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A Variational Approach to Calculating IBM1 Parameters and Properties of Even Tellurium Isotopes

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Abstract—A variational approach to determining Bogolyubov's parameters, the amplitudes of a collective quadrupole phonon that is an image of IBM1 *d*-boson, and the boson composition of wave functions is applied to even Te isotopes with $A = 116–128$. A satisfactory description of the energies and $B(E2)$ probabilities of low-lying collective states is obtained. The calculation of quadrupole moments for the first 2_1^+-states requires some alterations to be made to the single-particle spin–orbital potential, compared to the one that was fixed for nuclei adjacent to double-magic Sn isotopes with $Z = 50$ and $A = 50, 82$.

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INTRODUCTION

Theoretical study of the properties of low-lying collective excitations in even Te isotopes is of interest as a way of testing different versions of boson mapping techniques [1–11]. Many theoretical works devoted to tellurium and published after the year 2000 have used different versions of interacting boson models (IBMs).

A feature of even $_{52}$Te isotopes is that the properties of quadrupole-type collective states are manifested not as explicitly as in nuclei with a large number of protons because of the presence of only two protons in excess of filled shells. Although the energy of the first 2_1^+-level for Te isotopes with $A = 118–124$ is approximately half that of semimagic $_{50}$Sn isotopes, and the reduced probability of $E2$ transitions from the 2_1^+-level to the ground state $B(E2; 2_1^+ \to 0_1^+)$ is roughly three times higher than for Sn with the same values of A and varies from 31 to 36 Weisskopf units, these values of $B(E2)$ are approximately half those in neighboring $_{54}$Xe isotopes. Nevertheless, fairly long yrast bands (up to 14^+ in ^{118}Te) are known to exist in telluria with $A =$ 118, 120, and the values of $B(E2; I \to I - 2)$ in these bands grow, compared to $B(E2; 2_1^+ \to 0_1^+)$, testifying to the collective nature of these bands.

Quadrupole moments $Q(2_1^+)$ of the 2_1^+ states have been measured for Te isotopes with $A = 122–130$ and are negative, corresponding qualitatively to the start of protons filling a degenerate shell. The absolute value of $Q(2_1^+)$ is approximately 1.5 times higher for $A = 122$, 124, while for $A = 126–130$ it is less than a single-particle estimate by about the same factor. Since the values of $Q(2_1^+)$ are not large, their theoretical reproduction is quite sensitive to the details of description. For example, Sorensen [1, 2] failed to produce the correct sign of $Q(2_1^+)$ for ^{122}Te, while Kishimoto and Tamura [3], who used a fuller set of residual interactions and allowed for more than the most collective excitation modes, managed to calculate values of $Q(2_1^+)$ that were in agreement with experimental values. In addition, Tamura et al. [4] noted that the choice of single-particle spectrum is of great importance.

In [12–17], we developed the IBM1 version, in which one type of quadrupole bosons is used (the IBM2 treats proton and neutron bosons separately). The model parameters and effective boson charges for $E2$ transitions were calculated microscopically by minimizing the energy of each collective state. In [12–17], we considered the properties of low-lying collective states in $^{114–134}$Xe, ^{126}Ba, and ^{128}Ce. Our description was essentially based on a quasi-particle random phase approximation (QRPA). Applying this method to Te isotopes in which there are only two protons in an excess of filled shells introduces some uncertainty, due to the quasi-particle treatment of protons in the description. A poor excuse for such an approach is the possibility of pairing even for the weak force of monopole particle–particle interaction for open degenerate shells, for which there is no critical pairing constant.

Our method also assumes a considerable value of the matrix element of quadrupole transition from the most collective phonon state into the ground state and a low energy for such a phonon, compared to all other phonons. These conditions are obviously not met for the lightest and heaviest Te isotopes, so we restrict our analysis in this work to most collectivized isotopes with $A = 116–128$. In the first section, we briefly describe our method; in the second, we present some calculation results and discuss how they correspond to the experimental data.

MICROSCOPIC CALCULATION OF IBM1 PARAMETERS AND EFFECTIVE CHARGES OF *E*2 TRANSITIONS

Our method was described in detail in [13, 15, 17], so here we give only its main features and consider the procedure for calculating one of the parameters of the IBM1 Hamiltonian (H_{IBM}). We refer to this parameter as k_2, and it is responsible for the mixing of boson configurations that differ only by one *d*-boson. The sign of this parameter determines the sign of $Q(2_1^+)$ ($\text{sign}(Q(2_1^+)) = -\text{sign}(k_2)$).

We assume that the fermion image of the IBM1 *d*-boson is a paired quasi-particle *D*-phonon constructed according to the QRPA:

$$D_\mu^+ = \frac{1}{\sqrt{2}}\sum_{12\tau}(\psi_{12}a_1^+a_2^+ + \varphi_{12}a_{\bar{2}}a_{\bar{1}})_\tau(j_1j_2m_1m_2|2\mu), \quad (1)$$

where 1, 2 denote single-particle states in a spherical basis, and $\bar{1}, \bar{2}$ are time conjugates of 1, 2. Amplitudes ψ_{12} and φ_{12} do not depend on magnetic quantum numbers and are normalized in the standard QRPA manner $\sum_{12\tau}(\psi_{12}^2 - \varphi_{12}^2) = 1$. Amplitudes ($\psi$, φ) and Bogolyubov's parameters (u,ν) are determined from the condition of minimum of an energy functional that includes the energy of quasi-particle vacuum, the energy of phonon vacuum, and the mean value of H_{IBM}, calculated with boson wave functions, which in turn depend on (ψ,φ) and (u,ν) through H_{IBM} parameters ε_d, k_1, k_2, C_0, C_2, C_4:

$$H_{\text{IBM1}} = \varepsilon_d\hat{n}_d + k_1\hat{P}_1 + k_2\hat{P}_2 + \frac{1}{2}\sum_L C_L\hat{C}_L,$$
$$\hat{n}_d = \sum_\mu d_\mu^+d_\mu; \quad \hat{P}_1 = (d^+d^+ss + \text{h.c.}); \quad (2)$$
$$\hat{P}_2 = (d^+d^+)^{(2)}ds + \text{h.c.}; \quad \hat{C}_L = (d^+d^+)^{(L)}(dd)^{(L)}.$$

The dot between the operators in Eq. (2) denotes the scalar product; $(\ldots)^{(L)}$, the vector connection of the operators at moment L. Equation (2) implicitly contains one more (the seventh) parameter of the Hamiltonian H_{IBM}—the maximum number of *d*-bosons (Ω) that can be in the wave functions. This number appears when mapping the *D*-phonon onto *d*-bosons [18]:

$$D^+ \to d^+\sqrt{1 - \hat{n}_d/\Omega} \to d^+s\Omega^{-1/2}, \quad (3)$$

where *s* is a scalar IBM1 boson that replaces the square root in Eq. (3) and does not have any physical sense of its own.

To obtain realistic values of the parameters in H_{IBM}, they must be renormed with respect to other high-energy phonons with all possible moments that do not contradict the law of conservation of total angular momentum. Below, these phonons are denoted by letter *B*. Interaction between *D*-phonons and other *B*-phonons (no more than one), which results in renormalization of parameters ε_d, k_1, and C_L,was considered in [13, 14]. Processes that renormalize k_2 are illustrated with graphs in the next section.

The energy functional is minimized under additional conditions that include those of normalization, and of an integer-valued Ω as a characteristic of a symmetric representation of the SU(6) algebra, along with a regulator of correlations in the ground state that allows us to attain low values of $\sum\varphi^2/\sum\psi^2$, making the QRPA applicable [17]. This regulator is not found in the standard QRPA, so the version that we use was referred to as a modified QRPA in [17].

Variation of the functional that includes the energy of the collective state, and additional conditions produce a system of nonlinear equations that is solved via iteration. The equations obtained when the functional is varied over (u,ν) or (ψ,φ) incorporate the mean values of boson operators that appear in H_{IBM}, *i.e.*, $((I_\nu|\hat{n}_d|I_\nu),(I_\nu|\hat{P}_1|I_\nu)$, *et cetera*, where $|I_\nu)$ is a boson function of the collective state with spin and relevant number. The solution is reached when these values become self-consistent with (u,ν), (ψ,φ), which determine the parameters of H_{IBM}. This means that by substituting the ultimate values of the mean values of boson operators into the equations, we determine those values of (u,ν), (ψ,φ) that yield values of the parameters in H_{IBM} such that diagonalization of the latter yields the substituted values of the means. It follows that each collective state $|I_\nu)$ has its own system of IBM1 parameters. Below, we show that allowing for these differences in the parameters results in better agreement with the experimental data.

HAMILTONIAN PARAMETER k_2 AND $Q(2_1^+)$

Interaction between one and two *D*-phonons, which is illustrated in Figs. 1a and 1b, makes the main contribution to parameter k_2. The process in Fig. 1b is possible because, given the method for determining

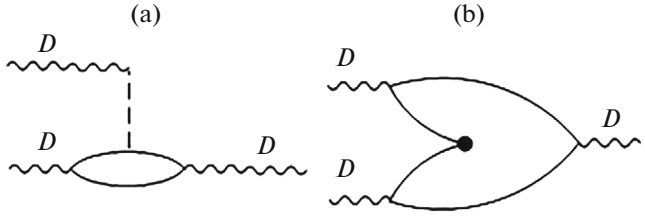

Fig. 1. Graph of matrix elements that determine Hamiltonian parameter k_2 in the first order over interaction. Wavy lines denote D-phonons; fine lines, quasi-particles; vertical dashed lines, interaction. The black dot corresponds to the term in the Hamiltonian H_{20+02}.

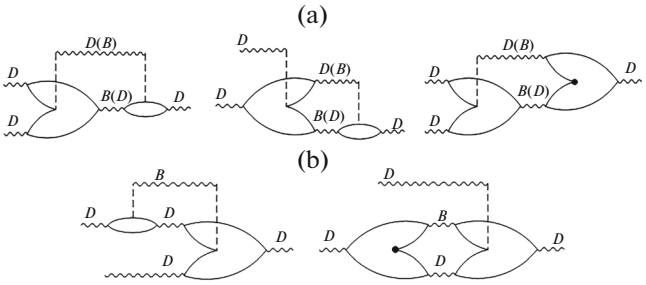

Fig. 2. Second-order processes that result in renormalization of k_2, in which the intermediate states are (a) two-phonon $(B^+D^+)^{(2)}$ and (b) three-phonon $(B^+D^+D^+)^{(2)}$. The key is the same as in Fig. 1.

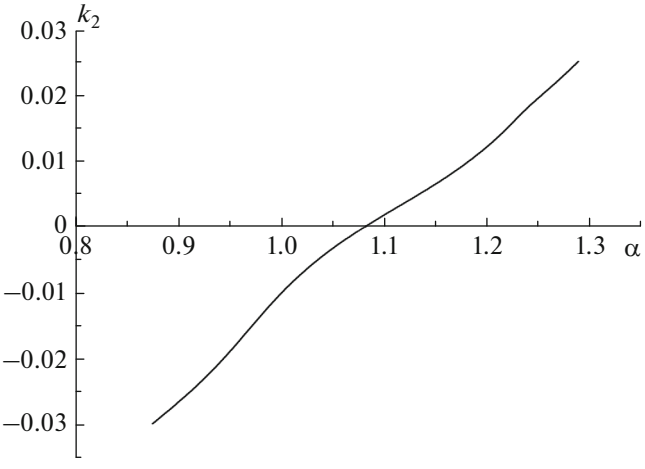

Fig. 3. Dependence of parameter k_2 on α for ^{122}Te.

(u, v) described in section 1, term $H_{20+02} \sim a_1^+ a_{\bar{1}}^+ + a_{\bar{1}} a_1$ in the fermion Hamiltonian does not disappear as it does when minimizing only the energy of a quasi-particle vacuum. This summand obviously can lead to annihilation of two quasi-particles, as illustrated in Fig. 1b.

The interaction in Fig. 1a includes factor $u_1u_2 - v_1v_2$, which is quite sensitive to the disposition of single-particle levels. The interaction in Fig. 1b contains factor $(\varepsilon_1 - \lambda)2u_1v_1 - \Delta(u_1^2 - v_1^2)$, which is equal to zero in the standard theory ($\varepsilon_1 - \lambda$ is the energy of single-particle level 1, counted from the chemical potential, and Δ is the pairing gap). In our case, this factor is very small for the ground state but grows along the yrast band. Figure 2 presents second-order processes with respect to interaction that renorm the values of parameter k_2.

To demonstrate how sensitive parameter k_2 is to the above disposition of single-particle levels, we varied the depth of spin–orbital interaction V_{ls} in the single-particle potential by introducing extra parameter α (i.e., the depth of these forces becomes αV_{ls}), as was done in [17]. The other parameters of the mean field, including V_{ls}, were assumed to be the same as in [19]. Figure 3 demonstrates how parameter k_2 depends on α for ^{122}Te with fixed parameters of the effective two-nucleon forces, which is discussed below. The contribution from processes illustrated in Figs. 1 and 2 to the value of parameter k_2 for ^{122}Te is given in Table 1. The table shows that k_2 changes as the spin in the yrast band grows.

The values of Ω listed in Tables 1 and 2 exceed canonical IBM values Ω_{can}, which are equal to half the minimum number of valent nucleons or holes. Numbers Ω were calculated in the same manner as in our previous works (see, e.g., [13, 17]) and were approximately twice those of the IBM1 canonical value (Table 2), due to the wide single-particle basis used to construct the D-phonon. The regulator of correlations (see section 1) plays an important role, since it strengthens the contribution from high-lying paired quasi-particle states. Only one value of Ω was used for all of the states in each nucleus.

The numerical values of parameter α were determined from experimental data on $Q(2_1^+)$ (Fig. 4); for all other isotopes, from the values of $B(E2; 2_2^+ \to 0_1^+)$. This was possible because $Q(2_1^+)$ is in fact proportional to k_2 and has an opposite sign. The energy spectrum of yrast states in telluria with $A = 116$–128 is fairly close to the O(6) IBM1 limit. This means that states with odd numbers of bosons make the main contribution to the wave function of 2_1^+. The admixture of states with even numbers of d-bosons can be estimated via perturbation theory, which produces, e.g., $-k_2\sqrt{2(\Omega - 1)} \times (E_2 - E_1)^{-1}$ for the amplitude of a two-boson admixture, where E_2 and E_1 are the energies of two and one d-bosons.

The IBM1 quadrupole-moment operator $\hat{Q}$ can be expressed through the operator of $E2$ transition $\hat{T}_{\mu=0}(E2)$; $\hat{Q} = 4\sqrt{\pi/5}\hat{T}_{\mu}(E2)$ in the usual manner:

$$\hat{T}_{\mu}(E2) = e^*\left(d^+s + s^+d + \chi d^+d\right)^{(2)}_{\mu} + e_0^*\left(s^+(d^+d)^{(0)}d + d^+(d^+d)^{(0)}s\right)^{(2)}_{\mu}, \quad (4)$$

where $e^*, e^*\chi, e_0^*$ are boson charges [15]. Since the value of χ in Te isotopes is determined mainly by the rather small proton contribution to the D-phonon and is therefore quite low ($\chi = -0.125$ for ^{122}Te), quadrupole moment $Q(2_1^+)$ is reduced to the matrix element of transition between a component of the wave function with one and three d-bosons and admixtures (two and four d-bosons); i.e., $Q(2_1^+) = -k_2 q$, where q is a positive numerical coefficient that contains e^*. The value of e^* (without introducing nucleon effective charges [15]) agrees satisfactorily with the experimental data on $B(E2)$. We may therefore establish the value of parameter α using $Q(2_1^+)$.

In all cases where we have $\alpha > 1$, the spin-orbital splitting in single-particle spectra is larger than the one established in [19] for odd nuclei in the vicinity of double-magic $Z = 50$ and $N = 50, 82$. However, the values of α selected in this manner do not contradict the spectra of neighboring odd-neutron nuclei, in which levels $\frac{1}{2}^+$, $\frac{3}{2}^+$, and $\frac{11}{2}^-$ are fairly close to one another (no more than 300 keV for a number of neutrons that ranges widely from 63 to 79). Calculated single-particle energies give a larger interval for $3s_{1/2}$, $2d_{3/2}$, and $1h_{11/2}$ states. If pairing is considered, however, this interval should shrink and have some effect on the position of these levels via quasi-particle–phonon interaction.

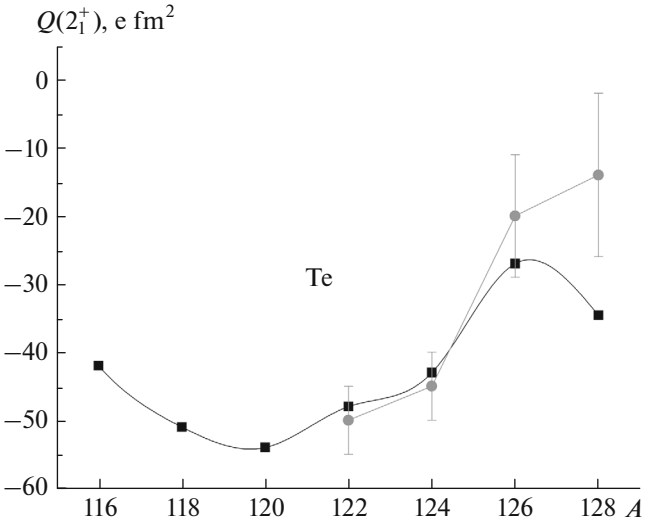

Fig. 4. Experimental and theoretical values of quadrupole moment $Q(2_1^+)$ of the 2_1^+ state for Te isotopes versus A.

CALCULATION RESULTS

All calculations of the H_{IBM} parameters and boson charges in the operator of $E2$ transitions were performed using a single-particle basis that included all bound and resonance states with a root-mean square radius of ≤ 10 fm. The single-particle basis was calculated using the Saxon-Woods potential (see the previous section), where a nucleus resides at the center of a sphere with totally reflecting walls and a radius that is approximately seven times that of the nucleus.

The matrices of particle–hole (p–h) and hole–hole (h–h) forces contained in the variational equations above were factorized in the traditional manner, i.e., as the product of matrix elements of single-particle quadrupole operators with a radial dependence in the form of a radius derivative of the Saxon–Woods function in both the p–h and h–h channels. The constant of isoscalar quadrupole p–h forces $\kappa^{(2)}$ varied somewhat from isotope to isotope and was on average

Table 1. Contributions from the different processes shown in Figs. 1 and 2 to the values of parameter k_2 for the yrast-band states in ^{124}Te ($\Omega = 14$, $\alpha = 1$). The values are given in MeV

I^π	Fig. 1a	Fig. 1b	Fig. 2a	Fig. 2b	$k_2\sqrt{\Omega - 1}$
0^+	0.06056	−0.0088	0.0100	0.0209	0.0827
2^+	0.0616	−0.0078	0.0109	0.0178	0.0825
4^+	0.0669	−0.0056	0.0124	0.0165	0.0902
6^+	0.0751	−0.0031	0.0133	0.0166	0.1019
8^+	0.0844	−0.0017	0.0136	0.0190	0.115
10^+	0.0913	−0.0042	0.0125	0.0203	0.120

Table 2. Constants of p–p forces $G^{(2)}$ and isoscalar p–h $\kappa^{(2)}$ in the units introduced in [20], and the parameter of the strengthening of spin-orbital bonding α and Ω

A	$G^{(2)}$	$\kappa^{(2)}$	α	Ω	A	$G^{(2)}$	$\kappa^{(2)}$	α	Ω
116	0.816	0.816	1.24	14	124	0.88	0.880	1	11
118	0.795	0.795	1.3	13	126	0.894	0.894	0.9	10
120	0.806	0.806	1.35	13	128	0.893	0.893	1	10
122	1.025	0.930	1.26	13					

Table 3. Comparison of experimental energy values (MeV) counted from the ground-state energy and theoretical values calculated by different means for a number of isotopes (see text for details)

	^{118}Te			^{122}Te			^{124}Te		
I^{π}	$E(0)$	$E(I)$	E-exp.	$E(0)$	$E(I)$	E-exp.	$E(0)$	$E(I)$	E-exp.
0^+	0	0	0	0	0	0	0	0	0
2^+	0.548	0.628	0.606	0.526	0.562	0.564	0.516	0.612	0.603
4^+	1.209	1.170	1.206	1.237	1.255	1.181	1.163	1.215	1.249
6^+	1.955	1.842	1.821	2.102	2.051	1.751	1.914	1.779	1.747
8^+	2.762	2.774	2.574						

≈ 0.85 (see Table 2) of the isoscalar constant proposed by Bohr and Mottelson [20]. The value of the isovector quadrupole constant was also taken from [20]. According to [3, 21, 22], constant of quadrupole h–h forces $G^{(2)}$ was assumed to be close to $\kappa^{(2)}$, and to be the same for neutrons and protons. The matrix elements of monopole h–h forces were assumed to be equal to pairing constant $G_\tau = 18.4A^{-1} \times \left(1 + \tau 0.37(N-Z)A^{-1}\right)$, with $\tau = -1$ for neutrons and $\tau = +1$ for protons.

The results from calculating the energies of yrast states for telluria with $A = 116$–128 and the value of $B(E2;\ 2_1^+ \to 0_1^+)$ are presented in Figs. 5a and 5b, respectively. It was indicated above that we varied the parameters in our calculations somewhat from state to state. Table 3 compares the experimental energies of the yrast states, counted from the ground state, and values calculated with parameters determined for the ground state and parameters obtained for each state with spin $I, E(I)$. It can be seen that the method in which parameters are calculated for each state produces a somewhat better description of energies with $I = 2,4,6$ in ^{124}Te (the matching for each state was done separately for isotopes with mass numbers $A =$ 116, 118, 122, 124). The energies (Fig. 5a) and values of $B(E2;\ 2_1^+ \to 0_1^+)$ (Fig. 5b) were calculated for other isotopes using parameters determined for the ground state. It should be noted that $B(E2;\ 2_1^+ \to 0_1^+)$ was approximately the same for the two methods of calculating the parameters.

The experimental values of $B(E2;\ I \to I-2)$ along the yrast band for ^{118}Te (not shown in the figures) are reproduced within the experimental errors in our calculations. The validity of the description is due to the term in the operator in Eq. (4) that is proportional to e_0^*. At the same time, when $e_0^* = 0$, the experimental data for this nucleus may be reproduced only if Ω increases with spin [24]. The calculated values of $B(E2;\ 2_2^+ \to 0_1^+)$ versus mass number A (not shown in the figures) agree with the experimental ones. The sole exception is A = 124, where the calculated values are two times higher than the experimental ones. Thus, our variational approach provides an entirely acceptable description of these quantities. The calculated energies of states outside the yrast bands (which are

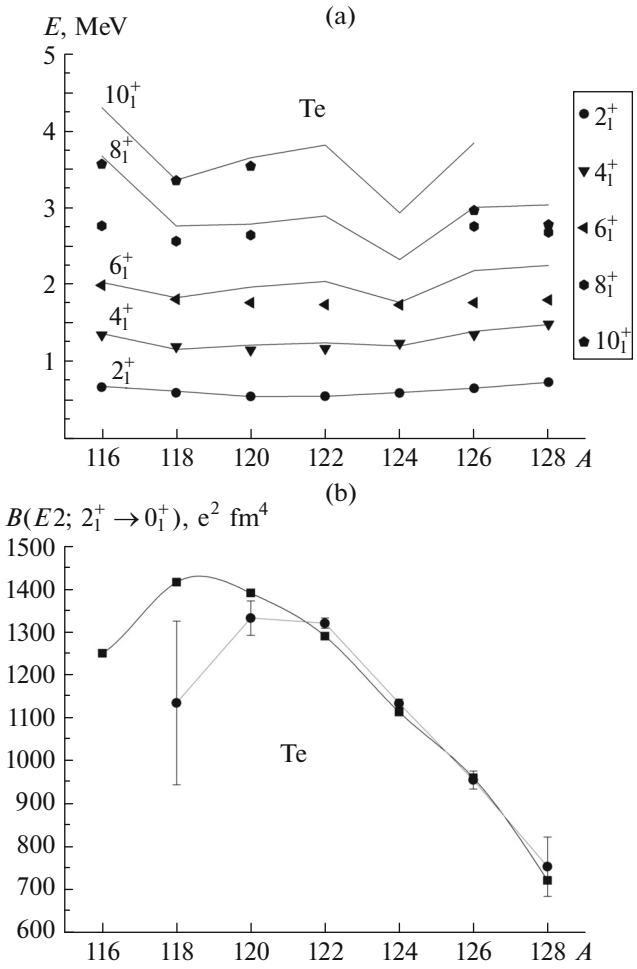

Fig. 5. (a) Experimental (designated by symbols) and calculated values of energies of yrast-band states in Te isotopes; (b) experimental and calculated values of $B(E2; 2_1^+ \to 0_1^+)$ in Te isotopes. The experimental data are borrowed from [10, 23].

not presented here) are in reasonable agreement with the experiment.

CONCLUSIONS

In this work and in [12–17], we developed a variational method for determining the values of such quantities as Bogolyubov's parameters, the amplitudes of the most collective quadrupole paired quasiparticle phonons, and the boson composition of wave functions, which together characterize the properties of the low-lying collective states of even–even nuclei.

The calculations performed here and in [12–17] showed that this method produces an entirely acceptable description of the experimental data on energies and quadrupole transitions. It was established in this work and in [17] that to obtain a more thorough description, we need to vary the mean field, which we affect via the single-particle spin–orbital potential.

A fixed mean field and factorized forces are not mandatory components of our method. Their use greatly simplifies calculations, but it is quite possible to employ Skyrme effective forces instead (see, e.g., the review in [25]). Self-consistent calculations can then consider fully the effect phonons have on the mean field. In addition, our method explicitly gives the energy of the ground state with allowance for correlations by using the more complicated boson structure of the ground-state wave function. Minimization of the energy functional with allowance for correlations in the ground state could thus refine the parameters of the effective forces.

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