

Proton-neutron symmetry in ^{92}Zr , ^{94}Mo with Skyrme interactions in a separable approximationA. P. Severyukhin,¹ N. N. Arsenyev,¹ and N. Pietralla²¹*Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, 141980 Dubna, Moscow region, Russia*²*Institut für Kernphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany*

(Received 1 June 2012; revised manuscript received 26 July 2012; published 24 August 2012)

Starting from a Skyrme interaction we study the properties of the low-energy spectrum of quadrupole excitations in $^{90,92}\text{Zr}$ and $^{92,94}\text{Mo}$. The coupling between one- and two-phonon terms in the wave functions of excited states are taken into account. We use the finite-rank separable approximation which enables one to perform the QRPA calculations in very large two-quasiparticle spaces. Our results from the SGII Skyrme interaction in connection with the volume pairing interaction are in reasonable agreement with experimental data. In particular, we present the successful description of the $M1$ transition between low-energy quadrupole excitations.

DOI: [10.1103/PhysRevC.86.024311](https://doi.org/10.1103/PhysRevC.86.024311)

PACS number(s): 21.60.Jz, 23.20.-g, 21.60.Ev, 27.60.+j

I. INTRODUCTION

Properties of the quadrupole-collective isovector excitations of the valence shell of heavy nuclei reflect three main aspects: collectivity, shell structure, and the isospin degree of freedom. The balance between these aspects has been studied within a series of experiments on so-called mixed-symmetry (MS) states. A rather complete list of references on that subject is given in Ref. [1]. These isovector excitations were predicted in the proton-neutron version of the interacting boson model (IBM-2) [2], where the proton-neutron symmetry of the wave functions is quantified by the bosonic analog of the isospin, F spin [3–5]. In particular, there are the symmetric states with maximum F spin ($F = F_{\text{max}}$) and the MS ones with $F < F_{\text{max}}$. One of the well-known examples is the MS quadrupole state with $F = F_{\text{max}} - 1$ in the nucleus ^{94}Mo which was identified by the measured strong $M1$ transitions and weakly collective $E2$ transitions to low-lying symmetric states [6–8]. In contrast to the case for ^{94}Mo , the next-lighter even-even $N = 52$ isotope ^{92}Zr has the proton subshell closure $Z = 40$ and the collectivity of the 2_1^+ state decreases. As a result, the collective MS structure and the structures showing considerable F -spin breaking have been observed experimentally [9–11]. This sensitivity makes the MS states highly appealing objects for studies in microscopic approaches.

The results of the conventional shell-model (SM) calculations in strongly restricted spaces [9,12,13] and of large-scale SM calculations [14–16] have indicated the occurrence of MS quadrupole states in nuclei of the $A \approx 130$ and $A \approx 90$ mass regions along with a substantial breaking of F -spin symmetry in ^{92}Zr . For the case of ^{94}Mo , the wave functions and the $M1$ and $E2$ matrix elements support the MS assignments for the 2_3^+ state, and the consistency with the IBM-2 predictions proves the collective character of the observed low-lying levels. For ^{92}Zr , the calculated $2_{1,2}^+$ states are predominantly the pure neutron and isovector excitations, respectively. This means that the single-particle and collective degrees of freedom are present in the low-energy spectrum.

An alternative powerful microscopic approach is the quasiparticle-phonon model (QPM) [17]. Its ability to describe low-energy nuclear spectroscopy has recently been reviewed in Ref. [18]. The model Hamiltonian is diagonalized in a

space spanned by states composed of one, two, and three phonons which are generated in the quasiparticle random-phase approximation (QRPA). The separable form of the residual interaction is the practical advantage of the QPM which allows one to perform the structure calculations in large configurational spaces. For ^{94}Mo , the QPM confirms the IBM-2 level scheme, selection rules, and, in particular, the dominant one-phonon structure of the transitions to the first and third 2^+ states [8,19]. Also, the QPM gives a satisfactory and comprehensive description of the large variety of data measured for ^{92}Zr [11,20,21]. The QPM wave functions of the two lowest 2^+ states are dominated by the lowest neutron and proton two-quasiparticle components and the structures are very similar to results of the shell-model calculations. Thus, the QPM can provide microscopic support to the IBM-2 scheme. However, it is difficult to extrapolate the model parameters to new regions of nuclei.

The properties of MS states are particularly sensitive to the proton-neutron interaction [22,23]. On the other hand, the dominance of the proton-neutron attraction is one of the main characteristics of the effective nucleon-nucleon interaction. It can be traced back to the cooperation of its $T = 0$ and $T = 1$ channels. This is a good possibility for examining microscopic approaches using effective nucleon-nucleon interactions. One of the successful tools for nuclear structure studies is the QRPA with the Skyrme interaction [24,25]. These QRPA calculations allow one to relate the properties of the ground states and excited states through the same energy density functional. Although such an approach describes the properties of the low-lying states less accurately than more phenomenological ones, the results are still in a reasonable agreement with experimental data, in particular, with respect to qualitative features of the properties of the 2_1^+ states of predominantly one-phonon excitations, see for example Refs. [26–29].

The complexity of calculations taking into account the coupling between one-phonon and more complex states increases rapidly with the size of the configurational space. Making use of the finite rank separable approximation (FRSA) [30,31] for the residual interaction enables one to perform QRPA calculations in very large two-quasiparticle spaces. Taking into account the basic QPM ideas, the approach has been generalized to take into account the coupling between

one- and two-phonon components of the wave functions [32]. The FRSA has been used to study the electric low-lying states and giant resonances within the QRPA and beyond [30–34]. Alternative schemes to factorize the residual interaction have also been considered in Refs. [35–37]. A trial to describe MS states on the basis of a Skyrme mean field is given in Ref. [38] where approximations are made with respect to the simplified separable forces. Using the FRSA we will avoid those approximations in our study.

Before investigating the occurrence of MS states in neutron-rich nuclei one needs to be sure that the approach is sufficiently good to reproduce characteristics of the low-energy spectrum of quadrupole excitations of nuclei in the mass range $A \approx 90$, in particular, the $M1$ transitions between the excitations. This initial paper gives an illustration of our approach for ^{92}Zr and ^{94}Mo in comparison to the $N = 50$ isotones ^{90}Zr and ^{92}Mo with closed neutron shell. Preliminary results of our studies for ^{94}Mo are reported already in Ref. [39].

This paper is organized as follows. In Sec. II, we sketch the method that allows us to consider the phonon-phonon coupling. In particular, the QRPA equations in the case of the finite-rank separable form of the residual interaction are discussed in Sec. II A. The coupling between one- and two-phonon terms in the wave functions of excited states are taken into account in Sec. II B. In Sec. III, we discuss the details of our calculations and show how this approach can be applied to treating the proton-neutron mixed-symmetry states. Results of our calculations for properties of the quadrupole states in $^{90,92}\text{Zr}$ and $^{92,94}\text{Mo}$ are given in Sec. IV. Section IV A is devoted to a QRPA analysis, while the effects of the phonon-phonon coupling are discussed in Sec. IV B. Conclusions are finally drawn in Sec. V.

II. METHOD

This method has already been introduced in Refs. [30–33]; hence, let us briefly summarize the different steps. For the present study, the anharmonicity of the low-energy vibrations is constrained by the coupling between one- and two-phonon terms in the wave functions of excited states.

A. Implementation of QRPA

The starting point of the method is the Hartree-Fock (HF)-BCS calculation [40] of the ground state, where spherical symmetry is imposed on the quasiparticle wave functions. The continuous part of the single-particle spectrum is discretized by diagonalizing the Skyrme HF Hamiltonian on a harmonic oscillator basis. As effective interactions, Skyrme interactions are used in the particle-hole (p-h) channel, and the pairing correlations are generated by a density-dependent zero-range force

$$V_{\text{pair}}(\mathbf{r}_1, \mathbf{r}_2) = V_0 \left[1 - \eta \left(\frac{\rho(r_1)}{\rho_0} \right)^\alpha \right] \delta(\mathbf{r}_1 - \mathbf{r}_2), \quad (1)$$

where $\rho(r_1)$ is the particle density in coordinate space; ρ_0 is equal to the nuclear saturation density; α , η , and V_0 are model parameters. We use $\alpha = 1$; $\eta = 0$, $\eta = 0.5$, and $\eta = 1$

are the cases of a volume interaction, a mixed interaction, and a surface-peaked interaction, respectively. The strength V_0 is fitted to reproduce the odd-even mass difference in the region of nuclei considered here. To limit the pairing single-particle space, we have used the smooth cutoff at 10 MeV above the Fermi energies [31,41,42].

The residual interaction in the p-h channel $V_{\text{res}}^{\text{ph}}$ and in the particle-particle (p-p) channel $V_{\text{res}}^{\text{pp}}$ can be obtained as the second derivative of the energy density functional with respect to the particle density and the pair density, accordingly. As proposed in Ref. [30], we simplify $V_{\text{res}}^{\text{ph}}$ by approximating it by its Landau-Migdal form. All Landau parameters with $l > 1$ are equal to zero in the case of Skyrme interactions. We keep only the $l = 0$ terms in $V_{\text{res}}^{\text{ph}}$. In this work we study only normal parity states and one can neglect the spin-spin terms since they play a minor role [26,33]. Also, the two-body Coulomb and spin-orbit residual interactions are dropped. Therefore we can write the residual interaction as

$$V_{\text{res}}^a(\mathbf{r}_1, \mathbf{r}_2) = N_0^{-1} [F_0^a(r_1) + F_0^a(r_1)\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2] \delta(\mathbf{r}_1 - \mathbf{r}_2), \quad (2)$$

where a is the channel index $a = \{\text{ph}, \text{pp}\}$; $\boldsymbol{\tau}_i$ are the isospin operators, and $N_0 = 2k_F m^* / \pi^2 \hbar^2$ with k_F and m^* standing for the Fermi momentum and nucleon effective mass.

The expressions for F_0^{ph} , F_0^{pp} and F_0^{pp} , F_0^{pp} can be found in Refs. [43] and [31], respectively. Since the definition of the pairing force (1) involves the energy cutoff of the single-particle space to restrict the active pairing space within the mean-field approximation, this cutoff is still required to eliminate the p-p matrix elements of the residual interaction in the case of the subshells that are far from the Fermi energies, as in Ref. [31].

The p-h matrix elements and the antisymmetrized p-p matrix elements can be written as the separable form in the angular coordinates [30,31]. After integrating over the angular variables we use an N -point integration Gauss formula for the radial integrals. Thus, the residual interaction can be expressed as the sum of N terms in FRSA for the Skyrme residual interaction [30,31].

We introduce the phonon creation operators

$$Q_{\lambda\mu}^+ = \frac{1}{2} \sum_{jj'} [X_{jj'}^{\lambda i} A^+(jj'; \lambda\mu) - (-1)^{\lambda-\mu} Y_{jj'}^{\lambda i} A(jj'; \lambda - \mu)], \quad (3)$$

$$A^+(jj'; \lambda\mu) = \sum_{mm'} \langle jmj'm' | \lambda\mu \rangle \alpha_{jm}^+ \alpha_{j'm'}^+, \quad (4)$$

where λ denotes the total angular momentum and μ is its z projection in the laboratory system. α_{jm}^+ (α_{jm}) is the quasiparticle creation (annihilation) operator and jm denote the quantum numbers $nljm$. One assumes that the ground state is the QRPA phonon vacuum $|0\rangle$ and the one-phonon excited states are $Q_{\lambda\mu}^+ |0\rangle$ with the normalization condition

$$\langle 0 | Q_{\lambda\mu} Q_{\lambda'\mu'}^+ | 0 \rangle = \delta_{\lambda\lambda'} \delta_{\mu\mu'} \frac{1}{2} \sum_{jj'} (X_{jj'}^{\lambda i} X_{jj'}^{\lambda' i} - Y_{jj'}^{\lambda i} Y_{jj'}^{\lambda' i}) = \delta_{ii'}. \quad (5)$$

Making use of the linearized equation-of-motion approach, one can get the QRPA equations [40]. Solutions of this set of linear equations yield the one-phonon energies $\omega_{\lambda i}$ and the amplitudes $X_{jj'}^{\lambda i}$, $Y_{jj'}^{\lambda i}$ of the excited states. There are two types of QRPA matrix elements: the $A_{(j_1 j_1')(j_2 j_2')}^{(\lambda)}$ matrix related to forward-going graphs and the $B_{(j_1 j_1')(j_2 j_2')}^{(\lambda)}$ matrix related to backward-going graphs, and the dimension of these matrices is the space size of the two-quasiparticle configurations. Using the FRSA for the residual interaction, the eigenvalues of the QRPA equations can be obtained as the roots of a relatively simple secular equation, where the matrix dimensions never exceed $6N \times 6N$ independently of the two-quasiparticle configuration space size [30,31]. The studies [31–33] enable us to conclude that $N = 45$ for the rank of our separable approximation is enough for the electric excitations ($J \leq 6$) in nuclei with $A \leq 208$.

B. Phonon-phonon coupling

In the next stage, we construct the wave functions from a linear combination of one-phonon and two-phonon configurations

$$\Psi_\nu(\lambda\mu) = \left(\sum_i R_i(\lambda\nu) Q_{\lambda\mu i}^+ + \sum_{\lambda_1 i_1 \lambda_2 i_2} P_{\lambda_2 i_2}^{\lambda_1 i_1}(\lambda\nu) \times [Q_{\lambda_1 \mu_1 i_1}^+ Q_{\lambda_2 \mu_2 i_2}^+]_{\lambda\mu} \right) |0\rangle. \quad (6)$$

with the normalization condition

$$\sum_i R_i^2(\lambda\nu) + 2 \sum_{\lambda_1 i_1 \lambda_2 i_2} [P_{\lambda_2 i_2}^{\lambda_1 i_1}(\lambda\nu)]^2 = 1. \quad (7)$$

Because of the completeness and orthogonality conditions for the phonon operators, the bifermion operators $A^+(jj'; \lambda\mu)$ and $A(jj'; \lambda\mu)$ can be expressed by the phonon ones. The Hamiltonian can be rewritten in terms of quasiparticle and phonon operators [17,32].

The amplitudes $R_i(\lambda\nu)$ and $P_{\lambda_2 i_2}^{\lambda_1 i_1}(\lambda\nu)$ are determined from the variational principle

$$\delta(\langle \Psi_\nu(\lambda\mu) | H | \Psi_\nu(\lambda\mu) \rangle - E_\nu(\langle \Psi_\nu(\lambda\mu) | \Psi_\nu(\lambda\mu) \rangle - 1)) = 0, \quad (8)$$

which leads to a set of linear equations [17,32]

$$(\omega_{\lambda i} - E_\nu) R_i(\lambda\nu) + \sum_{\lambda_1 i_1 \lambda_2 i_2} U_{\lambda_2 i_2}^{\lambda_1 i_1}(\lambda i) P_{\lambda_2 i_2}^{\lambda_1 i_1}(\lambda\nu) = 0, \quad (9)$$

$$2(\omega_{\lambda_1 i_1} + \omega_{\lambda_2 i_2} - E_\nu) P_{\lambda_2 i_2}^{\lambda_1 i_1}(\lambda\nu) + \sum_i U_{\lambda_2 i_2}^{\lambda_1 i_1}(\lambda i) R_i(\lambda\nu) = 0. \quad (10)$$

The Pauli principle corrections are dropped here since the effect on the lowest excited states is small [17].

The rank of the set of linear equations (9) and (10) is equal to the number of one- and two-phonon configurations included in the wave function (6). Its solution requires us to compute the matrix elements coupling one- and two-phonon configurations

$$U_{\lambda_2 i_2}^{\lambda_1 i_1}(\lambda i) = \langle 0 | Q_{\lambda i} H [Q_{\lambda_1 i_1}^+ Q_{\lambda_2 i_2}^+]_{\lambda} | 0 \rangle. \quad (11)$$

Equations (9) and (10) have the same form as the QPM equations [17], but the single-particle spectrum and the parameters of the residual interaction are calculated with the Skyrme forces.

III. DETAILS OF CALCULATIONS

We apply the approach to the study of the low-energy spectrum of 2^+ excitations in the nuclei $^{90,92}\text{Zr}$ and $^{92,94}\text{Mo}$. In our calculations the single-particle continuum is discretized by diagonalizing the HF Hamiltonian on a basis of 12 harmonic oscillator shells and cutting off the single-particle spectra at the energy of 100 MeV. This is sufficient to exhaust practically all the energy-weighted sum rule. Because of the large configurational space, we do not use effective charges.

The single-particle structure around the Fermi level is a key ingredient in the microscopic analysis. For the investigation, we adopt five Skyrme interactions, namely, SGII [43], SLy4 [44], SLy5 [44], SLy5 + T [45], and T44 [46]. The SGII parametrization is the successful attempt to describe the spin-dependent properties from a standard Skyrme force. In particular, one obtains a good description of experimental energies of the Gamow-Teller resonance of ^{90}Zr [43]. The parameters of the forces SLy4 and SLy5 have been adjusted to reproduce nuclear matter properties, as well as nuclear charge radii and binding energies of doubly magic nuclei. The forces SLy5 + T and T44 involve the tensor terms added with (T44) and without (SLy5 + T) refitting the parameters of the central interaction. These five parametrizations describe correctly the subshell order near the Fermi level of $^{90,92}\text{Zr}$ and $^{92,94}\text{Mo}$. To see this, the calculated neutron and proton single-particle energies for the case of ^{92}Zr and the experimental data [47] are plotted in Fig. 1. The calculations with SGII reproduce well the experimental data, and other choices of the Skyrme forces do not improve the agreement.

We employ the isospin-invariant pairing force (1), with the value $\rho_0 = 0.16 \text{ fm}^{-3}$ of the nuclear saturation density corresponding to the SGII force. The strength V_0 is fitted to get a reasonable description of the experimental neutron and proton pairing energies of $^{90,92}\text{Zr}$ and $^{92,94}\text{Mo}$,

$$P_N = \frac{1}{2} [B(N, Z) + B(N - 2, Z) - 2B(N - 1, Z)], \quad (12)$$

for neutrons, and similarly for protons. Thus, the strength V_0 is taken equal to -270 , -420 , and -870 MeV fm^3 for the cases of the volume, mixed, and surface-peaked interaction, respectively. To make the choice of the pairing interaction, it is very useful to analyze the three lowest two-quasiparticle states in ^{92}Zr . Since the $2d_{5/2}$ neutron subshell is partially filled and the $2p_{1/2}$ proton subshell is filled, one can expect that the first level is the $\{2d_{5/2}, 2d_{5/2}\}$ neutron state while the second level is the $\{1g_{9/2}, 1g_{9/2}\}$ proton one; see, for example, Refs. [1,20,21]. As seen in Fig. 2 the different choices have a strong impact on the unperturbed two-quasiparticle excitations. Only the volume pairing interaction gives the $\{1g_{9/2}, 1g_{9/2}\}$ proton state as the second level. Thus, hereafter we use the Skyrme interaction SGII in the particle-hole channel together with the volume zero-range force acting in the particle-particle channel.

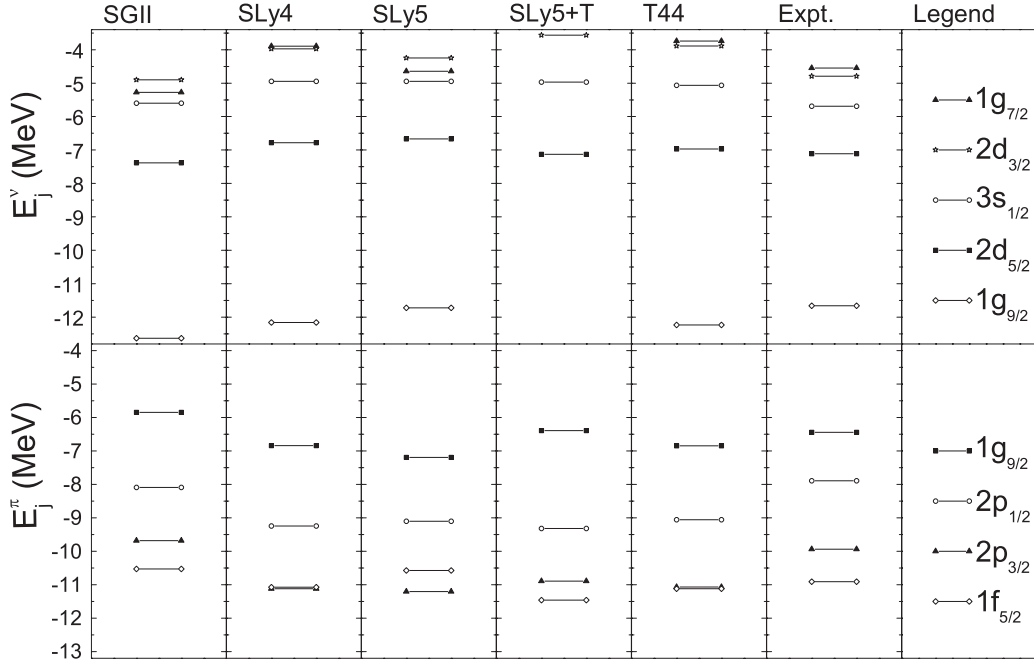


FIG. 1. Neutron (top) and proton (bottom) single-particle energies (in MeV) near the Fermi energies for ^{92}Zr calculated with SGII, SLy4, SLy5, SLy5 + T, and T44. The experimental spectra are taken from Ref. [47].

The Landau parameters F_0^{ph} , $F_0^{\text{ph}'}$ expressed in terms of the Skyrme force parameters [43] depend on k_F . As pointed out in our previous works [30,33] one needs to adopt some effective value for k_F to give an accurate representation of the original p-h Skyrme interaction. For the present calculations we use the value $k_F = 1.45 \text{ fm}^{-1}$ adjusted so as to have the spurious center-of-mass state at zero energy.

It is worth mentioning the effect of the residual p-p interaction within the QRPA. Figure 3 shows the effect on the $2_{1,2}^+$ energies and the $B(E2)$ values of ^{92}Zr . Including the quadrupole p-p interaction results in a decrease of the $2_{1,2}^+$ energies (about 0.1 MeV), and the $B(E2)$ values do not change practically.

Finally, we discuss the extension of the space for one- and two-phonon configurations. To construct the wave functions (6) of the low-lying 2^+ states up to 4 MeV we use only the 2^+ phonons for computational convenience. This restriction can be justified by the result of the recent QPM calculations with large configurational space [20,21], which demonstrate a

dominance ($\geq 90\%$) of the 2^+ phonons in the wave functions of the 2_1^+ and 2_{ms}^+ states that are at our focus. It is worth mentioning that all one- and two-phonon configurations with energies up to 8 MeV are included. We have checked that the inclusion of the high-energy configurations plays a minor role in our calculations.

IV. RESULTS

A. QRPA analysis

First, properties of the low-lying quadrupole states are studied within the one-phonon approximation. Results of our calculations for the $2_{1,2}^+$ states in $^{90,92}\text{Zr}$ and $^{92,94}\text{Mo}$ for the energies, the $B(E2)$ and $B(M1)$ values, and the contributions greater than 10% to the normalization conditions (5) are given in Table I. Note that the $B(M1)$ values have been calculated with the g factors of free protons and neutrons.

One can see that we find a satisfactory description of the isotopic dependence of the 2_1^+ energies near closed shells.

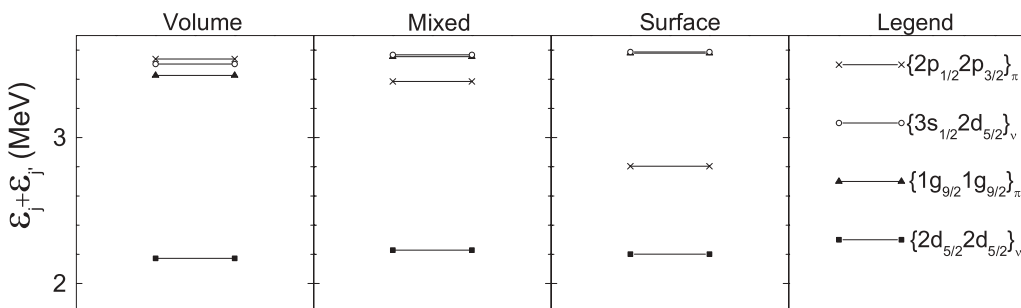


FIG. 2. Energies (in MeV) of lowest two-quasiparticle states in ^{92}Zr . The results of calculations with the volume, mixed, and surface-peaked pairing interactions are shown.

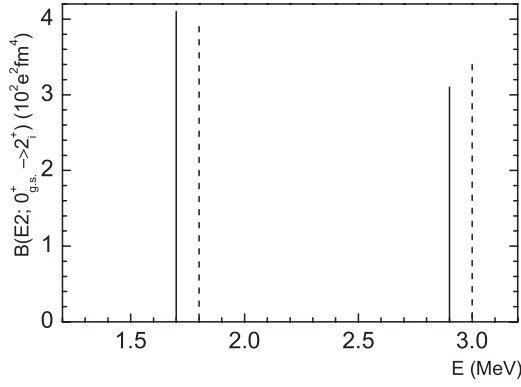


FIG. 3. Energies and $B(E2)$ values of the lowest quadrupole states in ^{92}Zr . The QRPA calculations are performed without (dashed line) and with (solid line) the residual p-p interaction.

The closure of the neutron subshell $1g_{9/2}$ in ^{90}Zr and ^{92}Mo leads to the vanishing of the neutron pairing, and as a result, the energies of the first two-quasiparticle poles $\{1g_{9/2}, 1g_{9/2}\}_\pi$ in ^{90}Zr and ^{92}Mo are larger than energies of the first poles $\{2d_{5/2}, 2d_{5/2}\}_\nu$ in ^{92}Zr and ^{94}Mo . This yields that the 2_1^+ state has collective (noncollective) structure with the domination of the proton configuration $\{1g_{9/2}, 1g_{9/2}\}$ for the case of ^{90}Zr (^{92}Mo). On the other hand, in ^{92}Zr the leading neutron configuration $\{2d_{5/2}, 2d_{5/2}\}$ gives a contribution of 79% that is almost twice larger than in ^{94}Mo . The structure peculiarities are reflected in the $B(E2; 0_{g.s.}^+ \rightarrow 2_1^+)$ values, as is shown in Table I. The dominant neutron and proton phonon amplitudes X, Y of the 2_1^+ states of ^{92}Zr and ^{94}Mo are in phase. This resembles an analogy to the full-symmetry states of the

interacting boson model, although for ^{92}Zr we observe a dominance of neutron components due to the proton subshell closure at $Z = 40$.

There are the second 2^+ states in ^{92}Zr and ^{94}Mo below 3 MeV within the one-phonon approximation. The dominant neutron and proton amplitudes of the fairly collective 2_2^+ state are out of phase. As a consequence, the isovector character of the 2_2^+ states are reflected in the remarkable values of $B(M1; 2_2^+ \rightarrow 2_1^+)$, as given in Table I. The first calculations of the isovector behavior of 2_2^+ QRPA excitations in ^{92}Zr and ^{94}Mo based on the analysis of the phonon amplitudes within the QPM have been done in Refs. [19–21].

We turn now to the structures of the 2_2^+ states of ^{90}Zr and ^{92}Mo . The proton configurations exhaust about 99% and 56% of the wave function normalization in ^{90}Zr and ^{92}Mo , respectively. It means that the second pole $\{2p_{1/2}, 2p_{3/2}\}_\pi$ in ^{92}Mo is closer to the neutron poles than that in ^{90}Zr . As expected, the negligible size of the $B(M1; 2_2^+ \rightarrow 2_1^+)$ value of ^{90}Zr is obtained. The 2_2^+ state in ^{92}Mo has the main neutron and proton phonon amplitudes in phase (Table I) and this results in the comparable $B(M1)$ value of the $M1$ transitions between the noncollective 2_1^+ state and the isoscalar 2_2^+ state.

This analysis within the one-phonon approximation can help us to identify the MS state, but it is only a rough estimate. Some overestimate of the experimental energies (Table II) indicates that there is room for two-phonon effects.

B. Effects of phonon-phonon coupling

Let us now discuss the extension of the space to one- and two-phonon configurations. The calculated 2^+ state energies, the largest contributions of the wave function normalization

TABLE I. Energies, transition probabilities, and structures of the QRPA quadrupole states in $^{90,92}\text{Zr}$ and $^{92,94}\text{Mo}$. Phonon amplitude contributions greater than 10% are given.

	State	Energy (MeV)	$B(M1; 2_1^+ \rightarrow 2_1^+)$ (μ_N^2)	$B(E2; 0_{g.s.}^+ \rightarrow 2_1^+)$ ($e^2\text{fm}^4$)	$\{n_1 l_1 j_1, n_2 l_2 j_2\}_\tau$	X	Y	%
^{90}Zr	2_1^+	2.8		630	$\{2d_{5/2}, 1g_{9/2}\}_\nu$	-0.37	-0.11	13
					$\{1g_{9/2}, 1g_{9/2}\}_\pi$	1.03	0.06	53
	2_2^+	3.4	0.00	10	$\{2p_{1/2}, 2p_{3/2}\}_\pi$	-0.52	-0.03	26
					$\{1g_{9/2}, 1g_{9/2}\}_\pi$	0.79	0.00	63
^{92}Zr	2_1^+	1.7		410	$\{2d_{5/2}, 2d_{5/2}\}_\nu$	0.85	0.00	36
					$\{1g_{9/2}, 1g_{9/2}\}_\pi$	1.26	0.12	79
	2_2^+	2.9	0.53	310	$\{2d_{5/2}, 2d_{5/2}\}_\nu$	-0.63	0.09	20
					$\{3s_{1/2}, 2d_{5/2}\}_\nu$	-0.45	-0.04	20
^{92}Mo	2_1^+	1.9		1170	$\{1g_{9/2}, 1g_{9/2}\}_\pi$	0.85	0.04	36
					$\{2p_{1/2}, 2p_{3/2}\}_\pi$	-0.36	-0.02	13
	2_2^+	4.4	0.25	230	$\{2d_{5/2}, 1g_{9/2}\}_\nu$	-0.35	-0.16	10
					$\{1g_{9/2}, 1g_{9/2}\}_\pi$	1.32	0.19	86
^{94}Mo	2_1^+	1.2		1730	$\{2d_{5/2}, 1g_{9/2}\}_\nu$	-0.65	-0.07	42
					$\{2p_{1/2}, 2p_{3/2}\}_\pi$	-0.63	-0.02	40
	2_2^+	2.4	1.23	160	$\{1g_{9/2}, 1g_{9/2}\}_\pi$	-0.49	0.10	11
					$\{2d_{5/2}, 2d_{5/2}\}_\nu$	0.92	0.27	39
					$\{1g_{9/2}, 1g_{9/2}\}_\pi$	0.99	0.37	42
					$\{2d_{5/2}, 2d_{5/2}\}_\nu$	-1.08	0.07	58
					$\{1g_{9/2}, 1g_{9/2}\}_\pi$	0.89	0.02	40

TABLE II. Energies, transition probabilities, and dominant components of phonon structures of the low-lying quadrupole states in $^{90,92}\text{Zr}$ and $^{92,94}\text{Mo}$. Experimental data are taken from Refs. [6,7,10,48,49].

	$\lambda_i^\pi = 2_i^+$	Energy (MeV)		Structure	$B(E2; 0_{\text{g.s.}}^+ \rightarrow 2_i^+)$ ($e^2\text{fm}^4$)		$B(E2; 2_i^+ \rightarrow 2_1^+)$ ($e^2\text{fm}^4$)		$B(M1; 2_i^+ \rightarrow 2_1^+)$ (μ_N^2)	
		Expt.	Theory		Expt.	Theory	Expt.	Theory	Expt.	Theory
^{90}Zr	2_1^+	2.186	2.6	93% $[2_1^+]_{\text{QRPA}}$	643 ± 22	600				
	2_2^+	3.308	3.2	95% $[2_2^+]_{\text{QRPA}}$	53 ± 14	1	65 ± 17	1	0.088 ± 0.025	0.00
^{92}Zr	2_1^+	0.934	1.6	96% $[2_1^+]_{\text{QRPA}}$	790 ± 62	420				
	2_2^+	1.847	2.7	87% $[2_2^+]_{\text{QRPA}}$	419 ± 49	230	10_{-7}^{+12}	4	0.37 ± 0.04	0.41
	2_3^+	2.067	2.6	45% $[2_4^+]_{\text{QRPA}} +$ 37% $[2_1^+ \otimes 2_1^+]_{\text{QRPA}}$	< 0.62	50	<395	160	<0.024	0.17
^{92}Mo	2_1^+	1.509	1.9	99% $[2_1^+]_{\text{QRPA}}$	1036 ± 62	1160				
	2_2^+	3.091	3.8	91% $[2_1^+ \otimes 2_1^+]_{\text{QRPA}}$	254 ± 20	50	96 ± 27	420	0.043 ± 0.007	0.03
^{94}Mo	2_1^+	0.871	0.5	73% $[2_1^+]_{\text{QRPA}}$	2031 ± 25	1280				
	2_2^+	1.864	1.8	53% $[2_1^+ \otimes 2_1^+]_{\text{QRPA}} +$ 21% $[2_3^+]_{\text{QRPA}}$	32 ± 7	170	720 ± 260	190	0.06 ± 0.02	0.07
	2_3^+	2.067	2.3	87% $[2_2^+]_{\text{QRPA}}$	279 ± 25	310	124_{-58}^{+76}	10	0.56 ± 0.05	0.68

(7), the $B(E2)$ and $B(M1)$ values, and the experimental data [6,7,10,48,49] are shown in Table II. It is worth pointing out that we get the wrong energy order of the second and third 2^+ states in the case of ^{92}Zr . On the other hand, the energy difference equal to 0.1 MeV is close to the expected accuracy of our calculations.

One can see that the inclusion of the two-phonon terms results in a decrease of the 2_1^+ energies and in a reduction of the $B(E2; 0_{\text{g.s.}}^+ \rightarrow 2_1^+)$ values, except for ^{92}Zr . Our calculations reproduce well a general behavior for energies and transition probabilities. There is some underestimation of the $B(E2)$ values of the $N = 52$ isotones in comparison with the experimental data; this probably points to a particular problem due to the effective interaction rather than to a deficiency of our variational space. In all four nuclei, the crucial contribution in the wave function structure of the first 2^+ state comes from the $[2_1^+]_{\text{QRPA}}$ configuration, but the two-phonon contributions are appreciable. This means that the structures of the first 2^+ states do not change practically due to the effects of the phonon-phonon coupling. As a result, we get the isoscalar collective structure of the 2_1^+ state in ^{94}Mo and the neutron dominated 2_1^+ excitation of ^{92}Zr which indicates the F -spin breaking.

The second 2^+ state contains a dominant two-phonon configuration $[2_1^+ \otimes 2_1^+]_{\text{QRPA}}$ in $^{92,94}\text{Mo}$ and such contribution leads to the small $B(E2; 0_{\text{g.s.}}^+ \rightarrow 2_2^+)$ values and the noticeable $B(E2; 2_2^+ \rightarrow 2_1^+)$ values. Moreover, the calculated $B(M1)$ value is sensitive to the phonon composition: the two-phonon configuration composed of the isoscalar collective phonons in the case ^{94}Mo and the noncollective phonons of ^{92}Mo . In $^{90,92}\text{Zr}$, the wave function of the 2_2^+ state is dominated by the $[2_2^+]_{\text{QRPA}}$ configuration and we can follow the QRPA estimate discussed in Sec. IV A. In addition, the dominance of the one-phonon configurations plays a key role in explaining the negligible size of the $B(E2; 2_2^+ \rightarrow 2_1^+)$ values. For the case of ^{92}Zr we obtain the isovector collective 2_2^+ state and the dominant one-phonon structure of the $M1$ transition between

the first and second 2^+ states in ^{92}Zr . The results are close to those that were previously calculated in the shell model [9,10,13] and in the QPM [11,20,21].

Finally, we examine the occurrence at low energy (below 3 MeV) of the third 2^+ states. One can see that the collective state in ^{94}Mo is dominated by the isovector one-phonon $[2_2^+]_{\text{QRPA}}$ structure. The calculated values of the 2_3^+ energy and the transition probabilities are in reasonable agreement with the experimental data. In other words, we reproduce the IBM-2 level scheme, and the calculated $B(M1; 2_3^+ \rightarrow 2_1^+)$ value supports the MS assignments observed experimentally and theoretically for the first time in Ref. [6]. It is noteworthy that this conclusion for ^{94}Mo remains valid for the SLy5+T parameter set [39]. For the 2_3^+ state of ^{92}Zr , one of the main components of the wave function is the $[2_1^+ \otimes 2_1^+]_{\text{QRPA}}$ configuration. As can be seen from Table II, the two-phonon contribution is reflected in the $B(E2)$ and $B(M1)$ values, but there is some overestimation in comparison with the experimental data. One can expect an improvement if the variational space is enlarged by the phonon composition with hexadecapole multipolarity and the three-phonon configurations are taken into account. Such calculations are now in progress.

We have examined the amount of the spin contribution to the $M1$ transition strength between the MS and first 2^+ states. In fact, we find orbital contributions $\mathcal{M}1(g_s = 0)/\mathcal{M}1_{\text{full}}$ of 31% for ^{92}Zr and of 50% for ^{94}Mo to the total $M1$ matrix elements, respectively. These numbers would result in pure orbital (spin) $M1$ strengths of 0.04 (0.19) μ_N^2 out of 0.41 μ_N^2 in total for ^{92}Zr and of 0.17 (0.17) μ_N^2 out of 0.68 μ_N^2 in total for ^{94}Mo . This observation agrees qualitatively with the situation reported previously on the orbital contribution to the $B(M1; 2_{\text{ms}}^+ \rightarrow 2_1^+)$ value from the QPM calculations [19–21].

Thus the microscopic approach [30–32] describes the properties of the low-lying states in ^{92}Zr and ^{94}Mo less accurately than more phenomenological ones [8,19–21], but the results are still in a reasonable agreement with the experimental data [6,7,10,48,49].

V. CONCLUSIONS

Starting from the Skyrme mean-field calculations, we have studied the effects of the phonon-phonon coupling on the properties of the low-energy spectrum of 2^+ excitations and, in particular, on the $M1$ transitions between the excited states of nuclei in the mass range $A \approx 90$. The finite-rank separable approach for the QRPA enables one to perform the calculations in very large configurational spaces.

The parametrization SGII of the Skyrme interaction is used for all calculations in connection with the volume zero-range pairing interaction. Using the same set of parameters we have studied the behavior of the energies and the $B(E2; 0_{g.s.}^+ \rightarrow 2_i^+)$, $B(E2; 2_i^+ \rightarrow 2_1^+)$, and $B(M1; 2_i^+ \rightarrow 2_1^+)$ values of the lowest 2^+ states in $^{90,92}\text{Zr}$ and $^{92,94}\text{Mo}$. Part of our initial motivation was the search for MS states in ^{92}Zr and ^{94}Mo in comparison to the $N = 50$ isotones ^{90}Zr and ^{92}Mo with closed neutron shell. Our results indicate indeed the occurrence of MS states in our calculation for the nuclei ^{92}Zr and ^{94}Mo that were successfully predicted within the IBM-2 before. Our results from the Skyrme interaction are in reasonable agreement with experimental data. We stress that they represent the first successful comparison between experimental $M1$ transition values and those calculated with the Skyrme interaction. The coupling between one- and two-phonon terms in the wave functions of excited states is essential. The QRPA results

tend to overestimate the 2_1^+ energies and the inclusion of the two-phonon configurations results in a decrease of the energies. There is a clear influence on the structure of the $2_{2,3}^+$ states. The structures of the low-lying 2^+ states calculated in our approach are close to those that were calculated within the QPM before. We conclude that the present approach may provide a valuable globally applicable microscopic analysis of the properties of the lowest quadrupole excitations.

Our model would probably be improved by enlarging the variational space for the 2^+ states with the inclusion of the two-phonon configurations constructed from phonons with hexadecapole multipolarity and taking into account the three-phonon configurations. The computational developments that would allow us to conclude on this point are still underway.

ACKNOWLEDGMENTS

We are grateful to R.V. Jolos, Nguyen Van Giai, V. Yu. Ponomarev, Ch. Stoyanov, and V. V. Voronov for useful discussions. A.P.S. and N.N.A. thank the hospitality of Institut für Kernphysik, Technische Universität Darmstadt, where a part of this work was done. This work was partly supported by the Heisenberg-Landau program, by the DFG under Grant No. SFB634, and by the RFBR Grant No. 110291054.

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