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Nuclear structure calculations with a separable approximation for Skyrme interactions

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A finite rank separable approximation for the quasiparticle RPA calculations with Skyrme interactions that was proposed in our previous work is extended to take into account the coupling between one- and two-phonon terms in the wave functions of excited states. It is shown that characteristics calculated within the suggested approach are in a good agreement with available experimental data.

1. INTRODUCTION

Many properties of the collective nuclear excitations can be described within the random phase approximation (RPA) [1–4]. The most consistent models employ the Gogny's [5] or Skyrme-type [6] effective interactions which can describe the ground states in the framework of the Hartree-Fock (HF) approximation and the excited states within the RPA. Such models are quite successful for predicting nuclear states properties [7–11].

Due to the anharmonicity of vibrations there is a coupling between one-phonon and more complex states [2,4] and the complexity of calculations beyond standard RPA increases rapidly with the size of the configuration space, so one has to work within limited spaces. Using simple separable forces one can perform calculations of nuclear characteristics in very large configuration spaces since there is no need to diagonalize matrices whose dimensions grow with the size of configuration space. For example, the well-known quasiparticle-phonon model (QPM) [4] can do very detailed predictions for nuclei away from closed shells[12].

The possibility for such a simplification was the motivation for proposing in our previous work [13] a finite rank approximation for the particle–hole (p-h) interaction resulting from Skyrme-type forces. Thus, the self-consistent mean field can be calculated in the standard way with the original Skyrme interaction whereas the RPA solutions would be obtained with the finite rank approximation to the p-h matrix elements. It was found that the finite rank approximation reproduces reasonably well the dipole and quadrupole strength distributions in Ar isotopes [13].

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Recently, we extended the finite rank approximation for p-h interactions of Skyrme type to take into account pairing [14]. In this paper we generalize our approach to take into account a coupling between the one- and two-phonon components of wave functions. As an application we present results of our first calculations for the quadrupole and octupole states in ^{112}Sn.

2. METHOD OF CALCULATIONS

We start from the effective Skyrme interaction[6] 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. The continuous part of the single-particle spectrum is discretized by diagonalizing the HF hamiltonian on the harmonic oscillator basis[16]. The p-h residual interaction $\tilde{V}_{res}$ 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[13] we simplify $\tilde{V}_{res}$ 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. Here, we keep only the $l = 0$ terms in V_{res} and in the coordinate representation one can write it in the following form:

$$V_{res}(\mathbf{r}_1, \mathbf{r}_2) = N_0^{-1} \left[F_0(r_1) + G_0(r_1)\sigma_1\sigma_2 + (F_0'(r_1) + G_0'(r_1)\sigma_1\sigma_2)\tau_1\tau_2\right] \delta(\mathbf{r}_1 - \mathbf{r}_2) \quad (1)$$

where σ_i and τ_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]. Because of the density dependence of the interaction the Landau parameters of Eq.(1) are functions of the coordinate $\mathbf{r}$.

The p-h residual interaction can be presented as a sum of N separable terms. Let us explain this procedure for making the finite rank approximation by examining only the contribution of the term F_0. In what follows we use the second quantized representation and V_{res} can be written as:

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

where a_1^+ (a_1) is the particle creation (annihilation) operator and 1 denotes the quantum numbers $(n_1 l_1 j_1 m_1)$,

$$V_{1234} = \int \phi_1^*(\mathbf{r}_1)\phi_2^*(\mathbf{r}_2) V_{res}(\mathbf{r}_1, \mathbf{r}_2)\phi_3(\mathbf{r}_1)\phi_4(\mathbf{r}_2)\mathbf{dr}_1\mathbf{dr}_2, \quad (3)$$

$$V_{1234} = \sum_{JM} \hat{J}^{-2} \langle j_1 || Y_J || j_3 \rangle \langle j_2 || Y_J || j_4 \rangle I(j_1 j_2 j_3 j_4) \times \quad (4)$$

$$(-)^{J+j_3+j_4-M-m_3-m_4} \langle j_1 m_1 j_3 - m_3 \mid J - M \rangle \langle j_2 m_2 j_4 - m_4 \mid JM \rangle.$$

In the above equation, $\langle j_1||Y_J||j_3\rangle$ is the reduced matrix element of the spherical harmonics $Y_{J\mu}$, $\hat{J} = \sqrt{2J+1}$, and $I(j_1j_2j_3j_4)$ is the radial integral:

$$I(j_1j_2j_3j_4) = N_0^{-1}\int_0^\infty F_0(r)u_{j_1}(r)u_{j_2}(r)u_{j_3}(r)u_{j_4}(r)\frac{dr}{r^2}, \tag{5}$$

where $u(r)$ is the radial part of the HF single-particle wavefunction. As it is shown in [13,14] 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 and weights r_k, w_k.

$$I(j_1j_2j_3j_4) \simeq N_0^{-1}\frac{R}{2}\sum_{k=1}^{N}\frac{w_kF_0(r_k)}{r_k^2}u_{j_1}(r_k)u_{j_2}(r_k)u_{j_3}(r_k)u_{j_4}(r_k) \tag{6}$$

So we employ the hamiltonian including an average nuclear HF field, pairing interactions, the isoscalar and isovector particle–hole residual forces in the finite rank separable form [14]. This hamiltonian has the same form as the QPM hamiltonian with N separable terms [4,18], but in contrast to the QPM all parameters of this hamiltonian are expressed through parameters of the Skyrme forces.

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

$$a_{jm}^+ = u_j\alpha_{jm}^+ + (-1)^{j-m}v_j\alpha_{j-m}. \tag{7}$$

The single-particle states are specified by the quantum numbers (jm) The quasiparticle energies, the chemical potentials, the energy gap and the coefficients u,v of the Bogoliubov transformations (7) are determined from the BCS equations.

We introduce the phonon creation operators

$$Q_{\lambda\mu i}^+ = \frac{1}{2}\sum_{jj'}\left(X_{jj'}^{\lambda i}A^+(jj';\lambda\mu) - (-1)^{\lambda-\mu}Y_{jj'}^{\lambda i}A(jj';\lambda-\mu)\right) \tag{8}$$

where

$$A^+(jj';\lambda\mu) = \sum_{mm'}\langle jmj'm' \mid \lambda\mu\rangle\alpha_{jm}^+\alpha_{j'm'}^+. \tag{9}$$

The index λ denotes total angular momentum and μ is its z-projection in the laboratory system. One assumes that the quasiparticle RPA (QRPA) ground state is the phonon vacuum $\mid 0\rangle$, i.e. $Q_{\lambda\mu i}\mid 0\rangle = 0$. We define the excited states for this approximation by $Q_{\lambda\mu i}^+\mid 0\rangle$.

Making use of the linearized equation-of-motion approach [1] one can derive the QRPA equations [3,4]:

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B} & -\mathcal{A} \end{pmatrix}\begin{pmatrix} X \\ Y \end{pmatrix} = w\begin{pmatrix} X \\ Y \end{pmatrix}. \tag{10}$$

In QRPA problems there appear two types of interaction matrix elements, the $\mathcal{A}^{(\lambda)}_{(j_1j_1')(j_2j_2')}$ matrix related to forward-going graphs and the $\mathcal{B}^{(\lambda)}_{(j_1j_1')(j_2j_2')}$ matrix related to backward-going graphs [14]. Solutions of this set of linear equations yield the eigen-energies and the

amplitudes X, Y of the excited states. A dimension of the matrixes $\mathcal{A}, \mathcal{B}$ is a space size of the two-quasiparticle configurations.

Using the finite rank approximation we need to invert a matrix having a dimension $4N \times 4N$ independently of the configuration space size. One can find a prescription how to solve the system (10) within our approach in [13,14]. The QRPA equations in the QPM [4,18] have the same form as the equations derived within our approach[13,14], but the single-particle spectrum and parameters of the p-h residual interaction are calculated making use of the Skyrme forces.

In this work we use the standard parametrization SIII [19] of the Skyrme force. Spherical symmetry is assumed for the HF ground states. It is well known [10,11] that the constant gap approximation leads to an overestimating of occupation probabilities for subshells that are far from the Fermi level and it is necessary to introduce a cut-off in the single-particle space. Above this cut-off subshells don't participate in the pairing effect. In our calculations we choose the BCS subspace to include all subshells lying below 5 MeV. The pairing constants are fixed to reproduce the odd-even mass difference of neighboring nuclei. In order to perform RPA calculations, the single-particle continuum is discretized [16] by diagonalizing the HF hamiltonian on a basis of twelve harmonic oscillator shells and cutting off the single-particle spectra at the energy of 190 MeV. This is sufficient to exhaust practically all the energy-weighted sum rule.

Our investigations [14] enable us to conclude that N=45 is enough for multipolarities $\lambda \leq 3$ in nuclei with $A \leq 208$. Increasing N, for example, up to N=60 in ^{208}Pb does not change results for energies and transition probabilities practically. Our calculations show that, for the normal parity states one can neglect the spin-multipole interactions as a rule and this reduces by a factor 2 the total matrix dimension. For heavy nuclei our approach gives a large gain in comparison with an exact diagonalization [14].

To take into account the mixing of the configurations in the simplest case one can write the wave functions of excited states as:

$$\Psi_\nu(\lambda\mu) = \{\sum_i R_i(\lambda\nu) Q^+_{\lambda\mu i} + \sum_{\lambda_1 i_1 \lambda_2 i_2} P^{\lambda_2 i_2}_{\lambda_1 i_1}(\lambda\nu) \left[Q^+_{\lambda_1\mu_1 i_1} Q^+_{\lambda_2\mu_2 i_2}\right]_{\lambda\mu}\}|0\rangle \tag{11}$$

with the normalization condition:

$$\langle \Psi_\nu(JM) \mid \Psi_\nu(JM)\rangle = \sum_i R^2_i(J\nu) + 2 \sum_{\lambda_1 i_1 \lambda_2 i_2} (P^{\lambda_1 i_1}_{\lambda_2 i_2}(J\nu))^2 = 1 \tag{12}$$

The matrix element coupling one- and two-phonon configurations is:

$$\langle Q_{Ji}|H|\left[Q^+_{\lambda_1 i_1} Q^+_{\lambda_2 i_2}\right]_J\rangle = U^{\lambda_1 i_1}_{\lambda_2 i_2}(Ji) \tag{13}$$

$U^{\lambda_1 i_1}_{\lambda_2 i_2}(Ji)$ is some combination of the geometrical factors and the QRPA phonon amplitudes [4,20].

The energies of the states $\Psi_\nu(\lambda\mu)$ are solutions of the following equation [4]:

$$F(E_\nu) \equiv det\left|(\omega_{\lambda i} - E_\nu)\delta_{ii'} - \frac{1}{2}\sum_{\lambda_1 i_1, \lambda_2 i_2} \frac{U^{\lambda_1 i_1}_{\lambda_2 i_2}(\lambda i) U^{\lambda_1 i_1}_{\lambda_2 i_2}(\lambda i')}{\omega_{\lambda_1 i_1} + \omega_{\lambda_2 i_2} - E_\nu}\right| = 0 \tag{14}$$

The rank of the determinant equals the number of the one-phonon configurations included in the first term of the wave function $\Psi_\nu(\lambda\mu)$.

It is worth to point out that after solving the RPA problem with a separable interaction, to take into account the coupling with two-phonon configurations demands to diagonalize a matrix having a size that does not exceed 40 even for the giant resonance calculations in heavy nuclei whereas one would need to diagonalize a matrix with a dimension of the order of a few thousands at least for a non-separable case.

3. RESULTS OF CALCULATIONS

As an example we consider the 2_1^+, 3_1^- state energies and transition probabilities $B(E\lambda)$ in ^{112}Sn. The experimental data [21,22] and the results of our calculations within the QRPA (the second line) and with taking into account the two-phonon terms (the third line) are shown in Table 1. In our calculations the two-phonon terms of the wave function (11) include phonons with multipolarities $\lambda = 2, 3, 4, 5$. One can see that there is some overestimate of the energies and transition probabilities for the QRPA calculations. The inclusion of the two-phonon configurations results in a reduction of the enrgies and transition probabilities for the $2_1^+, 3_1^-$ states in ^{112}Sn. Generally there is a reasonable agreement between theory and experiment. The study of an influence of a choice for the Skyrme forces parameters on properties of the low-lying states within our approach and calculations for other nuclei are in progress now.

Table 1
Energies and B(Eλ)-values for up-transitions to the first 2^+, 3^- states in ^{112}Sn.

State	2_1^+		3_1^-	
	Energy (MeV)	B(E2) (e^2fm^4)	Energy (MeV)	B(E3) (e^2fm^6)
EXP.	1.26	2400±140	2.36	87000 ±12000
QRPA	1.49	2600	2.73	97000
2PH	0.90	2200	1.90	72000

4. CONCLUSION

A finite rank separable approximation for the QRPA calculations with Skyrme interactions that was proposed in our previous work is extended to take into account the coupling between one- and two-phonon terms in the wave functions of excited states.

It is shown that the suggested approach enables one to reduce remarkably the dimensions of the matrices that must be inverted to perform structure calculations in very large

configuration spaces.

As an illustration of the method we have calculated the energies and transition probabilities of the 2_1^+ and 3_1^- states in ^{112} Sn.

They are in a reasonable agreement with experimental data. A systematical study of an influence of the two-phonon terms on properties of the low lying states is in progress now.

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