Quasiparticle random phase approximation with a nonlinear phonon operator

F. Šimkovic,[1] M. Šmotlák,[1] and G. Pantis[2]
[1]*Department of Nuclear Physics, Comenius University, Mlynská dol., pav. F1, SK-842 15 Bratislava, Slovakia*
[2]*Department of Physics, University of Ioanina, GR-45100 Ioanina, Greece*
(Received 5 September 2002; published 28 July 2003)

We present model calculations of the quasiparticle random phase approximation (QRPA) with a new form of the phonon operator. This modification of the QRPA is applied to the proton-neutron Lipkin model and we shall review it briefly. The present calculations show that the inclusion of nonlinear terms in the phonon operator leads to a much better agreement with the exact results obtained by the diagonalization of the nuclear Hamiltonian. It is further found that if all relevant nonlinear terms of the phonon operator are taken into account, all odd excited states are also exactly reproduced.

DOI: 10.1103/PhysRevC.68.014309 PACS number(s): 21.60.Jz, 21.60.Fw, 21.60.Ev, 23.40.Hc

The random phase approximation (RPA) and its quasiparticle generalization (QRPA) have been, for a long time, very important theoretical tools in investigating the collective degrees of freedom of many-fermion systems. They have been extensively used in various branches of physics from metals in bulk to atomic nuclei.

The instability of the QRPA [based on the quasiboson approximation (QBA)] solution has been discussed extensively and several remedies have been proposed in the literature [1–8]. It was shown that the renormalized QRPA [1,2] and the self-consistent QRPA [5–7] improve the results since they go beyond the QBA by restoring the Pauli exclusion principle (PEP) partially. In fact, this renormalization causes a shift of the point where the QRPA becomes unstable. However, the method introduces an undesirable violation of the sum rules. Thus, their behavior still remains unsatisfactory beyond the point of collapse.

Theoretically, the validities of different approximation schemes are studied in models that offer the possibility of comparison with exact solutions [2–9]. The solution of QRPA with an exact consideration of the Pauli exclusion principle (EPP QRPA) was applied to the proton-neutron Lipkin model in Ref. [2] and compared with other methods. The importance of the PEP for a reliable description of the many-fermion system has been well demonstrated. It was found that the EPP QRPA was reproducing the exact results within the physical region of the strength of the particle-particle interaction, but it was still showing a strong disagreement beyond the point of the collapse of the standard QRPA. This was mainly ascribed to the simple structure of the QRPA phonon operator [2].

It is one of the aims of this work to present an extension of the QRPA by including nonlinear terms in the phonon operator and to check how these new terms will affect the results. Second, the dependencies of some physical observables will be investigated. Keeping in mind that theoretical results are of no use unless they allow unambiguous comparison with exact ones, we apply this approach also to the proton-neutron Lipkin model. It will be shown that the QRPA with a nonlinear phonon operator can be reliably applied far beyond the collapsing point. An earlier attempt by Rowe [10] was not followed further, probably due to difficulties related to the construction of the excited states. A recent application of the second RPA and its extensions is discussed in Ref. [11]. The nonlinear phonon operator that we propose here is different. It reproduces exactly the results obtained by the diagonalization of the nuclear Hamiltonian.

In what follows, we briefly review those equations that are essential to understand the implications of the introduction of a nonlinear operator in the QRPA formalism. Emphasis is put on presentation of the background of the formulas and on the numerical results. We limit our attention to study the case of one proton and one neutron level with angular momentum *j*. The Hamiltonian of the proton-neutron monopole Lipkin model is given by [2,3]

$$H_F=\epsilon(\hat{N}_p+\hat{N}_n)+\lambda_1 A^\dagger A+\lambda_2(A^\dagger A^\dagger+AA), \tag{1}$$

where $\hat{N}_p$ ($\hat{N}_n$) and $A^\dagger$ are the proton (neutron) number and proton-neutron pair quasiparticle operators, respectively [2]. The parameters λ_1 and λ_2 are related to the strengths of particle-hole (χ) and particle-particle (κ) *pn* interactions as follows:

$$\lambda_1=2\chi'(u_p^2v_n^2+v_p^2u_n^2)-2\kappa'(u_p^2u_n^2+v_p^2v_n^2),$$

$$\lambda_2=2(\chi'+\kappa')u_pv_pu_nv_n,\quad \kappa'=2\Omega\kappa,\quad \chi'=2\Omega\chi \tag{2}$$

and $\Omega=j+\frac{1}{2}$. u_p,v_p and u_n,v_n are the BCS occupation amplitudes for protons and neutrons, respectively. The eigenvalues and the eigenvectors of model Hamiltonian (1) can be obtained by diagonalizing H_F in the basis $|n\rangle=\mathcal{N}(A^\dagger)^n|0\rangle$, where $n=0,\ldots,2\Omega$ and $\mathcal{N}$ is the normalization factor. Within the QRPA, an excited state $|Q\rangle$ is created by applying a phonon creation operator $Q^\dagger$ on a state $|\mathrm{rpa}\rangle$ having the properties

$$|Q\rangle=Q^\dagger|\mathrm{rpa}\rangle,\qquad Q|\mathrm{rpa}\rangle=0. \tag{3}$$

In order to find an excited state for the model Hamiltonian (1), the corresponding QRPA equation has to be solved. For that purpose an appropriate form of the phonon operator should be considered.

The new form of the QRPA phonon operator which we propose contains nonlinear terms in the bifermionic operators A and $A^\dagger$ as follows:

$$Q^{+}=X_1A^{\dagger}-Y_1A+X_3AA^{\dagger}A^{\dagger}-Y_3AAA^{\dagger}. \tag{4}$$

Here, we use odd indices to discuss odd excited states while quadratic terms are omitted since these are related to even excited states. In looking for a proper form of the phonon operator, we eliminated all other possibilities including those with cubic AAA and $A^{+}A^{+}A^{+}$ terms. We note that a common feature of the terms by forward (backward) amplitudes is that the difference between number of creation A^{+} and annihilation A operators in the product is plus (minus) one. Obviously, by setting the additional variational amplitudes X_3 and Y_3 equal to zero, the linear phonon operator of the EPP QRPA is recovered [2].

As we shall see later, another advantage of this nonlinear phonon operator (4) is that it allows a simultaneous description of the first and third excited states for a given Hamiltonian. It might be argued that the inclusion of cubic terms will give rise to huge matrix dimensions and will present a formidable problem in solving the nonlinear RPA equations. However, this problem can be treated by a truncation of the configuration space related to the nonlinear part of the phonon operator. As for the solutions of the nonlinear equations, they are definitely more tedious but they can be easily handled numerically. We shall note here that a close but different form of nonlinear phonon operator was suggested by Sambataro and Suhonen for the boson space in Ref. [9]. In this interesting work the authors used a different variational approach to discuss separately the ground and the first-excited state.

By solving the equation $Q|\mathrm{rpa}\rangle=0$ for the RPA ground state we find

$$|\mathrm{rpa}\rangle=\mathcal{N}\sum_{n=0}^{\Omega}\alpha_n(A^{\dagger})^{2n}|0\rangle, \tag{5}$$

where

$$\alpha_n=\frac{Y_1m_{2n-1}+Y_3m_{2n}}{X_1m_{2n}+X_3m_{2n+1}}\alpha_{n-1},\quad \mathcal{N}^{-2}=\sum_{n=0}^{\Omega}\alpha_n^2m_{2n} \tag{6}$$

with

$$m_n\equiv\langle 0|A^n(A^{\dagger})^n|0\rangle=\frac{n!(2\Omega)!}{(2\ \ \Omega-n)!(2\Omega)^n}, \tag{7}$$

m_n are vanishing for $n>2\Omega$.

By using the machinery of the equation of motion, we get the eigenvalue equation

$$\begin{pmatrix}\mathcal{A} & \mathcal{B}\\ \mathcal{B} & \mathcal{A}\end{pmatrix}\begin{pmatrix}X\\ Y\end{pmatrix}=E_{\mathrm{RPA}}\begin{pmatrix}\mathcal{U} & \mathcal{V}\\ -\mathcal{V} & -\mathcal{U}\end{pmatrix}\begin{pmatrix}X\\ Y\end{pmatrix}. \tag{8}$$

The elements of the submatrices $\mathcal{A}$ and $\mathcal{B}$ of the Hamiltonian matrix $\mathcal{H}$ on the left-hand side of Eq. (8) are given by

$$\begin{aligned}\mathcal{A}_{11}&=\langle\mathrm{rpa}|[A,H,A^{\dagger}]|\mathrm{rpa}\rangle,\\ &=2\epsilon+\lambda_1+2\lambda_1p-2\lambda_1pF_{101}+\lambda_1p^2F_{020}\\ &\quad-2(\epsilon p+\lambda_1p+\lambda_1p^2)F_{010}-4\lambda_2pF_{002},\end{aligned}$$

$$\begin{aligned}\mathcal{A}_{12}=\mathcal{A}_{21}&=\langle\mathrm{rpa}|[A,H,AA^{\dagger}A^{\dagger}]|\mathrm{rpa}\rangle\\ &=(4\epsilon+4\epsilon p+2\lambda_1+10\lambda_1p+8\lambda_1p^2)F_{101}\\ &\quad-(4\epsilon p+4\lambda_1p+10\lambda_1p^2)F_{111}+2\lambda_1p^2F_{121}\\ &\quad-2\lambda_1pF_{202}+\lambda_2[-2(1+p)F_{002}+2(2p+p^2)F_{012}\\ &\quad-2p^2F_{022}-4pF_{103}],\end{aligned}$$

$$\begin{aligned}\mathcal{A}_{22}&=\langle\mathrm{rpa}|[AAA^{\dagger},H,AA^{\dagger}A^{\dagger}]|\mathrm{rpa}\rangle\\ &=-(4\epsilon+4\epsilon p+2\lambda_1+10\lambda_1p+8\lambda_1p^2)F_{101}\\ &\quad+(8\epsilon p+4\epsilon p^2+6\lambda_1p+20\lambda_1p^2+8\lambda_1p^3)F_{111}\\ &\quad+(6\epsilon+16\epsilon p+3\lambda_1+28\lambda_1p+48\lambda_1p^2)F_{202}\\ &\quad-(4\epsilon p^2+6\lambda_1p^2+10\lambda_1p^3)F_{121}+2\lambda_1p^3F_{131}\\ &\quad-(6\epsilon p+6\lambda_1p+28\lambda_1p^2)F_{212}-2\lambda_1pF_{303}\\ &\quad+3\lambda_1p^2F_{222}+\lambda_2[(14+50p+60p^2+24p^3)F_{002}\\ &\quad-(42p+100p^260p^3)F_{012}+(42p^2+50p^3)F_{022}\\ &\quad-(12+48p+64p^2)F_{103}+24(p+2p^2)F_{113}-12p^2F_{123}\\ &\quad-14p^3F_{032}-4pF_{204}],\end{aligned} \tag{9}$$

$$\begin{aligned}\mathcal{B}_{11}&=-\langle\mathrm{rpa}|[A,H,A]|\mathrm{rpa}\rangle\\ &=-2\lambda_1pF_{002}+\lambda_2[2(1+p)\\ &\quad-(4p+2p^2)F_{010}+2p^2F_{020}-4pF_{101}],\end{aligned}$$

$$\begin{aligned}\mathcal{B}_{12}=\mathcal{B}_{21}&=-\langle\mathrm{rpa}|[A,H,AAA^{\dagger}]|\mathrm{rpa}\rangle\\ &=\lambda_1(pF_{002}-2pF_{103}-p^2F_{012})+\lambda_2[-(1+p)\\ &\quad+(3p+2p^2)F_{010}-(3p^2+p^3)F_{020}\\ &\quad+(6+24p+20p^2)F_{101}-(12p+24p^2)F_{111}\\ &\quad+p^3F_{030}+2pF_{004}-6pF_{202}+6p^2F_{121}],\end{aligned}$$

$$\begin{aligned}\mathcal{B}_{22}&=-\langle\mathrm{rpa}|[AAA^{\dagger},H,AAA^{\dagger}]|\mathrm{rpa}\rangle\\ &=\lambda_1(4p+4p^2)F_{103}-4\lambda_1p^2F_{113}-2\lambda_1pF_{204}\\ &\quad+\lambda_2[-(12+48p+60p^2+24p^3)F_{101}+4pF_{105}\\ &\quad+(96p^2+36p+60p^3)F_{111}-8pF_{303}+6p^2F_{024}bf\\ &\quad-(36p^2+48p^3)F_{121}-(24p+96p^2)F_{212}\\ &\quad+(12+96p+156p^2)F_{202}+12p^2F_{222}+12p^3F_{131}\\ &\quad-(12p+18p^2)F_{014}+(6+18p+12p^2)F_{004}],\end{aligned} \tag{10}$$

and the submatrices $\mathcal{U}$ and $\mathcal{V}$ of the norm matrix $\mathcal{N}$ on the right-hand side (rhs) of Eq. (8) take the form

$$\mathcal{U}_{11}=\langle\mathrm{rpa}|[A,A^{\dagger}]|\mathrm{rpa}\rangle=1-pF_{010},$$

$$\begin{aligned}\mathcal{U}_{22}&=\langle \mathrm{rpa}|[AAA^\dagger,AA^\dagger A^\dagger]|\mathrm{rpa}\rangle\\&=-(2p+2)F_{101}+(4p+2p^2)F_{111}+(3+8p)F_{202}\\&\quad-2p^2F_{121}-3pF_{212},\\ \mathcal{U}_{12}&=\mathcal{U}_{21}=\langle \mathrm{rpa}|[A,AA^\dagger A^\dagger]|\mathrm{rpa}\rangle=(2+2p)F_{101}-2pF_{111},\\ \mathcal{V}_{12}&=-\mathcal{V}_{21}=-\langle \mathrm{rpa}|[A,AAA^\dagger]|\mathrm{rpa}\rangle=-F_{002}+pF_{012}\end{aligned} \tag{11}$$

and $\mathcal{V}_{11}=\mathcal{V}_{22}=0$. Here the double commutators are defined as $[A,B,C]=\frac{1}{2}[A,[B,C]]+\frac{1}{2}[[A,B],C]$ and

$$\langle \mathrm{rpa}|A^iC^j(A^\dagger)^k|\mathrm{rpa}\rangle=F_{ijk},\quad p=\frac{1}{2\Omega}. \tag{12}$$

After the diagonalization of the norm matrix $\mathcal{N}$ on the rhs of Eq. (8), the eigenvalue equation Eq. (8) takes the form of the standard QRPA equation

$$\begin{pmatrix}\overline{\mathcal{A}} & \overline{\mathcal{B}}\\ \overline{\mathcal{B}} & \overline{\mathcal{A}}\end{pmatrix}\begin{pmatrix}\overline{X}\\ \overline{Y}\end{pmatrix}=E_{\mathrm{RPA}}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\overline{X}\\ \overline{Y}\end{pmatrix}. \tag{13}$$

From the definition of the QRPA ground state $|\mathrm{rpa}\rangle$ in Eqs. (5) and (6) it follows that the elements of the $\overline{\mathcal{A}}$ and $\overline{\mathcal{B}}$ matrices are functions of the $\overline{X}$ and $\overline{Y}$ amplitudes. Thus, in numerical applications the solution of the QRPA with a nonlinear phonon operator (QRPA with nlo) will be obtained by an iteration process. A new point with respect to the QRPA studies with linear phonon operator is that in each iteration by diagonalizing Eq. (13) two sets of $\overline{X}$ and $\overline{Y}$ amplitudes are obtained. These are associated with the two different QRPA energies. For each next iteration we consider that set of $\overline{X}$, $\overline{Y}$, which produces the smaller expectation value for the ground state of the nuclear Hamiltonian $\langle \mathrm{rpa}|H|\mathrm{rpa}\rangle$.

An interesting issue here is what is the meaning of the second QRPA energy. We recall that in the QRPA with a linear phonon operator (QRPA with lo) only the first excited state is evaluated. There it is found that for $j=1/2$ the first excited state obtained by exact diagonalization of the H_F fully coincides with the one calculated within the QRPA with lo. For $j=1/2$ there are only two excited states within a studied model. It is important to mention that the exact wave functions of the odd (even) excited states of the nuclear Hamiltonian contain components proportional to $(A^\dagger)^n$ with only $n=$odd (even) $(n\leqslant 2\Omega)$. In the case of $j=1/2$, the wave function of the first excited state is just $A^\dagger|0\rangle$. In the model considered here the elements of $\mathcal{A}$, $\mathcal{B}$, $\mathcal{U}$, and $\mathcal{V}$ in Eqs. (9), (10), and (11) coming from the nonlinear phonon operator are equal to zero, i.e., their inclusion is meaningless. However, a different situation occurs in the case of $j=3/2$. Here there are four excited states, two with $n=$even components and two with $n=$odd components. The wave functions of the first and third excited states are of the form $[a_1A^\dagger+a_2(A^\dagger)^3]|0\rangle$. By solving the QRPA with nlo [Eq. (13)] we obtain exactly the first and third excited states of the Hamiltonian in Eq. (1). The two sets of QRPA amplitudes define the same ground state $|\mathrm{rpa}\rangle$ in Eq. (5) equally and fulfill the requirement $Q|\mathrm{rpa}\rangle=0$. From the above discussion it follows that in order to reproduce exactly the eigenvalues given by the diagonalization of the nuclear Hamiltonian (1) for the odd excited states in the case of $j>3/2$, one needs to add additional nonlinear terms in the phonon operator in Eq. (4) as follows:

$$\begin{aligned}Q^+=&X_1A^\dagger-Y_1A+X_3AA^\dagger A^\dagger-Y_3AAA^\dagger+X_5AAA^\dagger A^\dagger A^\dagger\\&-Y_5AAAA^\dagger A^\dagger+\cdots.\end{aligned} \tag{14}$$

Now we shall show the influence of the nonlinear terms of phonon operator (4) by evaluating some physical QRPA observables of interest for the model Hamiltonian with $j=9/2, \epsilon=1$ MeV $(Z=4,N=6)$. We use a fixed value of $\chi'=0.5$ MeV, while κ' is considered as a free parameter in the interval (0,3) MeV. The same model was considered also in several previous studies (see, e.g., Ref. [2–4]).

We note again that if only linear terms are included in the phonon operator in Eq. (4), our approach is reduced to the EPP QRPA method of Ref. [2]. We shall denote it here EPP QRPA with lo in contrast to our present approach, which we shall denote EPP QRPA with nlo. Our present results, which are the first reported for such an operator, will be compared with those obtained by the diagonalization of Hamiltonian (1), EPP QRPA with lo and the standard QRPA approaches. The quality of the agreement will be assessed by looking at the expectation values of the quasiparticle operators for the ground and excited states.

In Fig. 1 we show the ground state energy $E_{\mathrm{g.s.}}=\langle \mathrm{rpa}|H|\mathrm{rpa}\rangle$ calculated without any approximation and the QRPA energy E_{rpa} associated with the first excited state (relative to the ground state) obtained by the above mentioned methods as a function of κ'. We note a collapse of the standard QRPA solution for $\kappa'\approx 1.1$. Beyond this point the qualitative agreement of the EPP QRPA with lo with the results of the exact diagonalization is degraded. A significantly better agreement with the exact results is achieved in the case of the EPP QRPA with nlo. Obviously, this has to do with the inclusion of nonlinear terms in the phonon operator.

As a simple test on the quality of the wave functions, we performed a comparison between exact and approximate expectation values of the quasiparticle number $C/2$ in the ground and in the first excited state. These are defined as follows:

$$N_0=\langle \mathrm{g.s.}|\frac{C}{2}|\mathrm{g.s.}\rangle,\quad \Delta N=\langle 1_{\mathrm{exc.}}|\frac{C}{2}|1_{\mathrm{exc.}}\rangle-N_0, \tag{15}$$

where $|\mathrm{g.s.}\rangle$ is the ground state and $|1_{\mathrm{exc.}}\rangle$ is the first excited state of the system. In Fig. 2 we show N_0 and ΔN, given by the above approaches and by the exact calculation. We see again that the inclusion of the nonlinear terms in the phonon operator is of great importance. Indeed, for both N_0 and ΔN the results achieved by the EPP QRPA with nlo are in good agreement with the exact ones even far beyond the point at which the standard QRPA breaks down. It is worthwhile to notice that EPP QRPA with nlo reproduces the exact result for ΔN, up to the point of collapse, and still continues to follow qualitatively the same trend after this point, i.e., for

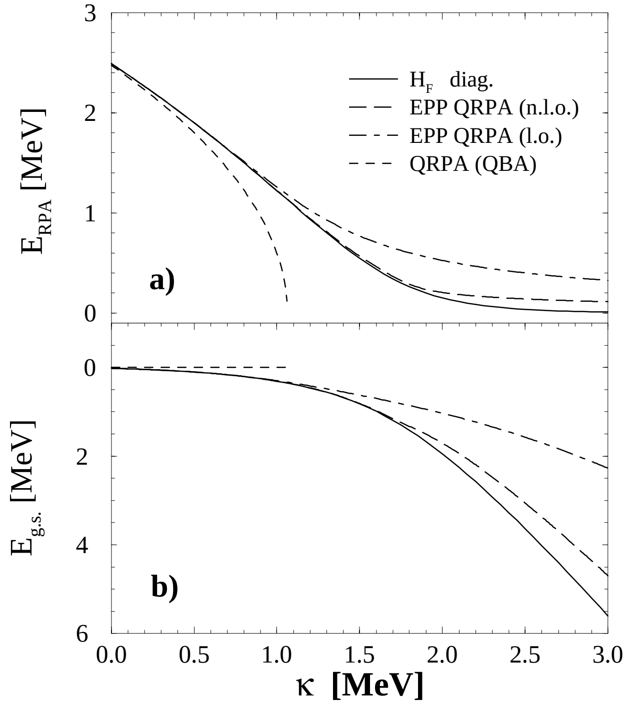

FIG. 1. The excitation energies $E_{\mathrm{rpa}}(=E_1-E_{\mathrm{g.s.}})$ (a) and the ground state energies $E_{\mathrm{g.s.}}$ (b) provided, by diagonalizing H_F (solid line), by the standard QRPA (dashed line), by the EPP QRPA with linear phonon operator (dot-dashed line), and by the EPP QRPA with nonlinear phonon operator (long dashed line) as a function of κ'.

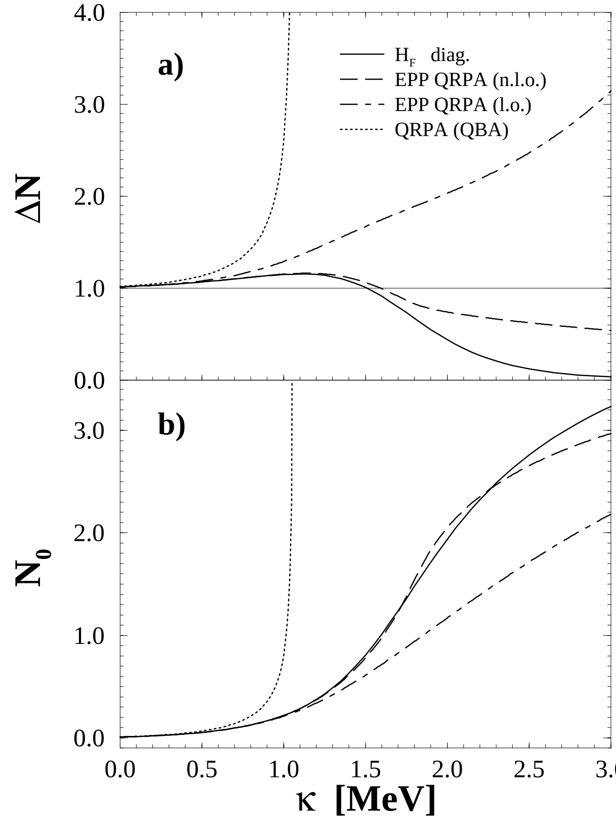

FIG. 2. (a) The difference ΔN of the expectation values (excited state−ground state) and (b) the expectation values N_0 (ground state) of the (half) quasiparticle number operator $C/2$ as a function of κ'. Notations as in Fig. 1.

$\kappa' > 1.2$. This change of behavior of the curve describing ΔN as a function of κ' was never seen before in any of the extensions of the standard QRPA.

In summary, in this work, using a QRPA with nonlinear phonon operator in the proton-neutron Lipkin model we arrive at the following conclusions.

(i) The inclusion of nonlinear terms in the phonon operator of the QRPA is feasible and leads to a very good agreement with the exact results obtained by the diagonalization of the nuclear Hamiltonian.

(ii) By adding more nonlinear terms the accuracy can be further increased. In the case all relevant nonlinear terms in the phonon operator are considered, the odd excited states of the nuclear Hamiltonian H_F in Eq. (1) are reproduced exactly.

This work has been a test case to see the influence of the nonlinear terms. For realistic calculations, one has to overcome the difficulties of dealing with large matrices and solving the nonlinear equations. This hopefully can be done by truncating the configuration space and using the matrix inversion techniques developed recently. Another difficult problem will be the definition of the ground state since in a realistic case the RPA ground state cannot be exactly evaluated. Here, a look at the boson space and an ansatz, e.g., in the way proposed in Ref. [2], might be very useful.

This work was supported by the VEGA Grant agency of the Slovak Republic under Contract No. 1/0249/03.

[1] F. Šimkovic, G. Pantis, and A. Faessler, Phys. At. Nucl. **61**, 1218 (1998).

[2] F. Šimkovic, A.A. Raduta, M. Veselský, and A. Faessler, Phys. Rev. C **61**, 044319 (2000).

[3] J.G. Hirsch, P.O. Hess, and O. Civitarese, Phys. Rev. C **54**, 1976 (1996); A. Mariano and J.G. Hirsch, *ibid.* **61**, 054301 (2000).

[4] F. Šimkovic, M. Šmotlák, and A.A. Raduta, J. Phys. G **27**, 1757 (2001).

[5] F. Krmpotić, E.J.V. de Passos, D.S. Delion, J. Dukelsky, and P. Schuck, Nucl. Phys. **A637**, 295 (1998).

[6] J. Dukelsky, J.G. Hirsch, and P. Schuck, Eur. Phys. J. A **7**, 155 (2000).

[7] A. Bobyk, W.A. Kaminski, and P. Zareba, Eur. Phys. J. A **5**, 385 (1999); Nucl. Phys. **A669**, 221 (2000).

[8] K. Hagino and G. Bertsch, Phys. Rev. C **61**, 024307 (2000).

[9] M. Sambataro and J. Suhonen, Phys. Rev. C **56**, 782 (1997); Europhys. Lett. **44**, 173 (1998).

[10] D.J. Rowe, *Nuclear Collective Motion* (Methuen, London, 1970), p. 277.

[11] M. Tohyama, Phys. Rev. C **64**, 067304 (2001).