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Nuclear Physics A 579 (1994) 1–12

NUCLEAR
PHYSICS A

Ground-state correlations beyond RPA

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Received 16 August 1993; revised 2 May 1994

Abstract

An approach is proposed which includes ground-state correlations beyond RPA. This is achieved by using a renormalized quasiboson approximation with reference to the correlated ground state of the system, rather than to the uncorrelated Hartree–Fock one, and by expressing the particle–particle and hole–hole pair operators in terms of the particle–hole ones. The set of the so-obtained nonlinear equations for the one-phonon energy and amplitudes are first solved within the Lipkin–Meshkov–Glick model and the results are compared with those of previous approaches as well as with the exact ones. Applications to realistic nuclei, starting from fully self-consistent HF + RPA calculations with a Skyrme force are also presented.

1. Introduction

The Random Phase Approximation (RPA) is one of the approximations to the many-body problem, which are more often employed in nuclear-structure physics. It provides a simple theory of excited states of the nucleus, including some correlations in the ground state. A large number of applications of the RPA, particularly for low-lying quadrupole and octupole vibrations as well as for giant resonances, has demonstrated its reliability [1,2].

A crucial point of the RPA resides in the so-called quasiboson approximation (QBA). This approximation treats particle–hole (ph) creation B_{ph}^+ and annihilation B_{ph} operators as if they were bosons, thus leading to a violation of the Pauli principle. As a consequence RPA breaks down at a certain value of the interaction strength, where it yields

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imaginary eigenvalues [1,2]. Various attempts have been made in the last three decades to go beyond the RPA to correct for this deficiency [3–9]. We also refer to a recent paper by Klein et al. [10] for an overview and criticism of some of these proposals.

The QBA can be obtained by substituting the commutator $[B_{ph}, B_{p'h'}^+]$ with its expectation value in the uncorrelated Hartree–Fock (HF) ground state. A method to go one step beyond QBA was proposed many years ago [5,6]. It basically consists in replacing the HF ground state by the correlated one $|0\rangle$ and leads to a set of RPA-like equations with a renormalized interaction. Since the latter turns out to be a function of the unknown forward X and backward Y amplitudes of the (ph) excitations, one has in fact a set of nonlinear equations to be solved self-consistently. In the following we will refer to this method as “Hara’s”.

In Ref. [6], by using the equations of motion method, a “renormalized RPA” was introduced which is essentially equivalent to Hara’s. A related approach, based on Green-function techniques, was also developed in Ref. [8]. Starting from the linear response function and restricting the class of pair operators to (ph) ones, the authors introduced some renormalized bosons. By inserting a complete set of states $|\nu\rangle$ into the static four-point densities appearing in the equation for the (ph) mass operator and neglecting amplitudes like $\langle 0|a_p^+ a_{p'}|\nu\rangle$, $\langle 0|a_h^+ a_{h'}|\nu\rangle$ and $\langle 0|a_p^+ a_h|0\rangle$, a system of highly nonlinear equations was obtained. These could reduce to Hara’s under appropriate approximations. Purpose of this method was that of realizing a self-consistent condition which could guarantee the equality between the ground state used in the evaluation of the RPA matrix elements and that emerging as solution. The same subject has been further elaborated in more recent publications [9] and has found applications within the schematic and exactly solvable model of Lipkin, Meshkov and Glick (LMG) [11].

In the present paper, we propose an alternative approach to Hara’s differing from this essentially in the way of evaluating expectation values of the commutator $[B_{ph}, B_{p'h'}^+]$ in the correlated ground state. We test the approach by comparing it with RPA and Hara’s within the LMG model. Further applications of all three methods are performed in realistic cases.

The paper is organized as follows. In Section 2 we derive the basic equations of our formalism, showing also the connection with Hara’s approach. In Section 3 we study an application of our method to the schematic LMG model. We also compare the results, obtained within our approach with the exact ones as well as with those obtained in RPA and in Hara’s approaches. In Section 4 we present for the first time the results of fully self-consistent calculations using a Skyrme interaction for ^{146}Gd and ^{208}Pb . The comparison is made between RPA and the two other approximations discussed above and concerns the energies and the $B(E\lambda)$ values. The results are summarized in Section 5, where some conclusions are drawn.

2. Formalism

Let us consider the particle–hole operators $B_{ph}^+ = a_p^+ a_h$ and $B_{ph} = (B_{ph}^+)^+$ with $p(= n_p, l_p, j_p)$ and $h(= n_h, l_h, j_h)$ denoting the single-particle and single-hole states, respectively. They satisfy the commutation relations:

$$[B_{ph}, B_{p'h'}^+] = \delta_{pp'} B_{hh'}^+ - \delta_{hh'} B_{pp'}, \quad (1)$$

$$[B_{ph}, B_{p'h'}] = [B_{ph}^+, B_{p'h'}^+] = 0. \quad (2)$$

In RPA the commutator of Eq. (1) is approximated by its expectation value in the HF ground state (g.s.) $|HF\rangle$, thus B^+ and B satisfy boson commutation relations. This approximation is referred to as QBA. The excited states $|\nu\rangle = Q_\nu^+ |RPA\rangle$ of the system are described in terms of the phonon operators

$$Q_\nu^+ = \sum_{ph} (X_{ph}^\nu B_{ph}^+ + Y_{ph}^\nu B_{ph}), \quad (3)$$

where the amplitudes X^ν and Y^ν are solutions of the equations

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = \omega_\nu \begin{pmatrix} X^\nu \\ -Y^\nu \end{pmatrix} \quad (4)$$

with

$$A_{ph,p'h'} = (\epsilon_p - \epsilon_h) \delta_{pp'} \delta_{hh'} + V_{h'p,p'h}, \quad (5)$$

$$B_{ph,p'h'} = V_{pp',hh'}, \quad (6)$$

where ϵ_p (ϵ_h) is the single-particle (hole) energy and $V_{ij,kl} = \langle kl|V|ij\rangle - \langle kl|V|ji\rangle$.

The amplitudes X_{ph}^ν and Y_{ph}^ν obey the orthonormalization condition:

$$\sum_{ph} (X_{ph}^\nu X_{ph}^{\nu'} - Y_{ph}^\nu Y_{ph}^{\nu'}) = \delta_{\nu\nu'}, \quad (7)$$

which implies that

$$[Q_\nu, Q_{\nu'}^+] = \delta_{\nu\nu'}. \quad (8)$$

The g.s. $|RPA\rangle$ is defined as the vacuum of the phonon operators Q_ν^+ , that is

$$Q_\nu |RPA\rangle = 0. \quad (9)$$

To go beyond RPA by incorporating ground-state correlations it has been suggested [5–7] to approximate the commutator of Eq. (1) by its expectation value in the correlated ground state $|0\rangle$, thus obtaining

$$[B_{ph}, B_{p'h'}^+] \simeq \delta_{pp'} \delta_{hh'} D_{ph} = \delta_{pp'} \delta_{hh'} (n_h - n_p) \quad (10)$$

with $n_p = \langle 0|a_p^+ a_p|0\rangle$ and $n_h = \langle 0|a_h^+ a_h|0\rangle$ being the single-particle and single-hole occupation probabilities in $|0\rangle$. In this approach one introduces [5,6] renormalized (ph) operators

$$\bar{B}_{ph}^+ = D_{ph}^{-1/2} B_{ph}^+ \quad (11)$$

and phonon operators

$$\bar{Q}_\nu^+ = \sum_{ph} (\bar{X}_{ph}^\nu \bar{B}_{ph}^+ + \bar{Y}_{ph}^\nu \bar{B}_{ph}). \quad (12)$$

From Eqs. (10) and (11) it follows that

$$[\bar{B}_{ph}, \bar{B}_{p'h'}^+] \simeq \delta_{pp'} \delta_{hh'}. \quad (13)$$

In the following we will denote the excited states of the system as $|\bar{\nu}\rangle = \bar{Q}_\nu^+ |0\rangle$ with the correlated ground state $|0\rangle$ defined as

$$\bar{Q}_\nu |0\rangle = 0. \quad (14)$$

By following the procedure of Ref. [6], based on the equations of motion method, and neglecting the renormalization of the single-particle energies considered there, one easily finds that the amplitudes \bar{X} and \bar{Y} satisfy RPA-like equations of the same form as Eq. (4), but with a renormalized interaction

$$\langle h'p|\bar{V}|p'h\rangle = D_{ph}^{1/2} \langle h'p|V|p'h\rangle D_{p'h'}^{1/2}, \quad (15)$$

$$\langle pp'|\bar{V}|hh'\rangle = D_{ph}^{1/2} \langle pp'|V|hh'\rangle D_{p'h'}^{1/2} \quad (16)$$

and the orthonormalization condition

$$\sum_{ph} (\bar{X}_{ph}^\nu \bar{X}_{ph}^{\nu'} - \bar{Y}_{ph}^\nu \bar{Y}_{ph}^{\nu'}) = \delta_{\nu\nu'}, \quad (17)$$

which guarantees that

$$[\bar{Q}_\nu, \bar{Q}_{\nu'}^+] = \delta_{\nu\nu'}. \quad (18)$$

Eq.(12) and its adjoint can be inverted to give

$$\bar{B}_{ph}^+ = \sum_{\nu} (\bar{X}_{ph}^\nu \bar{Q}_\nu^+ - \bar{Y}_{ph}^\nu \bar{Q}_\nu). \quad (19)$$

In order to calculate the renormalized interaction, Eqs. (15) and (16), one has to determine the quantity D_{ph} , i.e. the occupation numbers n_p and n_h . So far this has been done by making use of the Thouless theorem, which expresses the correlated ground state $|0\rangle$ in terms of the uncorrelated one $|\text{HF}\rangle$ as

$$|0\rangle = \mathcal{N} e^S |\text{HF}\rangle, \quad (20)$$

where S is a sum of products of two \bar{B}_{ph}^+ operators. In this approach one gets

$$D_{ph} = 1 - \sum_{p,\nu} (\bar{Y}_{ph}^\nu)^2 - \sum_{h,\nu} (\bar{Y}_{ph}^\nu)^2. \quad (21)$$

Thus the RPA-like equations with the renormalized interaction become nonlinear in the \bar{X} and \bar{Y} amplitudes. Recently, these equations have been solved [14] in a realistic case, within the quasiparticle representation and by using a separable isoscalar multipole–multipole interaction plus monopole pairing. The just described approach is what we have called Hara’s. We stress that the matrix elements of the double commutators of the equations of motion method have been calculated in the correlated ground state, so avoiding an inconsistency of RPA. However, some approximations have been introduced which make the resulting equations solvable in realistic cases.

We remark that Eq. (20) implies making use again of the approximation (13), that is treating the operators \bar{B}_{ph}^+ and \bar{B}_{ph} as bosons.

In the present paper we explore a different way of calculating the occupation probabilities, within the same renormalized QBA. It consists in expressing the $B_{hh'}^+$ and $B_{pp'}$ operators of Eq. (1) in terms of the mappings

$$B_{pp'}^+ \rightarrow \sum_h B_{ph}^+ B_{p'h}, \quad (22)$$

$$B_{hh'}^+ \rightarrow \delta_{hh'} - \sum_p B_{ph'}^+ B_{ph}, \quad (23)$$

which are known to preserve the commutation relations when the B_{ph}^+ and B_{ph} operators are bosons [12]. It is worthwhile mentioning, however, that even considering the operators at the r.h.s. of the mappings (22) and (23) as fermionic, the commutation relations are preserved up to the second order in the (ph) operators. For example, using exact fermionic commutation relations, one has

$$[B_{ph}, B_{p'p'}^+] = \delta_{pp'} B_{p'h} \quad (24)$$

and

$$[B_{ph}, \sum_{h'} B_{p'h'}^+ B_{p''h'}] = \delta_{pp''} B_{p''h} - \sum_{p_1} B_{p_1 h'}^+ B_{p_1 h} B_{p''h} - \sum_{h_1} B_{p h_1}^+ B_{p' h_1} B_{p''h}. \quad (25)$$

By using Eqs. (22) and (23), together with (11), (14) and (19) one gets

$$D_{ph} = 1 - \sum_{p'} D_{p'h} \sum_{\nu} (\bar{Y}_{p'h}^\nu)^2 - \sum_{h'} D_{ph'} \sum_{\nu} (\bar{Y}_{ph'}^\nu)^2, \quad (26)$$

which, in the limit of small ground-state correlations, i.e. when the amplitudes \bar{Y} are small, reduces to Eq. (21). Thus Eq. (26) includes Eq. (21) as a particular case.

In Section 4 we will report on some realistic calculations using a Skyrme force within the self-consistent HF + RPA scheme including ground-state correlations and compare the results obtained in the two approaches (Eqs. (21) and (26)) and in the bare RPA.

Before that we believe that it is useful to make such a comparison within the exactly solvable LMG model [11]. This will be discussed in the next section.

3. Application to the LMG model

In the LMG model one considers a system of two Ω -fold degenerate levels, one below and the other above the Fermi level, described by the hamiltonian:

$$H = \epsilon K_0 - \frac{1}{2} V (K_+^2 + K_-^2), \quad (27)$$

$$K_0 = \frac{1}{2} \sum_{m=1}^{\Omega} (B_{+m,+m}^+ - B_{-m,-m}^+), \quad (28)$$

$$K_+ = \sum_{m=1}^{\Omega} B_{+m,-m}^+, \quad K_- = (K_+)^+. \quad (29)$$

The exact result for the energy and the matrix elements $\langle \bar{\nu} | F | 0 \rangle$ of the excitation operator $F = K_+ + K_-$ is obtained by solving exactly the static Schrödinger equation by standard group techniques associated with the SU(2) Lie algebra structure of the operators K_0, K_{\pm} (see e.g. Ref. [13]). The RPA-like equations with ground-state correlations, assuming that there is only one collective phonon ($\bar{\nu} = 1$), have in both approaches the simple form

$$(\epsilon - \omega) \bar{X} - \Omega V D \bar{Y} = 0, \quad (30)$$

$$(\epsilon + \omega) \bar{Y} - \Omega V D \bar{X} = 0 \quad (31)$$

with the normalization condition

$$\Omega (\bar{X}^2 - \bar{Y}^2) = 1. \quad (32)$$

The renormalization factor D in our approach is (see Eq. (26))

$$D_1 = \frac{1}{1 + 2\bar{Y}^2}, \quad (33)$$

while, in Hara's approach, it is (see Eq. (21))

$$D_2 = 1 - 2\bar{Y}^2, \quad (34)$$

which may be seen as the first order of the expansion of Eq. (33) in powers of $(2\bar{Y}^2)$.

In Figs. 1–3 we show the energy (top), the square of the matrix element $|\langle 1 | F | 0 \rangle| / \Omega$ (middle) and their product $S_1 = (E_1 - E_0) |\langle 1 | F | 0 \rangle|^2 / (\Omega^2 \epsilon)$ (bottom) as functions of the interaction parameter $\Omega V / \epsilon$ for $\Omega = 8, 14$ and 30 . The thin solid lines represent the RPA results; the thick solid ones, the exact; the dashed ones, the results obtained with D_1 (Eq. (33)), and the dotted ones, those with D_2 (Eq. (34)). As expected, for small values of the strength both approaches give results close to the RPA ones.

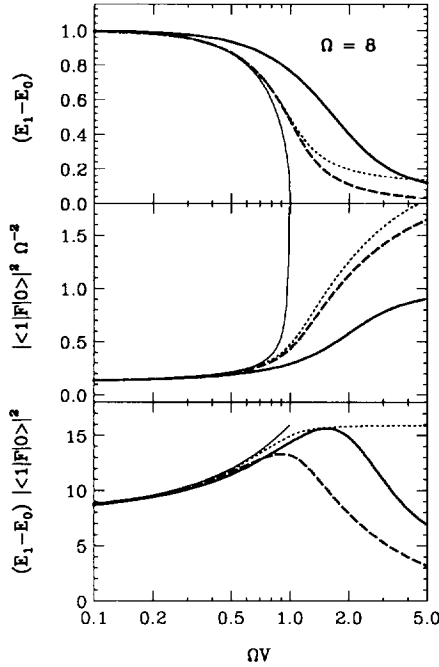
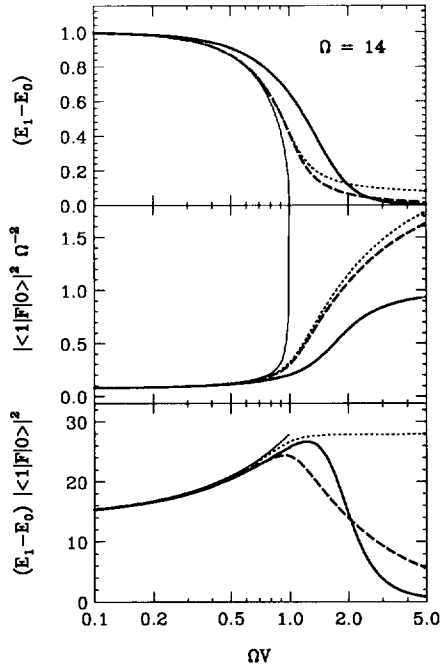
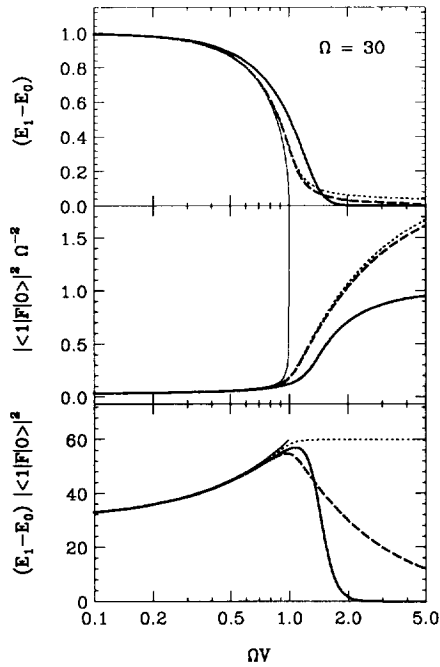


Fig. 1. Excitation energy of the first excited state above the ground state (in units of ϵ) (top); the square of the matrix element of the operator F corresponding to the transition from the ground state to the first excited one (divided by Ω^2) (middle) and their product (bottom) as a function of the interaction parameter ΩV (in units of ϵ) for the LMG model for particle number $\Omega = 8$. The thick solid curve represents the exact result; the thin solid, the RPA result; the dotted, the result of based on the renormalization (10); the dashed, the result of our approach.

When the interaction increases reaching the value 1, the bare RPA breaks down while the renormalized ones with ground-state correlations still give real solutions. The differences between the two renormalization schemes become sizeable for large interaction strength. In the limit of infinite strength one can see that using Eq. (33) the energy of the first excited state goes to zero in agreement with the exact result for $\Omega \geq 14$. On the contrary, with Eq. (34) the energy tends to the finite value $\epsilon/(\Omega+1)$. This different behaviour can be particularly appreciated looking at the quantity S_1 . In Figs. 1–3 (top and middle) one can see that the difference in the energy and the square of the matrix element between the results obtained within our and Hara’s approaches decreases with increasing the particle number from $\Omega = 8$ to 30. In the same figures (bottom) one also observes that the two approaches give quite different results for the quantity S_1 independently of the particle number, the results within our approach being in a qualitative agreement with the exact ones.

Fig. 2. Same as in Fig. 1 for $\Omega = 14$.Fig. 3. Same as in Fig. 1 for $\Omega = 30$.

4. Applications to realistic cases

In a recent application of Hara's formalism presented in Ref. [14] for the ^{64}Zn nucleus the inclusion of ground-state correlations beyond RPA was found to produce an upward shift of the low-lying 2_1^+ state and a substantial reduction of the associated $B(E2)$. In order to get good agreement with experimental data for both the energy and the $B(E2)$ value it was necessary to increase by 38% the isoscalar quadrupole–quadrupole strength of the residual interaction used in RPA. It was also found that the unphysical oscillations of the transition density in the interior part of the nucleus, present in RPA, were depleted.

In the present section we report on some calculations performed within a fully self-consistent scheme both in our and Hara's approaches. Using the SGII Skyrme interaction [15], we first made the self-consistent HF + RPA calculations for the closed-shell ^{146}Gd and ^{208}Pb nuclei. The results of these calculations have then been used as input for an iterative procedure to solve the nonlinear RPA-like equations for the renormalized \bar{X} and \bar{Y} amplitudes described in Section 2. We have found that the iterative procedure converges rapidly in both of the considered cases.

The single-particle wave functions have been expanded in a basis of 16 harmonic oscillators and all particle–hole configurations with unperturbed energies up to 35 and 45 MeV for ^{208}Pb and ^{146}Gd , respectively, have been included. The formalism of Section 2 has been modified by introducing angular-momentum coupling. Thus $\bar{\nu}$ now stands for (λ^π, i) with i denoting the different states for a given multipolarity λ and parity π . To calculate the renormalization factors D_{ph} of Eqs. (21) and (26) one must sum over all excited states $|\bar{\nu}\rangle$. In both calculations we have included all the $\lambda^\pi = 2^+, 3^-, 4^+$ and 5^- states in the summation. However, we will concentrate ourselves on the lowest 3_1^- state which, for spherical nuclei, is known to be well described by RPA. The calculated energies and $B(E3)$ values are collected in Table 1. First of all we remark that the results in our approach are very similar to those in Hara's for both the considered nuclei. With respect to the RPA results, the energy is shifted upward and the $B(E3)$ is considerably reduced, namely 20% in ^{208}Pb and 40% in ^{146}Gd . The trend found in Ref. [14] is thus confirmed in the present fully self-consistent calculations. The above results show that the inclusion of ground-state correlations beyond RPA reduces the collectivity of the low-lying 3^- states with respect to RPA. The effect was less pronounced for the low-lying 2^+ states and, as expected, negligible for the high-lying states as, for example, the GQR.

In order to push down again the energy of the 3^- states and increase their $B(E3)$ value, the parameters of the force should be varied so as to increase the collectivity. From the analysis of the previous section in the LMG model, we expect that the corrections due to the ground-state correlations beyond RPA will be magnified in this situation. Also, the differences between our and Hara's approaches should be more pronounced. Such a search of the best parameters would require however a great computational effort in the present self-consistent scheme starting from Hartree–Fock. We also remind that each iteration requires the solution of the RPA equations for all the considered multipolarities.

Table 1

Energy E , total occupancy ΔA of single-particle levels above the Fermi surface in the ground state, $B(E3)$ value and EWSR, associated with the 3_1^- state for ^{208}Pb and ^{146}Gd , obtained within RPA, our and Hara's approaches

Nucleus	Approximation	E (MeV)	ΔA	$B(E3)$ ($e^2\text{fm}^6$)	EWSR ($\text{MeV}\cdot e^2\text{fm}^6$)
^{208}Pb	RPA	3.585	3.149	0.332×10^7	0.588×10^8
	Only 3^- : Our	3.714	1.293	0.298×10^7	0.582×10^8
		Hara's	3.717	1.290	0.298×10^7
	All J^π : Our	3.812	2.798	0.272×10^7	0.575×10^8
		Hara's	3.821	2.789	0.272×10^7
^{146}Gd	RPA	1.569	4.394	0.892×10^6	0.267×10^8
	Only 3^- : Our	1.724	1.603	0.640×10^6	0.262×10^8
		Hara's	1.731	1.584	0.629×10^6
	All J^π : Our	1.798	3.404	0.531×10^6	0.258×10^8
		Hara's	1.812	3.363	0.510×10^6

In order to check their relative importance, we also made a calculation including only the 3^- states in the summation in Eqs. (21) and (26). The results, also reported in the table, are quite different from those of the complete calculation. To get a measure of the correlations present in the ground state, we have considered the quantity

$$\Delta A = \sum_{\text{h}} (n_{\text{h}}^{\text{HF}} - n_{\text{h}}) = A - \sum_{\text{h}} n_{\text{h}}, \quad (35)$$

i.e. the total occupancy of single-particle levels above the Fermi surface in the ground state. As shown in the table, this quantity is quite large both in our and in Hara's approach and its value is strongly increased when all multiplicities are included. As known, RPA overestimates this quantity. It is therefore worth noting that the value obtained by including ground-state correlations beyond RPA is quite smaller than the corresponding RPA one.

For the sake of completeness we also report the total 3^- energy-weighted sum rule. Since, as previously said, only the low-lying states are affected by the ground-state correlations we are considering, its value is only little modified with respect to the RPA one.

5. Summary and conclusions

In this work, we have illustrated a procedure for the description of particle-hole excitations including ground-state correlations beyond RPA. The procedure differs from RPA essentially in the way of evaluating the commutator between annihilation and creation particle-hole operators $[B_{\text{ph}}, B_{\text{p'h}}^+]$. This is realized in two steps. First, the commutator is expressed in terms of B_{ph} and B_{ph}^+ operators by mapping the (pp) and (hh) operators onto the products of the (ph) ones. Second, the result is replaced by its

expectation value in the correlated ground state. This step is common to the renormalized RPA and, as in this case, the procedure leads to a set of nonlinear equations in X and Y amplitudes, which are then solved by iteration. With respect to the renormalized RPA, however, our approach leads to a more general expression for the particle and hole occupation numbers.

We have first tested our procedure within the LMG model and found that while for small strengths of the interaction the energy of the first excited state is close to the RPA value, for large strengths the two results differ totally, our procedure approaching the exact eigenvalue. A comparison with the renormalized RPA has shown an increasing difference between the two approaches for increasing values of the strength above the critical point of RPA.

We have also reported for the first time on the results of fully self-consistent calculations, using the SGII Skyrme interaction, for ^{146}Gd and ^{208}Pb . In this case, we have first performed HF + RPA calculations and their results have been taken as input for an iterative procedure to solve the nonlinear RPA-like equations constructed within our approach. Calculations have concerned energies and $B(E\lambda)$ values, particular attention being devoted to the 3_1^- state. With respect to the RPA results, the energy of this state has been found shifted upward and the $B(E3)$ value considerably reduced. These results have shown that the inclusion of ground-state correlations beyond RPA reduces the collectivity of this state with respect to RPA. This effect has been found less pronounced for low-lying 2^+ states and negligible for high-lying ones.

The results of these calculations have been found close to those obtained within the renormalized RPA. This is not surprising as long as the calculations concern the region of the validity of RPA or the vicinity of its critical region. The analysis made in terms of LMG model, nevertheless allows us to believe that a better fit of parameters of the Skyrme interaction should lead to a more pronounced difference between the two mentioned approaches.

It would be interesting to consider a physical system for which the interaction is known better than for nuclei. This is, for example, the case of metallic clusters which have many analogies with nuclei [16] and can be described in the jellium model within the present scheme [17]. In such case the energy functional is derived essentially from the Coulomb interaction of the electrons among themselves and with the ionic component of the system. This study is now in progress.

Acknowledgement

Discussions with J.P. Blaizot (Saclay) and G. Brown (Stony Brook) are gratefully acknowledged.

N.D.D acknowledges the financial support of the Istituto Nazionale di Fisica Nucleare under the contract No. 091534/20.10.92 and of the Università di Catania during his stay in Catania.

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