NUCLEAR STRUCTURE CALCULATIONS WITH A SEPARABLE APPROXIMATION FOR SKYRME INTERACTIONS

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A finite rank separable approximation for the nuclear structure calculations with Skyrme interactions is presented. It is shown that characteristics of the low-lying states and giant multipole resonances calculated within the suggested approach are in a good agreement with available experimental data.

1. INTRODUCTION

The study of the structure of exotic nuclei far from the $\beta$-stability line has been at the forefront of nuclear physics research now. The main goal of such studies is to develop models by uncovering novel manifestations of nuclear structure when moving away from the $\beta$-stability line. One of the standard tools for nuclear structure calculations is the random phase approximation (RPA) [1, 2] with the self-consistent mean-field derived by making use of different effective nucleon-nucleon interactions [3, 4]. Such models are quite successful to reproduce the ground state properties [5, 6] within the Hartree-Fock (HF) or Hartree-Fock-Bogoliubov (HFB) approximations and the main features of nuclear excitations within the RPA and the quasiparticle RPA (QRPA) [7–9]. For the open-shell nuclei the pairing correlations are very important.

Due to the anharmonicity of vibrations there is a coupling between one-phonon and more complex states [1, 2] 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 [2], but it is very difficult to extrapolate the phenomenological parameters of the nuclear hamiltonian to new regions of nuclei.

That is why a finite rank approximation for the particle–hole (p-h) interaction resulting from the Skyrme forces has been suggested in our previous work [10]. 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.

The approach has been generalized to take into account the pairing correlations [11, 12] and the phonon-phonon coupling effects [13, 14]. The QRPA was used to describe characteristics of the low-lying 2+ and 3− states and giant resonances in different nuclei. Effects of the phonon-phonon coupling have been studied for low-lying 2+ states in neutron-rich Sn isotopes [14]. In this paper we give a brief review of our results within this approach.

2. METHOD OF CALCULATIONS

We start from the effective Skyrme interaction [4] and use the notation of Ref. [15] containing explicit density dependence and all spin-exchange terms. The single-particle spectrum is calculated within the HF method. Spherical symmetry is assumed for the HF ground states. The continuous part of the single-particle spectrum is discretized by diagonalizing the HF hamiltonian on a harmonic oscillator basis [16]. 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 [17]. Following our previous paper [10] we simplify $V_{res}$ by approximating it by its Landau-Migdal form. Here, we keep only the $l=0$ terms in $V_{res}$ and in the coordinate representation one can write it in the following form:

$$V_{res}(\mathbf{r}_1, \mathbf{r}_2) = N_0^{-1}[F_0(\eta_1) + G_0(\eta_1)(\sigma_1 \cdot \sigma_2) + (F_0'(\eta_1) + G_0'(\eta_1)(\sigma_1 \cdot \sigma_2))(\tau_1 \cdot \tau_2)]\delta(\mathbf{r}_1 - \mathbf{r}_2)$$  \hspace{1cm} (1)

where $\sigma_i$ and $\tau_i$ are the spin and 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 $F_0$, $G_0$, $F_0'$, $G_0'$ in terms of the Skyrme force parameters can be found in Ref. [15].

In what follows we use the second quantized representation and $V_{res}$ can be written as:

$$\hat{V}_{res} = \frac{1}{2} \sum_{1234} V_{1234} : a_{1\uparrow}^+ a_{2\downarrow}^+ a_3 a_4 :$$  \hspace{1cm} (2)

where $a_{1\uparrow}^+$ ($a_1$) is the particle creation (annihilation) operator and 1 denotes the quantum numbers $(n_1 l_1 j_1 m_1)$.
\[ V_{1234} = \int \phi_1^*(r_1) \phi_2^*(r_2) V_{res}(r_1, r_2) \phi_3(r_1) \phi_4(r_2) \, dr_1 \, dr_2. \]  

After integrating over the angular variables one needs to calculate the radial integrals. As it is shown in [10, 11] 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 [11]:

\[
H = \sum_{\tau} \sum_{jm} (E_j - \lambda_\tau) a_{jm}^\dagger a_{jm} - \frac{1}{4} V^{(0)}_{\tau} : P_0^\tau(\tau) P_0(\tau) : + \tilde{V}_{res},
\]

where

\[
P_0^\tau(\tau) = \sum_{jm} (-1)^{j-m} a_{jm}^\dagger a_{j\tau}.
\]

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. \( V^{(0)}_{\tau} \) is the interaction strength in the particle-particle channel. The hamiltonian (4) has the same form as the QPM hamiltonian with \( N \) separable terms [2], 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:

\[
a_{jm}^\dagger = \Omega_{jm} \alpha_{jm}^\dagger + (-1)^{j-m} \Omega_{mj} \alpha_{mj}.
\]

The hamiltonian (4) can be represented in terms of bifermion quasiparticle operators and their conjugates [2]:

\[
B(jj'; \lambda \mu) = \sum_{mm'} (-1)^{j+m'} \langle jnjm' | \lambda \mu \rangle \alpha_{jm}^\dagger \alpha_{j\mu}.
\]

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

We introduce the phonon creation operators
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 \( |0\rangle \). We define the excited states for this approximation by \( Q^+_{\lambda,\mu} |0\rangle \).

The quasiparticle energies \( (\varepsilon_j) \), the chemical potentials \( (\lambda_\tau) \), the energy gap and the coefficients \( u, v \) of the Bogoliubov transformations (6) 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.

In QRPA problems there appear two types of interaction matrix elements, the \( A^{(\lambda)}_{(\lambda,\mu)(\lambda,\mu)} \) matrix related to forward-going graphs and the \( B^{(\lambda)}_{(\lambda,\mu)(\lambda,\mu)} \) matrix related to backward-going graphs. Solutions of this set of linear equations yield the eigenenergies and the amplitudes \( X, Y \) of the excited states. The dimension of the matrices \( A, B \) is the space size of the two-quasiparticle configurations. For our case expressions for \( A, B \) and \( X, Y \) are given in [11]. Using the finite rank approximation we need to invert a matrix of dimension \( 4N \times 4N \) independently of the configuration space size [10, 11]. Therefore, this approach enables one to reduce remarkably the dimensions of the matrices that must be inverted to perform structure calculations in very large configuration spaces.

Our calculations [11] show that, for the normal parity states one can neglect the spin-multipole terms of the p-h residual interaction (1). 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 (4) can be rewritten in terms of quasiparticle and phonon operators in the following form:

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

\[
h_0 = \sum_{jm} e_j \alpha^+_j \alpha_{jm} \tag{11}\]

\[
h_{QQ} = -\frac{1}{4} \sum_{\lambda\mu\nu\tau} W^{\lambda\nu\mu\tau} (\tau) Q^+_{\lambda\mu} Q_{\lambda\mu\tau} \tag{12}\]

\[
h_{QB} = -\frac{1}{2} \sum_{\lambda,\mu,\tau} \sum_{jj'} \Gamma^{\lambda\mu}_{jj'} (\tau) \left( (-)^{\lambda-\mu} Q^+_{\lambda\mu} + Q_{\lambda-\mu} \right) \times B(jj'; \lambda - \mu) \tag{13}\]

The coefficients \( W, \Gamma \) of the hamiltonian (10) are sums of N combinations of phonon amplitudes, the Landau parameters, the reduced matrix element of the spherical harmonics and radial parts of the HF single-particle wave function (see [14]).
To take into account the mixing of the configurations in the simplest case one can write the wave functions of excited states as:

$$\Psi_\nu(\lambda_\nu\mu) = \sum_i R_i(\lambda_\nu\mu)Q^+_{\lambda_\nu\mu i} + \sum_{\lambda_i,\lambda_j,\lambda_k,\lambda_l} P_{\lambda_i,\lambda_j,\lambda_k,\lambda_l}^{\lambda_\nu\mu}(\lambda_\nu\mu) \left[ Q^+_{\lambda_i,\lambda_j,\lambda_k,\lambda_l} R_{\lambda_i,\lambda_j,\lambda_k,\lambda_l} \right]_{\lambda_\nu\mu i} [0]$$  \hspace{1cm} (14)

with the normalization condition:

$$\sum_i R_i^2(J\nu) + 2 \sum_{\lambda_i,\lambda_j,\lambda_k,\lambda_l} (P_{\lambda_i,\lambda_j,\lambda_k,\lambda_l}^{\lambda_\nu\mu}(J\nu))^2 = 1$$  \hspace{1cm} (15)

Using the variational principle in the form:

$$\delta \left( \left\langle \Psi_\nu(\lambda_\nu\mu) | H | \Psi_\nu(\lambda_\nu\mu) \right\rangle - E_\nu \left( \left\langle \Psi_\nu(\lambda_\nu\mu) | \Psi_\nu(\lambda_\nu\mu) \right\rangle - 1 \right) \right) = 0,$$  \hspace{1cm} (16)

one obtains a set of linear equations for the unknown amplitudes $R_i(J\nu)$ and $P_{\lambda_i,\lambda_j,\lambda_k,\lambda_l}^{\lambda_\nu\mu}(J\nu)$, where the number of linear equations equals the number of one- and two-phonon configurations included in the wave function (14). Note that the equations derived above have the same form as the basic QPM equations [2].

### 3. RESULTS OF CALCULATIONS

#### 3.1. HARMONIC APPROXIMATION

As a first example we examine the $2^+_1$ state energies and B(E2)-values in some Ar, Sn, Pb isotopes [11]. The results of our QRPA calculations making use of the Skyrme force SIII [18] and the experimental data [19] are shown in Table 1. One can see that there is a satisfactory agreement with experimental

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Energy [MeV]</th>
<th>B(E2↑) [e²fm⁴]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Exp.</td>
<td>Theory</td>
</tr>
<tr>
<td>$^{36}$Ar</td>
<td>1.97</td>
<td>1.91</td>
</tr>
<tr>
<td>$^{38}$Ar</td>
<td>2.17</td>
<td>2.51</td>
</tr>
<tr>
<td>$^{40}$Ar</td>
<td>1.46</td>
<td>2.17</td>
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<tr>
<td>$^{112}$Sn</td>
<td>1.26</td>
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<tr>
<td>$^{114}$Sn</td>
<td>1.30</td>
<td>1.51</td>
</tr>
<tr>
<td>$^{206}$Pb</td>
<td>0.80</td>
<td>0.96</td>
</tr>
<tr>
<td>$^{208}$Pb</td>
<td>4.09</td>
<td>5.36</td>
</tr>
</tbody>
</table>
data. Results of our calculations for Ar isotopes are close to those of QRPA with Skyrme forces [20]. The evolution of the B(E2)-values in the Ar isotopes demonstrates clearly the pairing effects. The experimental and calculated B(E2)-values in 38Ar are three times less than those in 36,40Ar. The neutron shell closure leads to the vanishing of the neutron pairing and a reduction of the proton gap. As a result there is a remarkable reduction of the E2 transition probability in 38Ar. Some overestimate of the energies indicates that there is room for two-phonon effects.

To test our approach for high lying states we examine the dipole strength distributions (GDR) in 36Ar, 112Sn and 208Pb [12]. For the energy centroids ($m_{i}/m_{0}$) we get 19.9 MeV, 15.8 MeV and 12.7 MeV in 36Ar, 112Sn and 208Pb respectively. The calculated energy centroid for 208Pb is in a satisfactory agreement with the experimental value [21] (13.4 MeV). The values of energy centroids for 36Ar and 112Sn are rather close to the empirical systematic $E_{c} = 31.2A^{-1/3} + 20.6A^{-1/6}$ MeV.

The octupole strength distribution in 208Pb is rather well studied in many experiments [22, 23]. The calculated octupole strength distribution up to the excitation energy 35 MeV is shown in Fig. 2. According to experimental data [22] for the $3^{-}$ state in 208Pb 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 \( E_c = 2.66 \text{ MeV} \) and EWSR = 21%. For the low-energy octupole resonance below 7.5 MeV our calculation gives the centroid energy \( E_c = 5.96 \text{ MeV} \) and EWSR = 12% and experimental values are 5.4 MeV and 15.2% accordingly. For the high-energy octupole resonance we get values \( E_c = 20.9 \text{ MeV} \) and EWSR = 61% that are in a good agreement with experimental findings \( E_c = 20.5 \pm 1 \text{ MeV} \) and EWSR = 75 \( \pm \) 15% [23]. One can conclude that present calculations reproduce correctly not only the \( 3^- \) 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 investigate effects of the phonon-phonon coupling on energies and transition probabilities $B(E2)$ to the $2^+_1$ state in $^{124-134}$Sn [14]. Results of our calculations with the parametrization SLy4 [24] of the Skyrme interaction, are compared with experimental data [19, 25] in Fig. 2. There is a remarkable increase of the $2^+_1$ energy and $B(E2 \uparrow)$ in $^{132}$Sn in comparison with those in $^{130,134}$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 $\{1h_{1/2},1h_{1/2}\}$ increases from 81.2% in $^{124}$Sn to 92.8% in $^{130}$Sn when neutrons fill the subshell $1h_{1/2}$. At the same time the contribution of the main proton configuration $\{2d_{5/2},1g_{9/2}\}$ is decreasing from 9.3% in $^{124}$Sn to 5.8% in $^{130}$Sn. The closure of the neutron subshell $1h_{1/2}$ in $^{132}$Sn leads to the vanishing of the neutron pairing. The energy of the first neutron two-quasiparticle pole $\{2f_{7/2},1h_{1/2}\}$ in $^{132}$Sn is greater than energies of the first poles in $^{130,134}$Sn and the contribution of the $\{2f_{7/2},1h_{1/2}\}$ configuration in the doubly magic $^{132}$Sn is about 61%. Furthermore, the first pole in $^{132}$Sn is closer to the proton poles. This means that the contribution of the proton two-quasiparticle configurations is greater than those in 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. It is worth to mention that the first prediction of the anomalous behaviour of $2^+$ excitations around $^{132}$Sn based on the QRPA calculations with a separable quadrupole-plus-pairing hamiltonian has been done in [26]. Other QRPA calculations with Skyrme [27] and Gogny [28] forces give similar results for the Sn isotopes.

One can see from Fig. 2 that the inclusion of the two-phonon terms results in a decrease of the energies and a reduction of transition probabilities. Note that the effect of the two-phonon configurations is important for the energies and this effect becomes weak in $^{132}$Sn. There is some overestimate of the energies for the QRPA calculations and taking into account the two-phonon terms improves the description of the $2^+_1$ energies. The reduction of the $B(E2)$ values is small in most cases due to the crucial contribution of the one-phonon configuration in the wave function structure.
4. CONCLUSION

We have proposed the finite rank separable approximation for the QRPA calculations with Skyrme interactions. As an illustration of the method we considered the energies and transition probabilities of the $1^-$, $2^+$ and $3^-$ states in some Ar, Sn and Pb isotopes. The calculated values are close to the QRPA ones with the full Skyrme interactions. They are in an agreement with available experimental data too.

The approach is extended to take into account the coupling between one and two-phonon terms in the wave functions of excited states. The finite rank separable approximation enables one to reduce remarkably the dimensions of the matrices that must be diagonalized to perform structure calculations in very large configuration spaces. As an application of our method we have studied the behaviour of the energies and transition probabilities to $2^+_1$ states in $^{124-134}$Sn. The inclusion of the two-phonon configurations results in a decrease of the energies and a reduction of transition probabilities. It is shown that the effect of the two-phonon configurations is important, but this effect decreases in $^{132}$Sn.

REFERENCES