Self-consistent calculations of quadrupole moments of the first 2^+ states in Sn and Pb isotopes

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A method of describing static moments of excited states and transitions between excited states is formulated for nonmagic nuclei within the Green's function formalism. Quadrupole moments of the first 2^+ states in tin and lead isotope chains are calculated self-consistently using the energy density functional by Fayans *et al.* [Nucl. Phys. A **676**, 49 (2000)]. Reasonable agreement with available experimental data is obtained. Quadrupole moments of unstable nuclei including ^{100}Sn and ^{132}Sn are predicted. A nontrivial dependence of the quadrupole moments on the neutron excess is found which can be traced to the negative proton contributions.

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I. INTRODUCTION

At present, spectroscopic information about unstable nuclei is of great interest because of the emergence of new magic numbers; see, for example, Ref. [1]. This phenomenon has important implications for astrophysics. To reliably predict properties of unstable nuclei, an approach based on a self-consistency relation between the mean field and effective interaction should be used. Self-consistency improves noticeably the predictive power of the theory; for a review, see Ref. [2].

Phonons are an important degree of freedom for nuclear structure. Widely used theoretical approaches including phonons are the quasiparticle-phonon model (QPM) [3], the quasiparticle random-phase approximation + phonon coupling (QRPA + PC) [4], and the extended theory of finite Fermi systems (ETFFS) [5]. Self-consistent extensions of these methods have been proposed recently, for example, (Q)RPA + PC [6] and the ETFFS in the quasiparticle time-blocking approximation (QTBA) [7] [ETFFS (QTBA)] [8]. For magic and semimagic nuclei, such approaches are based on the fact that in these nuclei there is a small parameter g^2, the dimensionless square of the phonon creation amplitude.

In the framework of the Green's function (GF) formalism, both PC and self-consistency have been realized and have shown their importance for stable nuclei [5,7,8]. However, all the above mentioned approaches dealing with the PC did not take into account *all* the g^2 terms, thus limiting themselves with the pole diagrams only; see the first diagram in Fig. 1 where diagrams for the mass operator are displayed. The second diagram represents the sum of all g^2 nonpole diagrams, usually called the tadpole.

The problem of consistent consideration of all g^2 terms including tadpoles was analyzed in the article by Khodel [9] based on the general self-consistency relations for finite Fermi systems [10]. The method developed was applied for magic nuclei, mainly for ground-state nuclear characteristics, within the self-consistent TFFS [11]. It was found that, as a rule, the tadpole contributions in magic nuclei are noticeable and are often of opposite sign as compared with those of the pole terms. The first attempts to include phonon tadpole effects for nuclei with pairing and for consideration of excited states were recently made in Refs. [12,13], respectively.

If one studies phonon effects in the binding energies, single-particle level positions, g^2 corrections are usually smaller than mean field predictions and could be partially hidden in the phenomenological parameters used. In this work, within the GF method, we concentrate our attention on more delicate characteristics which are proportional to g^2 themselves. Namely, we analyze the static moments of excited states and transitions between excited states. To ensure self-consistency, we use the self-consistent TFFS based on the energy density functional (EDF) by Fayans *et al.* [14] with the DF3-a set of parameters fixed previously in Ref. [15]. Thus, there are no fitted parameters in the present approach. We briefly describe the method for these characteristics in magic and generalize it for nonmagic even-even nuclei. Within this approach, we perform the first self-consistent calculations of static moments of the first 2^+ excited states in tin and lead isotopes.

The quadrupole moments of excited states in spherical nuclei with pairing have been calculated earlier within many-body approaches in Refs. [16,17] and within QPM in Refs. [18,19]. In Ref. [17], the authors use the nuclear field theory with a set of phenomenological parameters taken from experiment for each nucleus. In this article, a reasonable agreement was obtained with the experimental data for Sn and Ni isotopes available at that time. For magic nuclei, this problem was considered also within the self-consistent TFFS in Ref. [20]. The main difference of our approach from those of

FIG. 1. g^2 order corrections to the mass operator in magic nuclei. The circles with one wavy line in the first term are the phonon creation amplitudes g. The second term is the phonon tadpole.

Refs. [16–19] is its full self-consistency on the (Q)RPA level and absence of any phenomenological or fitted parameters.

II. MAGIC NUCLEI

To describe the PC effects in magic nuclei with the consistent account of all the g^2 terms, we follow the method by Khodel [9]. In the g^2 approximation, the matrix element M_{LL} for a static moment of the excited state (phonon) with the orbital angular moments L in a static external field V^0 is determined in terms of the change of the one-particle GF in the field of this phonon:

$$M_{LL} = \int V^0(\mathbf{r})\delta^{(2)}_{LL}G(\mathbf{r},\mathbf{r},\varepsilon)d\mathbf{r}\frac{d\varepsilon}{2\pi\imath}, \tag{1}$$

$$\begin{aligned}\delta^{(2)}_{LL}G &= \delta_L(Gg_LG) = G(\varepsilon)g_LG(\varepsilon+\omega_L)g_LG(\varepsilon)\\ &\quad + G(\varepsilon)g_LG(\varepsilon-\omega_L)g_LG(\varepsilon) + G(\varepsilon)\delta_Lg_LG(\varepsilon),\end{aligned} \tag{2}$$

where g_L is the amplitude for the production of the L phonon with the energy ω_L and δ_Lg_L is the variation of g_L in the field of other L phonon:

$$\delta_Lg_L = \delta_L(\mathcal{F}Ag_L) = \delta_L\mathcal{F}Ag_L + \mathcal{F}\delta_LAg_L + \mathcal{F}A\delta_Lg_L, \tag{3}$$

where $\mathcal{F}$ is the effective particle-hole (ph) interaction and A is the ph propagator (the integral over energy of the product of two single-particle GF's). Integration over intermediate coordinates is understood. By substituting Eq. (2) into Eq. (1), we obtain

$$M_{LL} = V^0Gg_LGg_LG + V^0A\delta_Lg_L, \tag{4}$$

It is convenient to transform this expression in such a way that the effective field V appears instead of the external field V^0. They are connected with the TFFS equation [21] $V = V^0 + \mathcal{F}AV$. After regrouping terms in Eqs. (3) and (4) (for details, see Refs. [11,13]), we obtain the ultimate expression

$$M_{LL} = VGg_LGg_LG + VA\delta_L\mathcal{F}Ag_L, \tag{5}$$

which is illustrated in Fig. 2. It contains now the effective field V, instead of V^0 in Eq. (4), and the quantity $\delta_L\mathcal{F}$ in the second

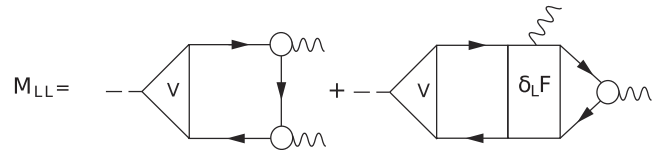

FIG. 2. Matrix element M_{LL} in the form of Eq. (5).

term, which denotes the variation of the effective ph interaction $\mathcal{F}$ in the field of the L phonon. For the density-dependent TFFS effective interaction $\mathcal{F}(\rho)$, the following ansatz can be readily obtained [9,11]:

$$\delta_L\mathcal{F}(\mathbf{r}) = \frac{\partial\mathcal{F}}{\partial\rho}\rho^{\rm tr}_L(r)Y_{LM}(\mathbf{n}), \tag{6}$$

where $\rho^{\rm tr}_L = Ag_L$ is the transition density for the L phonon excitation. The first term of Eq. (5) coincides with the result of Refs. [16,22], while the second one, with the $\delta_L\mathcal{F}$ quantity, is a generalization to take into account all the g^2 terms.

All the above equations can be readily modified for such processes as the transition between the excited states L and L' in the external field $V^0(\omega = \omega_{L'} - \omega_L)$ or the excitation of the two-phonon state $L + L'$ in the external field $V^0(\omega = \omega_{L'} + \omega_L)$. The static moment case corresponds to $\omega = 0$, $\omega_{L'} = \omega_L$.

III. NONMAGIC NUCLEI. COMPARISON WITH QRPA

In the case of nuclei with pairing, it is necessary to use four GF's (G, G^h, $F^{(1)}$, $F^{(2)}$ in Ref. [21]). To describe phonons, one has to use the complete set of the QRPA equations, which include the ph, hp, pp, and hh channels and four effective fields V, V^h, $d^{(1)}$, and $d^{(2)}$, respectively [21]. As the pp and hh channels give a small contribution in the case of the first 2^+ levels [23], which is considered in the article, we do not consider these channels and, accordingly, the fields $d^{(1)}$ and $d^{(2)}$. Then we obtain eight terms for $M^{(i)}_{LL'}$ instead of one in Eq. (5) and eight integrals of three GF's $A^{(i)\rm pair}_{123}$, where $i = 1$–8. The typical two terms, $M^{(1)}$ and $M^{(5)}$, are shown in Fig. 3.

The final formula for the static moment M_{LL} of the excited L state reads

$$\begin{aligned}M_{LL} = \sum_{123}(-1)^{L+1}&\begin{pmatrix} I & L & L\\ 0 & L & -L\end{pmatrix}\begin{Bmatrix} I & L & L\\ j_3 & j_2 & j_1\end{Bmatrix}\\ &\times\langle 1\|\,V\,\|2\rangle\langle 3\|\,g_L\,\|1\rangle\langle 2\|\,g_L\,\|3\rangle\sum_{i=1}^{8}A^{(i)\rm pair}_{123},\end{aligned} \tag{7}$$

where

$$\begin{aligned}\sum_{i=1}^{8}A^{(i)\rm pair}_{123} &= \left(\frac{1}{(\omega_L+E_{13})(\omega_L+E_{23})} + \frac{1}{(\omega_L-E_{13})(\omega_L-E_{23})}\right)\left[u_1^2u_2^2v_3^2 - v_1^2v_2^2u_3^2 + \frac{\Delta_1\Delta_2}{4E_1E_2}\left(u_3^2-v_3^2\right)\right.\\ &+ \frac{\Delta_1\Delta_3}{4E_1E_3}\left(u_2^2-v_2^2\right) + \frac{\Delta_2\Delta_3}{4E_2E_3}\left(u_1^2-v_1^2\right)\Big] + \frac{1}{E_{12}}\left[\frac{2E_{23}\left(u_1^2u_3^2v_2^2 - v_1^2v_3^2u_2^2\right)}{E_{23}^2-\omega_L^2} + \frac{2E_{13}\left(u_2^2u_3^2v_1^2 - v_3^2v_2^2u_1^2\right)}{E_{13}^2-\omega_L^2}\right.\\ &\left.\left. - \left(\frac{\Delta_1\Delta_2}{2E_1E_2}\left(u_3^2-v_3^2\right) + \frac{\Delta_1\Delta_3}{2E_1E_3}\left(u_2^2-v_2^2\right) + \frac{\Delta_2\Delta_3}{2E_2E_3}\left(u_1^2-v_1^2\right)\right)\left(\frac{E_{13}}{E_{13}^2-\omega_L^2} + \frac{E_{23}}{E_{23}^2-\omega_L^2}\right)\right)\right].\end{aligned} \tag{8}$$

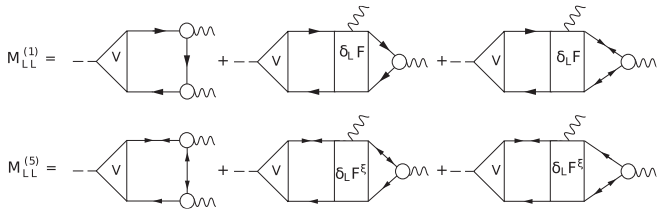

FIG. 3. Matrix elements for $M^{(1)}_{LL}$ and $M^{(5)}_{LL}$ for nonmagic nuclei.

Here $E_{12} = E_1 + E_2$, $E_1 = \sqrt{(\varepsilon_1 - \mu)^2 + \Delta_1^2}$, and the low index $1 = (n_1, l_1, j_1)$, spherical nuclei, is the set of single-particle quantum numbers.

Let us compare this expression with the QRPA approach. Here we mean the usual scheme [24], which uses the QRPA wave functions for the matrix element between two excited states. In Ref. [24] the expression for the $B(E2)$ quantity has been derived using the bare external field V^0 and the QRPA wave functions without the pp and hh channels. The first square brackets, in the first half of Eq. (8), coincide completely with the factor $v^-_{12}u^+_{23}u^+_{31}$ in Refs. [3,24]. Thus, the first half of Eq. (8) corresponds to the expression $v^-_{12}(\psi_{23}\psi_{31} + \phi_{23}\phi_{31})$ in Ref. [24] because the phonon amplitudes ψ_{12} and ϕ_{12} contain, by definition, the denominators $(E_{12} - \omega_L)$ and $(E_{12} + \omega_L)$, respectively. Therefore, the second half of Eq. (8), which contains the common factor $1/E_{12}$, generalizes the usual QRPA approach. This part of Eq. (8) describes the contribution of the ground-state correlations (GSC), the so-called backward-going diagrams, to the first diagrams of Fig. 3 with the integrals of three GF's ("triangle"). We calculate the contribution of such correlations below. The second generalization is the appearance of the effective field V, which depends in general on the frequency $\omega = \omega_L \pm \omega'_L$, instead of the external field V^0, which does not depend on the frequency. The terms with $\delta_L\mathcal{F}$ and $\delta_L\mathcal{F}^\xi$ are the third generalization of the QRPA approach. Note that these terms are also absent in Refs. [16–19,22].

In the problem under consideration, the terms of Fig. 3 referring to the density derivative of the force can be straightforwardly evaluated with the help of Eq. (6):

$$M_{\rm ddf} = C_{IL}\int \delta\rho_{\rm st}(r)\frac{\partial\mathcal{F}}{\partial\rho}(r)\left[\rho^{\rm tr}_L(r)\right]^2 d^3r, \tag{9}$$

$$C_{IL} = \frac{1}{2}(-1)^L(2L+1)(2I+1)\begin{pmatrix} I & L & L \\ 0 & L & -L\end{pmatrix}\begin{pmatrix} I & L & L \\ 0 & 0 & 0\end{pmatrix}, \tag{10}$$

TABLE I. Quadrupole moments Q (e b) of the first 2^+ states in Sn and Pb isotopes. (Q^n and Q^p are the neutron and proton contributions to the triangle diagram, $Q_{\rm tot} = Q^n + Q^p + Q_{\rm ddf}$.)

Nucl.	$Q^{\rm n}$	$Q^{\rm p}$	$Q_{\rm tot}$	$Q_{\rm exp}$ [26]	Q(GSC = 0)	$Q_{\rm QRPA}$
^{100}Sn	0.01	0.03	0.04	–	0.05	0.017
^{102}Sn	−0.05	−0.01	−0.07	–	−0.02	−0.001
^{104}Sn	−0.18	−0.03	−0.22	–	−0.08	−0.001
^{106}Sn	−0.28	−0.05	−0.34	–	−0.13	−0.002
^{108}Sn	−0.31	−0.07	−0.39	–	−0.14	−0.002
^{110}Sn	−0.38	−0.10	−0.50	–	−0.17	−0.003
^{112}Sn	−0.32	−0.11	−0.45	−0.03(11)	−0.15	−0.003
^{114}Sn	−0.15	−0.11	−0.28	0.32(3), 0.36(4)	−0.09	−0.004
^{116}Sn	0.00	−0.10	−0.12	−0.17(4), +0.08(8)	−0.03	−0.003
^{118}Sn	0.10	−0.09	−0.01	−0.05(14)	0.01	−0.003
^{120}Sn	0.12	−0.08	0.04	+0.022(10), −0.05(10)	0.03	−0.003
^{122}Sn	0.09	−0.07	0.01	$-0.28 < Q < +0.14$	0.02	−0.003
^{124}Sn	0.00	−0.06	−0.07	0.0(2)	−0.01	−0.003
^{126}Sn	−0.08	−0.05	−0.13	–	−0.04	−0.002
^{128}Sn	−0.10	−0.03	−0.14	–	−0.05	−0.002
^{130}Sn	−0.05	−0.01	−0.07	–	−0.03	−0.001
^{132}Sn	0.04	0.00	0.04	–	0.05	0.015
^{134}Sn	0.00	−0.01	−0.01	–	0.00	−0.001
^{190}Pb	−0.60	−0.29	−0.92	–	−0.30	−0.008
^{192}Pb	−0.77	−0.35	−1.15	–	−0.38	−0.008
^{194}Pb	−0.90	−0.39	−1.31	–	−0.44	−0.008
^{196}Pb	−0.85	−0.38	−1.26	–	−0.42	−0.008
^{198}Pb	−0.67	−0.35	−1.05	–	−0.35	−0.008
^{200}Pb	−0.27	−0.23	−0.52	–	−0.17	−0.006
^{202}Pb	0.02	−0.15	−0.15	–	−0.03	−0.005
^{204}Pb	0.18	−0.07	0.10	+0.23(9)	0.06	−0.003
^{206}Pb	0.11	−0.02	0.09	+0.05(9)	0.06	−0.002
^{208}Pb	0.01	0.04	0.05	−0.7(3)	0.07	0.043

where the transition density is $\rho_L^{\rm tr} = \mathcal{L}(\omega_L)g_L$, $\delta\rho_{\rm st} = \mathcal{L}(0)V$, and $\mathcal{L} = \int(GG - F^{(1)}F^{(2)})d\varepsilon/2\pi i$.

The problem of calculations of quadrupole moments of the first 2^+ states is connected with the study of the 2^+ state energies and $E2$ transitions to the ground state. To calculate these quantities one usually employs the (Q)RPA approach, which deals only with two quasiparticle excitations. PC modifies the propagation and interaction of the quasiparticles. A consistent theory of these anharmonic corrections to the QRPA is difficult because it requires including a self-consistency beyond the (Q)RPA and tadpole contributions. The realization of this program is beyond the scope of this paper since our calculations include dynamic quantities obtained only within the (Q)RPA and, thus, are fully self-consistent.

IV. CALCULATIONS OF STATIC QUADRUPOLE MOMENTS OF THE FIRST 2^+ STATES IN TIN AND LEAD ISOTOPES

The quadrupole moment of the excited state L is equal to the matrix element M_{LL}, Eq. (7), for $I = 2$, $V^0(\mathbf{r}) = e_q\, r^2 Y_{20}(\mathbf{n})$, and $e_q^p = 1$, $e_q^n = 0$. In the recent work [25], we have discussed the problem and calculated the quadrupole moment for the first 3^- level of ^{208}Pb, both without terms with $\delta_L\mathcal{F}$ and $\delta_L\mathcal{F}^\xi$.

In this article, we calculated the quadrupole moments of the first 2^+ states in tin and lead isotopes according to Eqs. (7)–(10) in the λ representation with self-consistent single-particle wave functions ϕ_λ obtained within the EDF method of Ref. [14] with the functional DF3-a [15]. A spherical box of the radius $R = 16$ fm is used to simulate the single-particle continuum. We examined the dependence of the results on the cutoff energy $E_{\rm max}$ and have found that the value of $E_{\rm max} = 100$ MeV ensures 1% accuracy. To calculate the quantities V and g_L, the results of Ref. [23] have been used where all the calculations were performed in the coordinate representation using the same self-consistent DF3-a basis as in the present calculation of the matrix element M_{LL}. Thus, the single-particle continuum is taken into account adequately in the present calculations. The contribution of the term with $M_{\rm ddf}$, Eq. (9), turned out to be rather small,

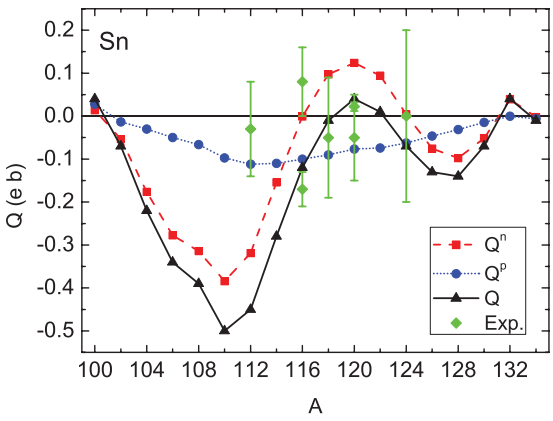

FIG. 4. (Color online) Quadrupole moments of the first 2^+ excited states in even Sn isotopes.

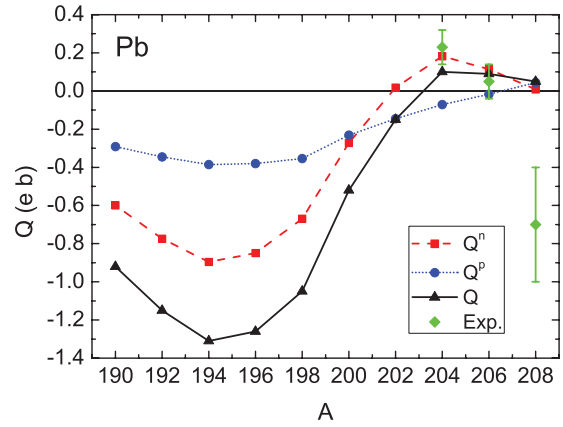

FIG. 5. (Color online) Same as in Fig. 4 but for Pb isotopes.

$Q_{\rm fdd} = -(0.01 \div 0.03)$ e b. However, there are cases where these corrections are comparable with the total $Q(2_1^+)$ value when the Q^n and Q^p values almost compensate each other, for example, in ^{118}Sn and ^{122}Sn. The term with $\delta_L\mathcal{F}^\xi$ contains the anomalous analogs of the quantities $\delta\rho_{\rm st}$ and $\rho_L^{\rm tr}$, which are small [23].

The results are given in Table I and Figs. 4 and 5. Except for ^{112}Sn and ^{208}Pb, we obtained a reasonable agreement with experimental data [26]. The contribution of the GSC term in Eq. (8) turned out to be large. Rather often it is more than $50 \div 60\%$ of all triangle contributions [column Q (GSC $= 0$)]. The usual QRPA (GSC $= 0$ and $V = V^0$), see the last column in Table I, results in considerably lower Q values.

V. CONCLUSION

We have formulated the method to describe static moments of the excited states and transitions between excited states, which are described within the QRPA, taking into account all the g^2 terms in magic and semimagic nuclei. We obtained a noticeable difference from the traditional QRPA approach. In particular, new terms with $\delta_L\mathcal{F}$ and $\delta_L\mathcal{F}^\xi$ appear, which contain the density derivatives of both the ph and pp effective interactions. In the problem under consideration, their contribution turned out, as a rule, to be rather small. However, for consistency, these terms should be included. We have performed the self-consistent calculations of the static quadrupole moments of the first 2^+ states for Sn and Pb isotopes using the known EDF parameter set DF3-a. Except for the ^{112}Sn and ^{208}Pb cases, a reasonable agreement has been obtained with the experimental results. Using the self-consistent method, which contains no newly adjusted parameters, we have also predicted the values of quadrupole moments of the first 2^+ states in several unstable lead and tin isotopes including the ^{100}Sn and ^{132}Sn nuclei. An unexpectedly large contribution of ground-state correlations to the $Q(2_1^+)$ values is found.

We have found that the static quadrupole moments of the first 2^+ states in both chains are small at the beginning of the shell. For isotopes in unfilled shells they are on average

much bigger. However, the function $Q(A)$ is rather irregular, especially for the tin chain, owing to the neutron component. In the left part of Fig. 4, the neutron and proton components are of the same sign, resulting in the large absolute value of $Q(2_1^+)$. On the right part of Fig. 4, the quadrupole moment is close to zero because two terms of the sum $Q = Q^p + Q^n$ compensate for each other. In the lead chain, the situation is similar but less pronounced. Similar behavior probably could be present in other isotope chains.

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