9/2}^2$  with  $j_{15/2}^2$ , seems hardly feasible due to smallness of the corresponding matrix elements.

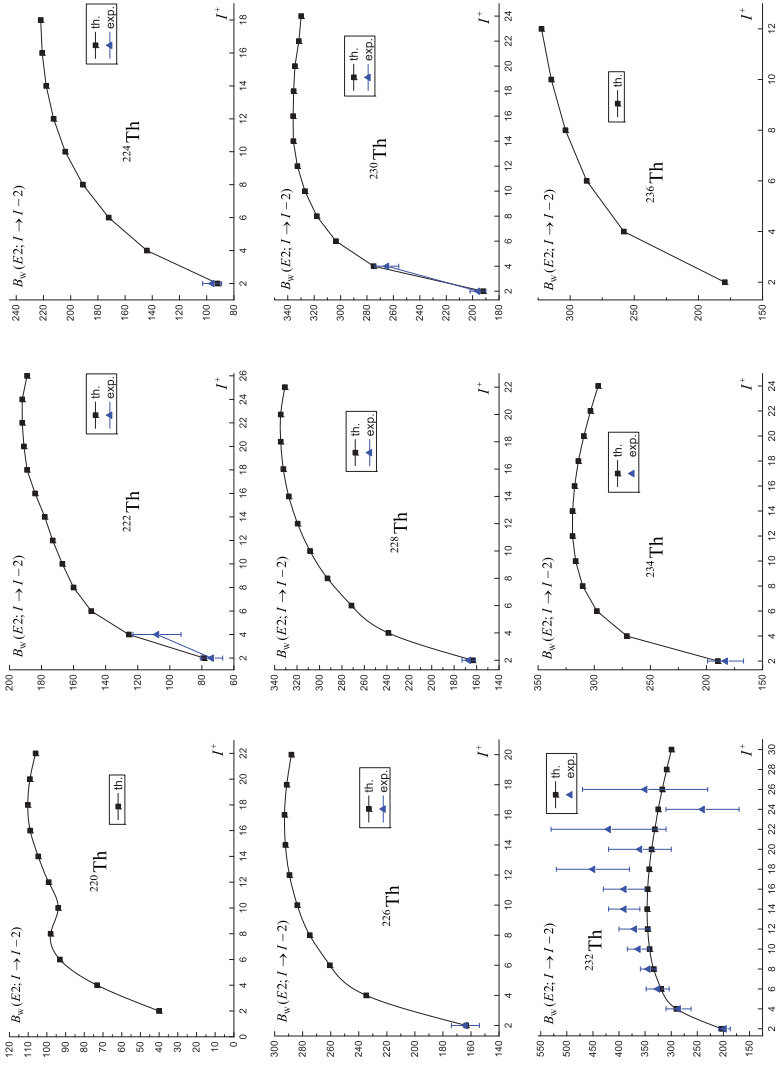


Fig. 11. Values of  $B(E2)$  in Th isotopes, experimental values are from [31]

**4.2. Nucleus  $^{222}\text{Th}$ .** In the  $^{222}\text{Th}$  nucleus, compared to a lighter isotope, there is a significant decrease in excitation energies, which leads to a change in the nature of the spectrum, which exhibits a weakly expressed parabolic character of the  $E(I)$  function (Fig. 7).

When implementing self-consistency of the calculated parameters of the boson Hamiltonian  $H_{\text{IBM}}$  and boson averages in heavy nuclei, at least starting from nuclei with  $Z = 90$ , there are certain difficulties, which turned out to be associated with increased sensitivity of the calculated energies and boson averages from the  $C_L$  parameters of the  $H_{\text{IBM}}$  Hamiltonian. This was not the case when calculating the properties of collective states in intermediate nuclei from Te [16], Xe [23], Ba [44], Ce [21] to  $^{156}\text{Dy}$  [45]. At the same time, it was already noted in the cited works that the calculated values of the parameters  $C_L$  ( $L = 0, 2, 4$ ) are determined by the difference between two quantities, which largely compensate each other. Some of these quantities,  $C_L^{(0)}$  for all  $L$  turn out to be significantly larger than those determined from the analysis of experimental data within phenomenology. This effect, called the kinematic effect [24, 46], is due to the fact that  $D$  phonons do not exactly map onto  $d$  bosons. In two-phonon states, this effect is a consequence of the Pauli principle regarding quasiparticles belonging to different  $D$  modes, as well as the result of the action of attractive forces between quasiparticles forming different phonons and specific phase relationships. All this does not depend on whether the nucleus is spherical or deformed. Expressions for  $C_L^{(0)}$  obtained from various processes are given in [26].

Compensation of the  $C_L^{(0)}$  values occurs due to dynamic effects, namely, by taking into account the connection between collective modes containing  $(D^2)^{(L)}$  with states containing  $B_J$  modes [21]. It is important to emphasize here that the increased sensitivity of the calculated energies and boson averages of the Hamiltonian  $H_{\text{IBM}}$  terms,  $C_L$ , leads to the problem of achieving agreement between microscopic boson parameters and boson averages. The estimates obtained for  $C_{L=0,2,4}^{(0)}$  are 0.525, 0.221 and 0.219 MeV. As a result of their renormalization, the values of  $C_L$  can become completely negative. The total number of bosons  $\Omega$  turns out to be 24.

Let us emphasize once again that all states containing non-collective bosons were shifted by  $E_0^{(b)}$ . This shift can be either positive or negative. The negative shift is explained by the unaccounted influence of four quasiparticle configurations or components in the wave function containing two non-collective bosons  $B_{J_1}$  and  $B_{J_2}$ . It was assumed that  $E_0^{(b)} = -0.4$  MeV. At the same time, at each iteration a constant number of particles on average was achieved. The number of particles is determined not only by Bogolyubov amplitudes, but also by the amplitudes of  $D$  phonons and boson averages. The total number of bosons is a calculated quantity, which is kept constant and equal, as already mentioned, to 24. In addition, at each iteration, the measure of correlations in the ground state was kept unchanged small, namely,  $\sum \varphi^2 / \sum \psi^2 = 0.01$ , which is achieved through modification of the quasiparticle random phase method [21].

Theoretical and experimental energy values for  $^{222}\text{Th}$  are given in Table 3 and Fig. 7. The values of the moments of inertia are shown in Fig. 8.

Figure 9 shows the boson composition of the wave functions. The component in the wave function with  $B_{J=8}$  becomes the main one when the spin of the yrast band is  $I^\pi = 14^+$ . In this case, a smooth replacement of the collective component with a quasiparticle component occurs. It is so smooth that it does not appear in the functional dependence of the moment of inertia on the square of the frequency and in the theoretical values of  $B(E2)$ , which are shown in Fig. 11. Experimental values are known only for the two lowest transitions, and these are reproduced. Everything that has been said regarding the  $^{222}\text{Th}$  nucleus suggests that, despite the absence of a reverse bend in the behavior of the moments of inertia from the square of the rotation frequency, the intersection of the bands still occurs, but quite smoothly as the spins of the observed states increase from  $I^\pi = 8^+$  to  $I^\pi = 16^+$ .

**4.3. Nucleus  $^{224}\text{Th}$ .** Figure 7 shows experimental and calculated energy values of  $^{224}\text{Th}$  nucleus depending on spin. Figure 8 shows the corresponding values of the effective moments of inertia. It can be seen that there is no manifestation of the intersection of bands. This gives grounds for understanding that almost all observed states up to the spin  $I^\pi = 18^+$  can be reproduced within the usual IBM phenomenology with the Hamiltonian (6). For this, it turned out to be sufficient to set the parameter  $E_0^{(b)} = 0.4$  MeV. The boson composition of the wave functions is shown in Fig. 8. Comparison of its composition with that obtained for  $^{222}\text{Th}$  shows that starting from  $^{224}\text{Th}$  no intersection of bands is observed. This is due, on the one hand, to the low energies of the lowest excitations, as well as to the value of  $E_0^{(b)}$ , which, starting from this isotope, in the chain of Th isotopes, turns out to be a positive value. The values of  $B(E2)$  along the yrast band are shown in Fig. 11, where the experimental value from the lowest excited state is noticeably larger than that of the previous nucleus.

**4.4. Nucleus  $^{226}\text{Th}$ .** Figure 7 shows experimental and calculated energy values of  $^{226}\text{Th}$  nucleus. A smooth and regular behavior of spin energy values is observed. Regularity is manifested to an even greater extent in the behavior of moments of inertia (Fig. 8). This indicates the absence of signs of band crossing and gives grounds for understanding that all observed states up to the spin  $I^\pi = 20^+$  can also be reproduced within the usual phenomenology of the IBM with the Hamiltonian (6). Therefore, this possibility was considered. Table 2 shows for this case the parameters of the Hamiltonian (6), designated as IBM-ph, which are close to those obtained within the theoretical consideration. The corresponding calculated energies, together with the experimental ones, are given in Table 4. Thus, the question arises about the role of possible high-spin excitation modes. The role of these modes can be partially reduced due to the value of  $E_0^{(b)}$ , which was taken equal to 0.6 MeV, but this turned out to be insufficient to adequately describe the energy values at high spins. The description was obtained by taking into account the possible difference in  $D$ -phonon amplitudes in purely collective

components of the wave function and the components in which non-collective excitation modes are present.

Table 4. **Comparison of experimental [31] and theoretical energy values in keV for  $^{226,228}\text{Th}$  nuclei**

$I^\pi$	$^{226}\text{Th}$			$^{228}\text{Th}$		
	Exp.	IBM-ph.	Th.	Exp.	IBM-ph.	Th.
$2^+$	72.2	72.6	72.1	57.8	58.1	55.2
$4^+$	226.4	225.7	227	186.8	187	193
$6^+$	447.3	445.1	445	378.2	378	383
$8^+$	721.9	719.6	717	622.5	623	629
$10^+$	1040.3	1040	1035	911.8	912	916
$12^+$	1395.2	1399	1391	1239.3	1239	1242
$14^+$	1781.5	1791	1781	1599.4	1599	1601
$16^+$	2195.8	2210	2196	1987.9	1986	1989
$18^+$	2635.1	2651	2632	2400.5	2395	2402
$20^+$	3097.1	3109	3090	2834.4	2823	2834
$22^+$				3283	3264	3283.5

Attenuation that reduces the interaction of states differing in the presence of a  $B$  phonon and determined by the parameter  $\varsigma$  in the relation

$$\langle D^{n'} B | H | D^{+n} \rangle \rightarrow \varsigma \langle D^{n'} B | H | D^{+n} \rangle \quad (59)$$

was taken into account in all works of this series related to the microscopic calculation of the parameters of the IBM1 Hamiltonian. When analyzing the mechanism of band crossing in even Ce isotopes [21], it was noted that this weakening can play an increasingly important role as the spin in the band increases.

To determine the dependence of  $\varsigma$  on the characteristics of the collective state,  $\varsigma(I)$ , in [45] it was assumed that this weakening is associated with a difference in the structure of  $D$ -phonon amplitudes depending on whether there is a  $B$  phonon in the component of the wave function, i.e., that in the presence of a  $B$  phonon, the  $D$  phonon changes somewhat, becoming a  $D'$  phonon. The difference is associated with both phonon amplitudes and superfluidity parameters. Let

$$\xi = \langle D' | D^+ \rangle, \quad (60)$$

then we can assume that  $\varsigma \sim \xi^{n_d(I)}$ . In this work, we used the parameterization

$$\varsigma = \varsigma_0 \xi^{\langle n_d - n_d(I=0) \rangle}. \quad (61)$$

For  $^{226}\text{Th}$  it was assumed that  $\varsigma_0^2 = 0.7$ ,  $\xi^2 = 0.78$ . Taking into account the boson averages  $\langle n_d \rangle$ , which for spins of states from  $I = 0^+$  to  $I = 20^+$  in accordance with microscopic calculations turned out to be respectively equal

to 14.95, 15.06, 15.29, 15.61, 15.99, 16.42, 16.88, 17.37, 17.88, 18.4, 18.94. This led to the values of the parameter  $\zeta^2$  for spins from  $I = 0^+$  to  $I = 20^+$  respectively equal to 0.7, 0.681, 0.643, 0.594, 0.541, 0.486, 0.433, 0.384, 0.338, 0.297, 0.260.

In this case, the parameter  $E_0^{(b)}$  was taken equal to 0.6 MeV. Figure 7 shows experimental, theoretical values and those obtained within the phenomenology of energy magnetic resonance. Table 4 gives their numerical values. Figure 8 compares the corresponding values of the moments of inertia. It should be noted that the moments of inertia obtained from experimental energies give a line that slightly deviates from a straight line. Both calculated curves in this figure are close to the one obtained from experimental energies, but still do not exhibit such smoothness. This reveals the non-random nature of highly collectivized states, which is violated when non-collective components are introduced into the wave functions of the analyzed states. When using the IBM as a phenomenological model, this regularity is preserved except for states with a small number of configurations, namely, for spins with  $I = 2\Omega - 2$  and  $I = 2\Omega$ , where  $\Omega$  is the maximum number of bosons. For the latter spin, the wave function consists of a single configuration, which leads to irregularity in the energy. In the presented calculation, it was possible to avoid noticeable deviations from the experimental data.

The boson composition of the wave functions is shown in Fig. 9, which implies a weak drop in the collective component, such that for the limiting spin it remains at the level of 80%. This indicates the absence of the effect of band crossing in this nucleus up to the maximum observed spin  $I = 20^+$ . Qualitatively, this was clear from the possibility of reproducing experimental energies in the IBM phenomenology.

The values of  $B(E2)$  along the yrast band for  $^{226}\text{Th}$  are shown in Fig. 11. To significantly increase the calculated value of  $B(E2)$  compared to previous nuclei, it was necessary to slightly change the spin-orbit splitting parameter. When calculating the mean-field levels, the Saxon-Woods potential was used and its parameters were taken in accordance with [49]. For  $^{226}\text{Th}$ , an exception was made for the spin-orbit splitting parameter. The value used differs by a factor of 1.0364. This turned out to be sufficient to reproduce the experimentally known value of  $B_W(E2; 2^+ \rightarrow 0^+) = 164(10)$ .

**4.5. Nucleus  $^{228}\text{Th}$ .** Figure 7 and Table 4 show the energy values for the  $^{228}\text{Th}$  nucleus. The quality of the description is better demonstrated by the behavior of  $J(\omega^2)$ , shown in Fig. 8. Some discrepancy between the calculated and experimental points in this figure for the first two transitions is due to the low energies of the corresponding states. This is caused by the discrepancy between theory and experiment for the  $2_1^+$  and  $4_1^+$  states at 2.6 and 7 keV, as can be seen from Table 4. It is interesting that at high spins the theoretical values of the moment of inertia provide a significantly better description of the experimental points than those obtained from the phenomenology of the IBM. In this case, a certain rise or lifting of  $J(\omega^2)$  (upbending) [52] is realized.



From Fig. 9, where the boson composition of the wave functions is shown, it is clear that there is a smooth decrease in the collective component to 65% and an increase in the component with the boson multipole  $J = 8^+$  up to 20% at the observed spin  $I = 22^+$ . This does not lead to the effect of bands crossing, but only to a slight increase in the moment of inertia.

In the theoretical calculation, the value of  $E_0^{(b)}$  was taken equal to 0.3 MeV,  $\zeta_0^2 = 0.7$ ,  $\xi^2 = 0.817$ . Taking into account the boson averages  $\langle n_d \rangle$ , which correspond to the microscopic parameters given in Table 2, the values of the parameter  $\zeta^2$  for spins from  $I = 0^+$  to  $I = 22^+$  are respectively equal to 0.7, 0.6878, 0.6617, 0.6266, 0.5859, 0.5426, 0.4988, 0.4557, 0.4143, 0.3752, 0.3385, 0.3046.

The values of  $B(E2)$  along the yrast band for  $^{228}\text{Th}$  are shown in Fig. 11. For  $^{228}\text{Th}$ , as well as for  $^{226}\text{Th}$ , the spin-orbit splitting parameter was increased compared to the value proposed in [49]. For  $^{228}\text{Th}$ , it differs by a factor of 1.0738. The experimental value  $B_W(E2; 2^+ \rightarrow 0^+) = 167(6)$  is reproduced.

**4.6. Nucleus  $^{230}\text{Th}$ .** Figures 7 and 8 show the values of energies and moments of inertia for  $^{230}\text{Th}$ . The maximum number of quadrupole bosons is  $\Omega = 30$ . Phenomenological calculations within the IBM lead to underestimated energy values for states with spins  $I = 22^+$ ,  $24^+$ , as can be seen from Table 5. As can be seen from Fig. 8, taking into account high-spin excitation modes does not completely correct the situation.

In the theoretical calculation, the value of  $E_0^{(b)}$  was taken equal to 0.4 MeV,  $\zeta_0^2 = 0.68$ ,  $\xi^2 = 0.7935$ . Taking into account the boson averages

Table 5. Comparison of experimental [31] and theoretical energy values in keV for  $^{230,232}\text{Th}$  nuclei

$I^\pi$	$^{230}\text{Th}$			$^{232}\text{Th}$		
	Exp.	IBM-ph.	Th.	Exp.	IBM-ph.	Th.
2 <sup>+</sup>	53.2	52.4	50.5	49.4	49.15	49.4
4 <sup>+</sup>	174.1	172.4	169.5	162	161.5	163.8
6 <sup>+</sup>	356.5	355.1	350	333.3	332.5	334.7
8 <sup>+</sup>	593.8	594.4	587	556.9	556.6	553.9
10 <sup>+</sup>	879.3	883.5	874	826.8	827.9	822.0
12 <sup>+</sup>	1206.6	1216	1204	1137.1	1141	1132.2
14 <sup>+</sup>	1571.8	1585	1572	1482.2	1490	1477.0
16 <sup>+</sup>	1969.5	1984	1974	1858.2	1871	1858.7
18 <sup>+</sup>	2396.3	2408	2399	2262.4	2280	2267.2
20 <sup>+</sup>	2848.6	2851	2851	2691	2710	2694
22 <sup>+</sup>	3324	3309	3321	3144	3160	3151.3
24 <sup>+</sup>	3819	3775	3800	3620	3624	3621.1
26 <sup>+</sup>				4117	4103	4108
28 <sup>+</sup>				4633	4582	4604
30 <sup>+</sup>				5164	5081	5123

$\langle n_d \rangle$ , the values of the parameter  $\zeta^2$  for spins from  $I = 0^+$  to  $I = 24^+$  are respectively equal to 0.68, 0.6702, 0.6488, 0.6180, 0.5808, 0.540, 0.4972, 0.4545, 0.4129, 0.3730, 0.3556, 0.3008, 0.2687.

The cases when, within the phenomenology, the energies of calculated states at high spins give underestimated values are quite rare; even Te isotopes can probably be attributed to them. One of the explanations may be related to the fact that if the maximum number of bosons  $\Omega$  turned out to be equal to 12 or 13, then already within the IBM phenomenology the states  $I = 22^+$  and  $I = 24^+$  would have a larger energy due to the extremely low number of boson configurations. The weakness of this explanation is due to the unfoundedness of using a small part of the maximum number of bosons. Another reason that can lead to an increase in high-spin states can be the increase in the number of quadrupole bosons in states as the spin increases. In consistent calculations (consistency of boson averages and microscopically calculated boson parameters), which were successfully carried out for Te to Dy isotopes, this increase is realized automatically due to a smooth change in the structure of collective  $D$  phonons.

Figure 9 shows the boson composition of the wave functions. As for the previous nuclei, there is a smooth decrease in the collective component. In  $^{230}\text{Th}$ , the collective component decreases to 50%, but remains predominant.

The values of  $B(E2)$  along the yrast band for  $^{230}\text{Th}$  are shown in Fig. 11. The spin-orbit splitting parameter was increased 1.18 times compared to the value proposed in [49]. The experimental values  $B_W(E2; 2^+ \rightarrow 0^+) = 196(6)$  and  $B_W(E2; 4^+ \rightarrow 2^+) = 265(9)$  are reproduced.

**4.7. Nucleus  $^{232}\text{Th}$ .** Figures 7 and 8 show the values of energies and moments of inertia for  $^{232}\text{Th}$ . Phenomenological calculations within the IBM lead to an accuracy of energy reproduction up to 7 keV for spins up to  $I^+ = 24^+$ ; for spins  $I^+ = 26^+$ ,  $28^+$ ,  $30^+$  the calculated energy values within the final calculation taking into account high-spin excitation modes are underestimated by 9, 29 and 42 keV, respectively, as can be seen from Table 5. A similar situation occurred for the previous nucleus,  $^{230}\text{Th}$ . The quality of the description could be improved if a self-consistent calculation were carried out for each band state separately. Such a calculation invariably leads to an increase in the energies of collective states. The fact that the calculated energies of states are significantly lower than the experimental ones at limiting values of spins may indicate an interruption of the band at these spins.

In the theoretical calculation, the value of  $E_0^{(b)}$  was taken equal to 1.35 MeV,  $\zeta_0^2 = 0.67$ ,  $\xi^2 = 0.7866$ . Taking into account the boson averages  $\langle n_d \rangle$  corresponding to the microscopic parameters given in Table 2, the values of the parameter  $\zeta^2$  for spins from  $I = 0^+$  to  $I = 30^+$  are respectively equal to 0.67, 0.659, 0.634, 0.600, 0.561, 0.518, 0.474, 0.431, 0.388, 0.349, 0.312, 0.278, 0.247, 0.219, 0.193, 0.1706.

Figure 9 shows the boson composition of the wave functions. As for the previous nuclei, there is a smooth decrease in the collective component. In  $^{232}\text{Th}$ , the collective component decreases to 56% with a spin of  $30^+$ .

The values of  $B(E2)$  along the yrast band for  $^{232}\text{Th}$  are shown in Fig. 11. The spin-orbit splitting parameter was increased 1.09882 times compared to the value proposed in [49]. The experimental values  $B_W(E2; 2^+ \rightarrow 0^+) = 198(11)$ ,  $B_W(E2; 4^+ \rightarrow 2^+) = 286(24)$  and subsequent ones up to  $B_W(E2; 26^+ \rightarrow 24^+) = 350(120)$  are reproduced. This is the only nucleus of thorium isotopes for which  $B(E2)$  values have been measured for almost the entire band.

**4.8. Nucleus  $^{234}\text{Th}$ .** Figures 7 and 8 show the values of energies and moments of inertia for  $^{234}\text{Th}$ . Theoretical calculation reproduces experimental energies with an accuracy of 1 keV up to the spin  $I^+ = 18^+$ ; for the spins  $I^+ = 20^+$ ,  $22^+$ ,  $24^+$  the calculated energy values are less than the experimental ones, respectively, by 3, 6 and 7 keV, as can be seen from Table 6. This quality of reproducing the energies of states is unique not only for thorium isotopes, but also for all nuclei in general. Similarly, a unique reproduction of the energies of the yrast band was obtained within the phenomenology of the IBM, which is also evident from Table 6. The appropriate quality of energy description leads to a precise reproduction of the moment of inertia in Fig. 8.

Table 6. **Comparison of experimental [31] and theoretical energy values in keV for  $^{234,236}\text{Th}$  nuclei**

$I^\pi$	$^{234}\text{Th}$			$^{236}\text{Th}$		
	Exp.	IBM-ph.	Th.	Exp.	IBM-ph.	Th.
$2^+$	49.6	49.3	49.6	48.4	48.5	48.1
$4^+$	163.1	162.6	164.2	160.0	159.7	159.6
$6^+$	336.5	336.1	338.0	329.4	329.6	329.5
$8^+$	564.7	564.8	564.8	553.4	553.3	553.8
$10^+$	842.5	843.6	842.7	826.1	825.3	826.4
$12^+$	1164.9	1167	1165.5		1140	1143.5
$14^+$	1526.6	1529	1525.6			
$16^+$	1923.4	1926	1924.2			
$18^+$	2351	2353	2350.2			
$20^+$	2805.1	2804	2801.9			
$22^+$	3281.4	3277	3275.9			
$24^+$	3775.1	3766	3767.9			

In the theoretical calculation, the value of  $E_0^{(b)}$  was taken equal to 1.6 MeV,  $\zeta_0^2 = 0.67$ ,  $\xi^2 = 0.7788$ . Taking into account the boson averages  $\langle n_d \rangle$ , corresponding to the microscopic parameters given in Table 2, the values of the parameter  $\zeta^2$  for spins from  $I = 0^+$  to  $I = 24^+$  are respectively equal to 0.67, 0.658, 0.634, 0.600, 0.561, 0.517, 0.472, 0.427, 0.385, 0.344, 0.306, 0.272, 0.240. The fact of a decrease in the values of  $\zeta^2$ , which are not

independent parameters, but are determined using the relation (61), where the most important quantity is  $\xi^2$ , allows relative compensation of the processes of interaction of collective states with high-spin excitation modes.

Figure 9 shows the boson composition of the wave functions. As for the previous nuclei, there is a smooth decrease in the collective component. In  $^{234}\text{Th}$ , the collective component decreases to 71% with a spin of  $24^+$ .

The values of  $B(E2)$  along the yrast band for  $^{234}\text{Th}$  are shown in Fig. 11. The spin-orbit splitting parameter is accepted as 1.09882 times larger than the value proposed in [49]. The only known experimental value  $B_W(E2; 2^+ \rightarrow 0^+) = 183(16)$  is reproduced.

**4.9. Nucleus  $^{236}\text{Th}$ .** For the  $^{236}\text{Th}$  nucleus, in comparison with the previous thorium isotopes, the experimental information is already relatively modest, the energies of the main band are known only up to the state with  $I^+ = 10^+$ , and there are no experimental values of  $B(E2)$ . Nevertheless, this nucleus was also included among those considered in this study. Figures 7 and 8 show the energy values and moments of inertia for  $^{236}\text{Th}$ . The final theoretical calculation leads to the reproduction of energies with an accuracy of 0.4 keV, as can be seen from Table 2. According to this accuracy, the moments of inertia are also reproduced.

In the theoretical calculation, the value of  $E_0^{(b)}$  was taken equal to 1.6 MeV,  $\zeta_0^2 = 0.67$ ,  $\xi^2 = 0.82225$ . Taking into account the boson averages  $\langle n_d \rangle$ , the values of the parameter  $\zeta^2$  for spins from  $I = 0^+$  to  $I = 12^+$  are respectively equal to 0.67, 0.6568, 0.627, 0.588, 0.545, 0.499, 0.454.

Figure 9 shows the boson composition of the wave functions. The collective component for the state with the spin  $I^+ = 10^+$  is over 96%, and this is greater than for the previous thorium isotopes.

The theoretical values of  $B(E2)$  along the yrast band for  $^{236}\text{Th}$  are shown in Fig. 11. The spin-orbit splitting parameter is accepted as 1.09882 times larger than the value proposed in [49]. For this nucleus, it is possible to change the number of bosons in a small interval, and its values in this case turned out to change the value of  $B_W(E2; 2^+ \rightarrow 0^+)$  (this does not happen automatically, since in each case different values of the parameters of the  $E2$ -transition operator are obtained). The maximum number of bosons was chosen to be 26, and the calculated value  $B_W(E2; 2^+ \rightarrow 0^+) = 179.5$ .

## CONCLUSIONS

The paper presents the microscopic theory of an extended version of IBM1, which makes it possible to calculate its parameters using a spherical single-particle basis and residual internucleon interactions, as well as numerous parameters for the connection of collective states with high-spin modes. For demonstration, calculations of even xenon isotopes were presented, for which the effect of band crossing is clearly visible. The properties of yrast bands in even thorium isotopes have been considered in more detail. For  $^{220,222}\text{Th}$  nuclei, the result obtained is that there is a soft intersection of bands in them,

which in the first of them leads to the observed backbending and a theoretical anomaly in the behavior of the  $B(E2)$  values. For the second nucleus, the intersection of the bands occurs so smoothly that backbending, as well as anomalies in the values of  $B(E2)$ , is not observed. For the remaining nuclei, as the mass number increases, the excitation energies decrease and  $B(E2)$  increases. The collective component of the wave function remains dominant up to the maximum observable spins.

## REFERENCES

1. *Beliaev S., Zelevinsky V.G.* // Nucl. Phys. 1962. V. 39. P. 582; Izv. Akad. Nauk SSSR, Ser. Fiz. 1964. V. 28. P. 127.
2. *Sorensen B.* // Phys. Lett. 1966. V. 21. P. 683; 1966. V. 23. P. 274; Nucl. Phys. A. 1967. V. 97. P. 1; Phys. Lett. B. 1967. V. 24. P. 328; Nucl. Phys. A. 1968. V. 119. P. 65; Prog. Theor. Phys. 1968. V. 39. P. 1468; Nucl. Phys. A. 1970. V. 142. P. 392, 411; 1973. V. 217. P. 505.
3. *Kishimoto T., Tamura T.* // Nucl. Phys. A. 1971. V. 163. P. 100; 1972. V. 192. P. 246; 1976. V. 270. P. 317.
4. *Tamura T., Weeks K., Kishimoto T.* // Phys. Rev. C. 1979. V. 20. P. 307; Nucl. Phys. A. 1980. V. 347. P. 359.
5. *Weeks K.J., Tamura T.* // Phys. Rev. C. 1980. V. 22. P. 888.
6. *Weeks K.J., Tamura T., Udagawa T., Hahne F.J.W.* // Phys. Rev. C. 1981. V. 24. P. 703.
7. *March N.H., Young W.H., Sampanthar S.* The Many-Body Problem in Quantum Mechanics. Cambridge Univ. Press, 1967.
8. *Janssen D., Jolos R.V., Donau F.* // Nucl. Phys. A. 1974. V. 224. P. 93.
9. *Jolos R. V., Donau F., Janssen D.* // Theor. Math. Phys. 1974. V. 20. P. 704.
10. *Jolos R. V., Donau F., Janssen D.* // Theor. Math. Phys. 1975. V. 23. P. 580.
11. *Jolos R. V., Donau F., Kartavenko V.G., Janssen D.* JINR Preprints P4-7223, P4-7533. Dubna, 1973.
12. *Arima A., Iachello F.* // Phys. Rev. Lett. 1975. V. 35. P. 1069; Ann. Phys. (N. Y.) 1978. V. 99. P. 253; 1978. V. 111. P. 201; 1979. V. 12. P. 468.
13. *Efimov A.D., Mikhajlov V.M.* // Bull. Russ. Acad. Sci.: Phys. 1992. V. 56. P. 96.
14. *Efimov A.D., Mikhajlov V.M.* // Bull. Russ. Acad. Sci.: Phys. 2011. V. 75. P. 890.
15. *Efimov A.D., Mikhajlov V.M.* // Bull. Russ. Acad. Sci.: Phys. 2012. V. 76. P. 857.
16. *Efimov A.D., Mikhajlov V.M.* // Bull. Russ. Acad. Sci.: Phys. 2016. V. 80. P. 898.
17. *Efimov A.D., Mikhajlov V.M.* // EPJ Web Conf. 2016. V. 107. P. 03013(1-5).
18. *Gelberg A., Zemel A.* // Phys. Rev. C. 1980. V. 22. P. 937.
19. *Yoshida N., Arima A., Otsuka T.* // Phys. Lett. B. 1982. V. 114. P. 86.
20. *Efimov A.D., Mikhajlov V.M.* // Phys. Rev. C. 1999. V. 59. P. 3153.
21. *Efimov A.D.* // Phys. At. Nucl. 2020. V. 83. P. 651.
22. *Efimov A.D., Izosimov I.N.* // Phys. At. Nucl. 2023. V. 86. P. 333.
23. *Efimov A.D., Mikhajlov V.M.* // Bull. Russ. Acad. Sci.: Phys. 2018. V. 82. P. 1266.
24. *Marumori T., Takada K., Sakata F.* // Prog. Theor. Phys. Suppl. 1981. V. 71. P. 1.
25. *Bohr A., Mottelson B.* // Nuclear Structure. New York: Benjamin, 1975. V. 2.

26. *Efimov A. D., Mikhajlov V. M.* // EPJ Web Conf. 2012. V. 38. P. 17005.
27. *Efimov A. D., Mikhajlov V. M.* // Bull. Russ. Acad. Sci.: Phys. 2013. V. 77. P. 862.
28. *Lakenbrink C.-D., Beckers M., Blazhev A., Dewald A. et al.* // Eur. Phys. J. A. 2023. V. 59. P. 290; <https://doi.org/10.1140/epja/s10050-023-01204-3>.
29. *Clement E., Lemasson A., Rejmund M., Jacquot B. et al.* // Phys. Rev. C. 2023. V. 107. P. 014324.
30. *Cromaz M., Drake T. E. et al.* // Phys. Rev. C. 1998. V. 58. P. 164; Erratum: *DeGraaf J., Cromaz M. et al.* // Phys. Rev. C. 1999. V. 59. P. 1818.
31. Brookhaven National Laboratory, National Nuclear Data Center (online). <http://www.nndc.bnl.gov/nndc/ensdf/>
32. *Katou T., Tendow Y. et al.* // Proc. Intern. Conf. on Nucl. Phys. Berkeley, 1980. P. 751.
33. *Govil I. M., Kumar A. et al.* // Phys. Rev. C. 2002. V. 66. P. 064318.
34. *Pasternak A. A., Sasaki Y., Efimov A. D., Mikhailov V. M., Hayakawa T., Toh Y., Oshima M., Hatsukawa Y., Katakura J., Shinohara N., Liu Z., Furuno K.* // Eur. Phys. J. A. 2000. V. 9. P. 293.
35. *Rainovski G., Pietralla N. et al.* // Phys. Lett. B. 2010. V. 683. P. 11.
36. *Coquard L., Rainovski G. et al.* // Phys. Rev. C. 2011. V. 83. P. 044318.
37. *Coquard L., Pietralla N. et al.* // Phys. Rev. C. 2009. V. 80. P. 061304.
38. *Rother W., Dewald A. et al.* // Nucl. Instrum. Methods Phys. Res. A. 2011. V. 654. P. 196.
39. *Srebrny J., Czosnyka T. et al.* // Nucl. Phys. A. 1993. V. 557. P. 663.
40. *Kanbe M., Kitao K.* // Nucl. Data Sheets. 2001. V. 94. P. 227.
41. *Cakirli R. B., Casten R. F., Jolie J., Warr N.* // Phys. Rev. C. 2004. V. 70. P. 047302.
42. *Zhang Yu, He Ying-Wen, Karlsson D., Qi Chong, Pan Feng, Draayer J. P.* // Phys. Lett. B. 2022. V. 834. P. 137443.
43. *Chabab M., El Batoul A. et al.* // Nucl. Phys. A. 2016. V. 953. P. 158.
44. *Efimov A. D., Mikhajlov V. M.* // Bull. Russ. Acad. Sci.: Phys. 2019. V. 83. P. 1136.
45. *Efimov A. D., Izosimov I. N.* // Phys. At. Nucl. 2021. V. 84. P. 408.
46. *Tazaki S., Takada K., Kaneko K., Sakata F.* // Prog. Theor. Phys. Suppl. 1981. V. 71. P. 123.
47. *Diebel M., Mosel U.* // Z. Phys. A. 1981. V. 303. P. 131.
48. *Dudek J., Nazarewicz W., Szymanski Z.* // Phys. Rev. C. 1982. V. 26. P. 1708.
49. *Isakov V. I., Erokhina K. I., Mach H., Sanchez-Vega M., Fogelberg B.* // Eur. Phys. J. A. 2002. V. 14. P. 29.
50. *Ahmed I. M., Al-Jubbori M. A., Kassim H. H., Abdullah H. Y., Sharrad F. I.* // Nucl. Phys. A. 2018. V. 977. P. 34.
51. *Delion D. S., Dumitrescu A.* // At. Data Nucl. Data Tables. 2015. V. 101. P. 1.
52. *Ackermann D., Theisen Ch.* // Phys. Scr. 2017. V. 92. P. 083002.

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