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Separabelized Skyrme Interactions and Quasiparticle RPA*

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Abstract—A finite rank separable approximation for the quasiparticle random phase approximation with Skyrme interactions is applied to study the low-lying quadrupole and octupole states in some S isotopes and giant resonances in some spherical nuclei. It is shown that characteristics calculated within the suggested approach are in good agreement with available experimental data. © *2003 MAIK "Nauka/Interperiodica".*

1. INTRODUCTION

The random phase approximation (RPA) [1–4] with the self-consistent mean field derived with the use of Gogny interaction [5] or Skyrme-type interactions [6, 7] is nowadays one of the standard tools to perform nuclear structure calculations. Many properties of the nuclear collective states can be described successfully within such models [7–14].

Due to the anharmonicity of vibrations, there is a coupling between one-phonon and more complex states [2, 4]. The main difficulty is that the complexity of calculations beyond the standard RPA increases rapidly with the size of the configuration space and one has to work within limited spaces. It is well known that, 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] belongs to such a model. Very detailed predictions can be made by QPM for nuclei away from closed shells [15–17].

That is why a finite rank approximation for the particle–hole (p–h) interaction resulting from Skyrme-type forces has been suggested in our previous work [18]. 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 [18].

Recently, we extended the finite rank approximation to p–h interactions of Skyrme type to take into account pairing [19]. We tested our approach to calculate characteristics of the low-lying quadrupole and octupole states in some spherical nuclei. In this paper, we apply our approach to study the low-lying quadrupole and octupole states in some S isotopes. Choosing as examples some spherical nuclei, we demonstrate an ability of the method to describe correctly the strength distributions in a broad excitation energy interval.

2. BASIC FORMULAS AND DETAILS OF CALCULATIONS

We start from the effective Skyrme interaction [6] and use the notation of [20] containing explicit density dependence and all spin-exchange terms. The single-particle spectrum is calculated within the Hartree–Fock (HF) method. The continuous part of the single-particle spectrum is discretized by diagonalizing the HF Hamiltonian on the harmonic oscillator basis [21]. The p–h residual interaction $\tilde{V}_{\rm res}$ 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 [22]. Following our previous papers [18, 19], we simplify $\tilde{V}_{\rm res}$ 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 $V_{\rm res}$, and

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in the coordinate representation, one can write it in the following form:

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

where σ_i and τ_i are the spin and isospin operators, and $N_0 = 2k_{\rm F}m^*/\pi^2\hbar^2$ with $k_{\rm F}$ and m^* standing for the Fermi momentum and nucleon effective mass. The expressions for F_0, G_0, F_0', and G_0' in terms of the Skyrme force parameters can be found in [20]. 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 represented as a sum of N separable terms. To illustrate a procedure for making the finite rank approximation, we examine only the contribution of the term F_0. In what follows, we use the second quantized representation and $V_{\rm res}$ can be written as

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

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

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

$$V_{1234} = \sum_{JM} \hat{J}^{-2}\langle j_1||Y_J||j_3\rangle\langle j_2||Y_J||j_4\rangle I(j_1j_2j_3j_4) \quad (4)$$
$$\times (-1)^{J+j_3+j_4-M-m_3-m_4}\langle j_1 m_1 j_3 - m_3|J - M\rangle\langle j_2 m_2 j_4 - m_4|JM\rangle.$$

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:

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

where $u(r)$ is the radial part of the HF single-particle wave function. As is shown in [18, 19], the radial integrals can be calculated accurately by choosing a sufficiently large cutoff radius R and using an N-point integration Gauss formula with abscissas r_k and weights w_k:

$$I(j_1j_2j_3j_4) \simeq N_0^{-1}\frac{R}{2} \quad (6)$$
$$\times \sum_{k=1}^{N} \frac{w_k F_0(r_k)}{r_k^2}u_{j_1}(r_k)u_{j_2}(r_k)u_{j_3}(r_k)u_{j_4}(r_k).$$

Thus, we employ the Hamiltonian including an average nuclear HF field, pairing interactions, and the isoscalar and isovector p–h residual forces in the finite rank separable form [19]. This Hamiltonian has the same form as the QPM Hamiltonian with N separable terms [4, 23], 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 Bogolyubov transformation:

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

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 Bogolyubov transformations (7) are determined from the BCS equations.

We introduce the phonon creation operators

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

where

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

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

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

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

Table 1. Energies, $B(E2)$ values, and $(M_n/M_p)/(N/Z)$ ratios for up-transitions to the first 2^+ states

Nucleus	Energy, MeV		$B(E2\uparrow)$, e^2 fm^4		$(M_n/M_p)/(N/Z)$	
	exp.	theor.	exp.	theor.	exp.	theor.
^{32}S	2.23	3.34	300 ± 13	340	0.94 ± 0.16	0.92
^{34}S	2.13	2.48	212 ± 12	290	0.85 ± 0.23	0.87
^{36}S	3.29	2.33	104 ± 28	130	0.65 ± 0.18	0.40
^{38}S	1.29	1.55	235 ± 30	300	1.09 ± 0.29	0.73

Table 2. Energies, $B(E3)$ values, and $(M_n/M_p)/(N/Z)$ ratios for up-transitions to the first 3^- states

Nucleus	Energy, MeV		$B(E3\uparrow)$, e^2 fm^6		$(M_n/M_p)/(N/Z)$
	exp.	theor.	exp.	theor.	theor.
^{32}S	5.01	7.37	12700 ± 2000	8900	0.89
^{34}S	4.62	5.66	8000 ± 2000	8500	1.06
^{36}S	4.19	3.86	8000 ± 3000	7200	1.15
^{38}S	–	5.68	–	6200	1.01

In QRPA problems, there appear two types of interaction matrix elements, the matrix related to forward-going graphs $\mathcal{A}^{(\lambda)}_{(j_1j_1')(j_2j_2')}$ and the matrix related to backward-going graphs $\mathcal{B}^{(\lambda)}_{(j_1j_1')(j_2j_2')}$. Solutions to this set of linear equations yield the eigenenergies and the amplitudes X, Y of the excited states. The dimension of the matrices $\mathcal{A}$, $\mathcal{B}$ is the space size of the two-quasiparticle configurations. Expressions for $\mathcal{A}$, $\mathcal{B}$ and X, Y are given in [19].

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 of how to solve the system (10) within our approach in [18, 19]. The QRPA equations in the QPM [4, 23] have the same form as the equations derived within our approach [18, 19], 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 [24] of the Skyrme force. Spherical symmetry is assumed for the HF ground states. It is well known [11, 12] that the constant gap approximation leads to an overestimation of occupation probabilities for subshells that are far from the Fermi level, and it is necessary to introduce a cutoff in the single-particle space. Above this cutoff, subshells do not 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 [21] by diagonalizing the HF Hamiltonian on a basis of twelve harmonic oscillator shells and cutting off the single-particle spectra at the energy of 160 MeV. This is sufficient to exhaust practically all the energy-weighted sum rule. Our investigations [19] enable us to conclude that $N = 45$ is sufficient for multipolarities $\lambda \leq 3$ in nuclei with $A \leq 208$. Increasing N, for example, up to $N = 60$ in ^{208}Pb, changes the results for energies and transition probabilities by no more than 1%, so all calculations in what follows have been done with $N = 45$. 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 example, for the octupole excitations in ^{206}Pb [19], we need to invert a matrix having a dimension $2N = 90$ instead of diagonalizing a 1376×1376 matrix as would be the case without the finite rank approximation. For light nuclei, the reduction of matrix dimensions due to the finite rank approximation is 3 or 4. Thus, for heavy nuclei our approach gives a large gain in comparison with an exact diagonalization. It is worth pointing out that, after solving the RPA problem with a separable interaction, to take into account the coupling with two-phonon configurations requires one to diagonalize a matrix having a size that does not exceed 40 for the giant resonance calculations in heavy nuclei, whereas one would need to diagonalize a matrix with a dimension

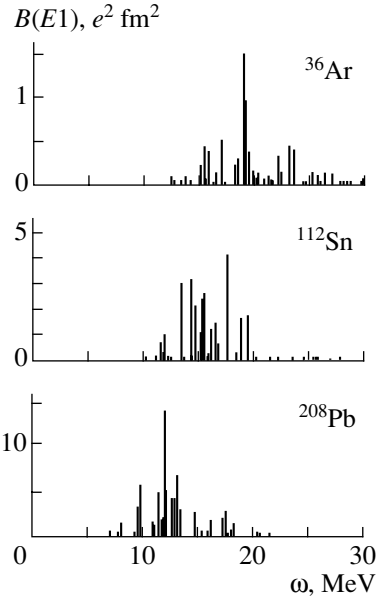

Fig. 1. Strength distributions of the GDR in ^{36}Ar, ^{112}Sn, and ^{208}Pb.

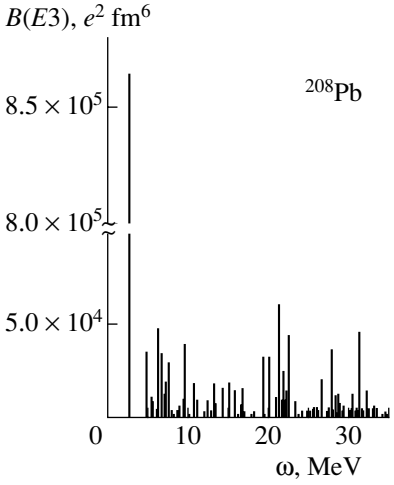

Fig. 2. The octupole strength distribution in ^{208}Pb.

of the order of a few thousand at least for a nonseparable case.

3. RESULTS OF CALCULATIONS

As a first example, we examine the 2_1^+ and 3_1^- state energies and transition probabilities in some S isotopes. The results of our calculations for the energies and $B(E2)$ values and the experimental data [25] are shown in Table 1. One can see that there is rather good agreement with experimental data. Results of our calculations for S isotopes are close to those of QRPA with Skyrme forces [26]. The evolution of the $B(E2)$ values in the S isotopes demonstrates clearly the pairing effects. The experimental and calculated $B(E2)$ values in ^{36}S are lower by a factor of two than those in ^{34,38}S. 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 ^{36}S. Some overestimate of the energies in ^{34,38}S indicates that there is room for two-phonon effects. The study of the influence of two-phonon configurations on properties of the low-lying states within our approach is in progress now.

Results of our calculations for the 3_1^- energies and the transition probabilities $B(E3)$ are compared with experimental data [27] in Table 2. Generally, there is good agreement between theory and experiment.

Additional information about the structure of the first $2^+, 3^-$ states can be extracted by looking at the ratio of the multipole transition matrix elements M_n/M_p that depend on the relative contributions of the proton and neutron configurations. In the framework of the collective model for isoscalar excitations, this ratio is equal to $M_n/M_p = N/Z$, and any deviation from this value can indicate an isovector character of the state. The M_n/M_p ratio can be determined experimentally by using different external probes [28–30]. Recently [26], QRPA calculations of the M_n/M_p ratios for the 2_1^+ states in some S isotopes have been done. The predicted results are in good agreement with experimental data [26]. Our calculated values of the M_n/M_p ratios for the 2_1^+ and 3_1^- states are shown in Tables 1 and 2, respectively. Our results support the conclusions of [26] about the isovector character of the 2_1^+ states in ^{36}S. As one can see from Table 2 our calculations predict that the M_n/M_p ratios for the 3_1^- states are rather close to N/Z, thus indicating their isoscalar character.

To test our approach for high-lying states, we examine the dipole strength distributions. The calculated dipole strength distributions (GDR) in ^{36}Ar, ^{112}Sn, and ^{208}Pb are displayed in Fig. 1. For the energy centroids (m_1/m_0), we get 19.9, 15.8, and 12.7 MeV in ^{36}Ar, ^{112}Sn, and ^{208}Pb, respectively. The calculated energy centroid for ^{208}Pb is in a satisfactory agreement with the experimental value [31] (13.4 MeV). The values of energy centroids for ^{36}Ar, and ^{112}Sn are rather close to the empirical systematics [32] $E_c = 31.2A^{-1/3} + 20.6A^{-1/6}$ (MeV). For ^{36}Ar the QRPA gives results that are very similar to our previous calculations with the particle–hole RPA [18] because the influence of pairing on the giant resonance properties is weak. It is worth mentioning that experimental data for the giant resonances in light nuclei are very scarce.

The octupole strength distribution in ^{208}Pb is rather well studied in many experiments [33, 34]. The calculated octupole strength distribution up to the excitation energy 35 MeV is shown in Fig. 2. According to experimental data [33] for the 3^-_1 state in ^{208}Pb, the excitation energy equals $E_x = 2.62$ MeV and the energy-weighted sum rule (EWSR) is exhausted by 20.4%, which 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 the experimental values are 5.4 MeV and 12%, accordingly. For the high-energy octupole resonance, we get values $E_c = 20.9$ MeV and EWSR = 61%, which are in good agreement with experimental findings $E_c = 20.5 \pm 1$ MeV and EWSR = (75 ± 15)% [34]. One can conclude that present calculations reproduce correctly not only the 3^-_1 characteristics but also the whole octupole strength distribution in ^{208}Pb.

4. CONCLUSION

A finite rank separable approximation for the QRPA calculations with Skyrme interactions that was proposed in our previous work is applied to study the evolution of dipole, quadrupole, and octupole excitations in several nuclei. 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 1^-, 2^+, and 3^- states in some S, Ar, Sn, and Pb isotopes. The calculated values are very close to those that were calculated in QRPA with the full Skyrme interactions. They are in agreement with available experimental data.

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