Complex configurations and nuclear structure problems

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Abstract. Starting from the quasi particle random phase approximation based on an effective
Skyrme interaction, we study the effects of phonon-phonon coupling (PPC) on the low-lying and
high-lying collective nuclear states. Many examples of such effects are presented. It is shown
that to reproduce experimental data one needs to take into account PPC in many cases.

1. Introduction
The experimental and theoretical studies of properties of the excited states in nuclei far from
the $\beta$-stability line are very active now. The random phase approximation (RPA) [1, 2, 3] is a
well-known and successful way to treat nuclear vibrational excitations. Using the Gogny’s [4] or
Skyrme-type [5] effective nucleon-nucleon interactions the most consistent models can describe
the ground states in the framework of the Hartree-Fock (HF) and Hartree-Fock-Bogoliubov
(HFB) approximations and the excited states within the RPA and quasiparticle RPA (QRPA).
Such models are quite successful not only to reproduce the nuclear ground state properties [6],
but also to describe the main features of nuclear excitations in closed-shell and open-shell nuclei
[7, 8]. In the latter case the pairing correlations are very important.

Due to the anharmonicity of vibrations there is a coupling between one-phonon and more
complex states [1, 3] and the complexity of calculations beyond standard RPA or QRPA increases
rapidly with the size of the configuration space, so one has to work within limited spaces. Making
use of separable forces one can perform calculations of nuclear characteristics in very large
configuration spaces since. For example, the well-known quasiparticle-phonon model (QPM)
[3] can do very detailed predictions for nuclei away from closed shells, but it is very difficult
to extrapolate the phenomenological parameters of the nuclear hamiltonian to new regions of
nuclei.

A finite rank approximation for the particle–hole (p-h) interaction resulting from the Skyrme
forces has been suggested in our previous work [9]. Thus, the self-consistent mean field can be
calculated with the original Skyrme interaction whereas the RPA solutions would be obtained
with the finite rank approximation to the p-h matrix elements. This approach has been
generalized to take into account the pairing correlations [10]. The QRPA was used to describe
characteristics of the low-lying $2^+$ and $3^-$ states and giant resonances in nuclei with very different
mass numbers [10]. It was found that there is room for the phonon-phonon coupling effects
in many cases. Following the QPM ideas [3, 11] one can extend our approach to take into
account the coupling between the one- and two-phonon terms in the wave functions of excited
states [12]. One can find examples of an influence of the complex configurations on the global B(E1) distributions including pygmy resonances in [13, 14]. The charge-exchange modes were considered in [15].

2. The model hamiltonian

We start from the effective Skyrme interaction[5] and use the notation of Ref.[16] containing explicit density dependence and all spin-exchange terms. The single-particle spectrum is calculated within the HF method. The continuous part of the single-particle spectrum is discretized by diagonalizing the HF hamiltonian on a harmonic oscillator basis[17]. The p-h residual interaction $V_{res}$ corresponding to the Skyrme force and including both direct and exchange terms can be obtained as the second derivative of the energy density functional with respect to the density[18]. Following our previous papers[9] we simplify $V_{res}$ by approximating it by its Landau-Migdal form. For Skyrme interactions all Landau parameters $F_l, G_l, F'_l, G'_l$ with $l > 1$ are zero.

The expressions for $F_0, G_0, F'_0, G'_0$ in terms of the Skyrme force parameters can be found in Ref.[16]. Because of the density dependence of the interaction the Landau parameters are functions of the coordinate $r$. In what follows we use the second quantized representation and $V_{res}$ can be written as:

$$\hat{V}_{res} = \frac{1}{2} \sum_{1234} V_{1234} : a_1^+ a_2^+ a_4 a_3 :$$  

where $a_1^+$ ($a_1^-$) is the particle creation (annihilation) operator and 1 denotes the quantum numbers $(n_1 l_1 j_1 m_1)$. $V_{1234}$ is an integral that can be reduced to the radial integral after integrating over the angular variables [9, 10].

As it is shown in [9, 10] the radial integrals can be calculated accurately by choosing a large enough cutoff radius $R$ and using a $N$-point integration Gauss formula with abscissas $r_k$ and weights $w_k$. Thus, the two-body matrix element is a sum of $N$ separable terms, i.e., the residual interaction takes the form of a rank $N$ separable interaction.

We employ a hamiltonian including an average HF field, pairing interactions, the isoscalar and isovector particle-hole (p-h) residual forces in a finite rank separable form [10]:

$$H = \sum_\tau \left( \sum_{jm} (E_j - \lambda_\tau) a^+_j a^+_{jm} a_{jm} - \frac{1}{4} V^{(0)}_r : P_0^+ (\tau) P_0 (\tau) : + \hat{V}_{res} \right),$$  

where

$$P_0^+ (\tau) = \sum_{jm} (-1)^j a^+_{jm} a^+_{j-m}.$$  

We sum over the proton($p$) and neutron($n$) indexes and the notation $\{ \tau = (n, p) \}$ is used. A change $\tau \leftrightarrow -\tau$ means a change $p \leftrightarrow n$. The single-particle states are specified by the quantum numbers $(jm)$, $E_j$ are the single-particle energies, $\lambda_\tau$ the chemical potentials. $V^{(0)}_r$ is the interaction strength in the particle-particle channel. The hamiltonian (2) has the same form as the QPM hamiltonian with $N$ separable terms [3], but the single-particle spectrum and parameters of the p-h residual interaction are calculated making use of the Skyrme forces.

In what follows we work in the quasiparticle representation defined by the canonical Bogoliubov transformation.

The hamiltonian (2) can be represented in terms of bifermion quasiparticle operators and their conjugates [3]:
\[ B(jj'; \lambda \mu) = \sum_{mm'} (-1)^{j'+m'} \langle jm' j' | \lambda \mu \rangle \alpha_{jm}^+ \alpha_{j'm'}^-; \tag{4} \]

\[ A^+(jj'; \lambda \mu) = \sum_{mm'} \langle jm' j' | \lambda \mu \rangle \alpha_{jm}^+ \alpha_{j'm'}^+; \tag{5} \]

We introduce the phonon creation operators

\[ Q^+_\lambda \mu = \frac{1}{2} \sum_{jj'} \left( X^{\lambda \mu}_{jj'} A^+(jj'; \lambda \mu) - (-1)^{\lambda - \mu} Y^{\lambda \mu}_{jj'} A(jj'; \lambda - \mu) \right). \tag{6} \]

where the index \( \lambda \) denotes total angular momentum and \( \mu \) is its z-projection in the laboratory system. One assumes that the ground state is the QRPA phonon vacuum \(|0\rangle\), i.e. \( Q^+_{\lambda \mu} |0\rangle = 0 \). We define the excited states for this approximation by \( Q^+_{\lambda \mu} |0\rangle \). The quasiparticle energies \( (\epsilon_j) \), the chemical potentials \( (\lambda_\tau) \), the energy gap and the coefficients \( u, v \) of the Bogoliubov transformations are determined from the BCS equations with the single-particle spectrum that is calculated within the HF method with the effective Skyrme interaction. Making use of the linearized equation-of-motion approach one can get the QRPA equations [2, 3]. Solutions of this set of linear equations yield the eigen-energies and the amplitudes \( X, Y \) of the excited states.

Using the completeness and orthogonality conditions for the phonon operators one can express bifermion operators \( A^+(jj'; \lambda \mu) \) and \( A(jj'; \lambda \mu) \) through the phonon ones and the initial hamiltonian (2) can be rewritten in terms of quasiparticle and phonon operators in the following form:

\[ H = h_0 + h_{QQ} + h_{QB} \]

\[ h_0 = \sum_{jm} \epsilon_j \alpha_{jm}^+ \alpha_{jm} \]

\[ h_{QQ} = -\frac{1}{4} \sum_{\lambda \mu \tau} W_{\lambda \mu \tau} X^{\lambda \mu}_{jj'} A^+(jj'; -\mu \lambda) + (-1)^{\lambda - \mu} Y^{\lambda \mu}_{jj'} A(jj'; -\mu \lambda) \]

\[ h_{QB} = -\frac{1}{2} \sum_{\lambda \mu \tau} \Gamma^{\lambda \mu \tau}_{jj'} \left( (-)^{\lambda - \mu} Q^+_{\lambda \mu} + Q_{\lambda - \mu} \right) B(jj'; -\mu \lambda) + h.c. \]

The coefficients \( W, \Gamma \) of the hamiltonian (7) are sums of \( N \) combinations of phonon amplitudes, the Landau parameters, the reduced matrix elements of the spherical harmonics and radial parts of the HF single-particle wave function.

It is worth to point out that the term \( h_{QB} \) is responsible for the mixing of the configurations and, therefore, for the description of many characteristics of the excited states of even–even nuclei [3].

To take into account the mixing of the configurations in the simplest case one can write the wave functions of excited states as a superposition of one- and two-phonon terms [3, 11].

3. Some examples
3.1. RPA
The RPA works very well in the closed shells nuclei and as an example we consider \(^{208}\)Pb. The octupole strength distribution in \(^{208}\)Pb is rather well studied in many experiments [19, 20]. The calculated octupole strength distribution up to the excitation energy 35 MeV is shown in Fig. 1.
According to experimental data [19] for the $3_{1}^{-}$ state in $^{208}\text{Pb}$ the excitation energy equals to $E_{x} = 2.62$ MeV and the energy-weighted sum rule (EWSR) is exhausted by 20.4% that can be compared with the calculated values $E_{x} = 2.66$ MeV and EWSR=21%. For the low-energy octupole resonance below 7.5 MeV our calculation gives the centroid energy $E_{c} = 5.96$MeV and EWSR=12% and experimental values are 5.4 MeV and 15.2% accordingly. For the high-energy octupole resonance we get values $E_{c} = 20.9$ MeV and EWSR=61% that are in a good agreement with experimental findings $E_{c} = 20.5 \pm 1$ MeV and EWSR=75$\pm$15% [20]. One can conclude that present calculations reproduce correctly not only the $3_{1}^{-}$ characteristics, but the whole octupole strength distribution in $^{208}\text{Pb}$.

3.2. Effect of phonon-phonon coupling

As an application of the method we demonstrate effects of the phonon-phonon coupling on energies and transition probabilities to $2_{1}^{+}$ states in $^{124-134}\text{Sn}$ [12]. Results of our calculations for the $2_{1}^{+}$ energies and transition probabilities $B(E2)$ are compared with experimental data [21, 22] in Table 1. Columns ”QRPA” and ”2PH” give values calculated within the QRPA and taking into account the phonon-phonon coupling, respectively.

As it is seen from Table 1 there is a remarkable increase of the $2_{1}^{+}$ energy and $B(E2 \uparrow)$ in $^{132}\text{Sn}$ in comparison with those in $^{130,134}\text{Sn}$. Such a behaviour of $B(E2 \uparrow)$ is related with the proportion between the QRPA amplitudes for neutrons and protons in Sn isotopes. The neutron amplitudes are dominant in all Sn isotopes and the contribution of the main neutron configuration $\{1h_{11/2},1h_{11/2}\}$ increases from 81.2% in $^{124}\text{Sn}$ to 92.8% in $^{130}\text{Sn}$ when neutrons fill the subshell $1h_{11/2}$. At the same time the contribution of the main proton configuration $\{2d_{5/2},1g_{9/2}\}$ is decreasing from 9.3% in $^{124}\text{Sn}$ to 3.9% in $^{130}\text{Sn}$. The closure of the neutron subshell $1h_{11/2}$ in $^{132}\text{Sn}$ leads to the vanishing of the neutron paring. The energy of the first neutron two-quasiparticle pole $\{2f_{7/2},1h_{11/2}\}$ in $^{132}\text{Sn}$ is greater than energies of the first poles in $^{130,134}\text{Sn}$ and the contribution of the $\{2f_{7/2},1h_{11/2}\}$ configuration in the doubly magic $^{132}\text{Sn}$ is about 61%. Furthermore, the first pole in $^{132}\text{Sn}$ is closer to the proton poles. This means that the contribution of the proton two-quasiparticle configurations is greater than those in
Table 1. Energies and $B(E2)$-values for up-transitions to the first $2^+$ states

| Nucleus | Energy (MeV) | $B(E2)^{↑}$ ($e^2b^2$) |
|---------|-------------|-----------------|
|         | Exp.        | QRPA            | 2PH          |
|         | Theory      | Exp.            | Theory       |
| $^{124}$Sn | 1.13         | 1.92 ± 0.0404   | 0.177         |
| $^{126}$Sn | 1.14         | 1.96 ± 0.03     | 0.177         |
| $^{128}$Sn | 1.17         | 2.08 ± 0.062    | 0.177         |
| $^{130}$Sn | 1.22         | 2.37 ± 0.005    | 0.177         |
| $^{132}$Sn | 4.04         | 4.47 ± 0.06     | 0.177         |
| $^{134}$Sn | 0.73         | 1.65 ± 0.006    | 0.177         |

the neighbouring isotopes and as a result the main proton configuration \(\{2d_{5/2}, 1g_{9/2}\}\) in $^{132}$Sn exhausts about 33%. In $^{134}$Sn the leading contribution (about 99%) comes from the neutron configuration \(\{2f_{7/2}, 2f_{7/2}\}\) and as a result the $B(E2)$ value is reduced. Such a behaviour of the $2^+_1$ energies and $B(E2)$ values in the neutron-rich Sn isotopes reflects the shell structure in this region.

The discovery of the double giant dipole resonance in nuclei (DGDR) [23] that is the giant dipole resonance (GDR) built on top of another GDR and the observation of small deviations from the harmonic picture of the excitation energy and spreading width, combined with the large deviations of the associated Coulomb excitation cross sections measured in relativistic heavy ion collisions [24], demand a better understanding of the role anharmonicities play in the spectrum of the DGDR. The study of the anharmonical effects within the QPM has been done in [25, 26].

The Pauli principle corrections are responsible for this energy shift [11]. Excluding four-quasiparticle configurations which violate the Pauli principle reduces somewhat collectivity of two-phonon configurations. Thus, from general arguments we should expect a positive sign of the shift for two-phonon states built up of two isoscalar phonons and a negative sign when we are dealing with isovector phonons as in the case of the DGDR.

According to predictions of different approaches for the A dependence of the anharmonicity shifts their value follows the $A^{-1}$ [1, 27] or $A^{-5/3}$ [28] dependence. The results of our calculations follow very well the $A^{-1}$ dependence, although both double- and semimagic nuclei have been included in the consideration. Weighing equally the $0^+$ and $2^+$ components of the DGDR we obtain from a $\chi^2$ analysis of the results a $|\Delta E| \sim A^{-\alpha}$ dependence with $\alpha = 1.08 \pm 0.06$. To better appreciate the results, one should point out that the present calculations of the shift have been performed with no free parameters. The most essential parameter for this calculation, the strength of the isovector dipole residual interaction, has been fixed to reproduce the energy of the GDR centroid in each nucleus known from experiment or systematics.

Let us compare the results of the present calculation for the anharmonical energy shifts with our previous calculations taking into account an additional coupling with 3-phonon configurations [26]. In Fig. 2b-c, the $B(E1) \times B(E1)$ quantity associated with the Coulomb excitation of the $J^= 0^+$ and $J^= 2^+$ components of the DGDR is shown. The $B(E1)$ quantity associated with the Coulomb excitation of the GDR is also shown in Fig. 2a. The calculated excitation functions displayed in Fig. 2b-c yield the following values for the centroid and width of the DGDR in $^{136}$Xe: $<E_{0^+}> = 36.68$ MeV and $\Gamma_{0^+} = 6.82$ MeV for the $0^+$ component of the DGDR and $<E_{0^+}> = 37.71$ MeV and $\Gamma_{2^+} = 6.84$ MeV for the $2^+$ component. These values have to be compared to $<E_{1^-}> = 15.40$ MeV and $\Gamma_{1^-} = 4.72$ MeV for the single GDR in this nucleus from our calculation. The anharmonical shifts $\Delta E_C(J^\pi) = E_{DGDR} - 2E_{GDR}$ in
this case are about -100 keV and they are underestimated in comparison with the present calculation. The calculated widths are quite close to the predictions of the harmonic model $\Gamma_{DGDR} = \sqrt{2} \Gamma_{GDR}$. The last ones are in a good agreement with experimental data [24] too. The large scale calculations taking into account a coupling of the DGDR with one- and tree-phonon terms can reproduce very well the integral characteristics of the DGDR in many nuclei [29].

Comparing the results of the present calculation of the DGDR properties with the previous ones [26] we should comment on the following. The main idea of the calculation in [26] was to describe the width of the DGDR and for this reason a three-phonon term was added to the wave function, but to make numerical calculations possible we had to truncate very strongly the basis of the two-phonon configurations. Thus, only a few most important two-phonon configurations of the type $[1^- \otimes 1^-]$ have been included in a model space. Also, an internal fermion structure of phonons was taken into account only for the one- and two-phonon configurations while the three-phonon ones were treated as constructed of bosons. For this reason, the shift of the DGDR centroid in [26] was underestimated and $0^+$ and $2^+$ components of the DGDR were practically degenerated. In the present calculation the model space of two-phonon configurations is rather complete and the $B([E1 \times E1]j)$ strength distribution over two components of the DGDR is different. It is presented in Fig. 2a) for $0^+$ and in Fig. 2b) for $2^+$ components of the DGDR in $^{136}$Xe in comparison with the strength distribution in the harmonic limit in Fig 2c).

In spite of that calculations discussed above have been done with the separable residual interaction, a comparison with other calculations for some double-magic nuclei within different approaches with making use of the Skyrme [30] or Migdal [31] forces supports the $A^{-1}$ dependence.

**Figure 2.** Fragmentation of the most collective a) one-phonon $1^-$ and b) two-phonon $[1^- \otimes 1^-]$ configurations. The results are presented with a smearing parameter $\Delta = 0.2$ MeV.
4. Conclusions
Many properties of the nuclear collective excitations in stable and unstable nuclei can be described within modern microscopic approaches. The complex configurations effects can influence on many nuclear characteristics and they are needed to be taken into account to describe experimental data.

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