Extended RPA within a solvable 3 level model

F. Catara $^{1,2*}$, M. Grasso $^3\dagger$, M. Sambataro $^{2\dagger}$

$^1$ Dipartimento di Fisica, Università di Catania

$^2$ Istituto Nazionale di Fisica Nucleare, Sez. di Catania

Corso Italia 57, I-95129 Catania, Italy

$^3$ Institut de Physique Nucléaire, IN2P3-CNRS,

Université Paris-Sud, 91406 Orsay Cedex, France

Abstract

Working within an exactly solvable 3 level model, we discuss an extension of the Random Phase Approximation (RPA) based on a boson formalism. A boson Hamiltonian is defined via a mapping procedure and its expansion truncated at four-boson terms. RPA-type equations are then constructed and solved iteratively. The new solutions gain in stability with respect to the RPA ones. We perform diagonalizations of the boson Hamiltonian in spaces containing up to four-phonon components. Approximate spectra exhibit an improved quality with increasing the size of these multiphonon spaces. Special attention is addressed to the problem of the anharmonicity of the spectrum. PACS numbers: 21.60.Jz, 21.10.Pc, 21.10.Re

* e-mail address: catara@ct.infn.it

† e-mail address: grasso@ipno.in2p3.fr

‡ e-mail address: samba@ct.infn.it

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I. INTRODUCTION

The most commonly used microscopic approach for the study of collective vibrational states in many-fermion systems is the Random Phase Approximation (RPA) [1]. In this theory the lowest collective excitations result from the action of phonon operators $Q^\dagger_\nu$ on a state $|RPA\rangle$ which is defined by the condition that $Q_\nu|RPA\rangle = 0$. This state represents the ground state of the system. It is a distinctive feature of RPA that multiphonon states, i.e. states obtained by repeated actions of phonon operators on the ground state, are eigenstates of the Hamiltonian with energies forming a harmonic spectrum. The existence of states which can be approximately described as corresponding to the multiple excitation of low-lying and/or high-lying phonons is well established in atomic nuclei. However, deviations from the harmonic picture are also observed and their influence on several processes has been analysed [2].

In a standard derivation of the RPA equations, a crucial point is represented by the so-called Quasi-Boson Approximation (QBA). This is a rather crude approximation which causes the $Q^\dagger_\nu$ operators to behave as boson operators in spite of their (composite) fermionic structure. Overcoming this approximation has represented the starting point of many attempts aiming at improving RPA [3–22]. One of the line of research in such a context has been based on a reformulation of the whole theory in a boson formalism [16–22]. In other words, the $Q^\dagger_\nu$ operators have been defined from the beginning in terms of true boson operators and all the fermion operators of interest have been replaced, via a mapping procedure, by their boson images. The RPA-type equations that one constructs in this formalism depend, of course, on the degree of expansion of the boson Hamiltonian. Truncating this expansion at the lowest order, i.e. at two-boson terms only, gives the boson counterpart of RPA. Including higher-order terms in the boson image of the Hamiltonian provides a natural way to reach a higher level of approximation. Besides that, the inclusion of these terms has another important effect: it leads to a coupling among multiphonon states. States which result from a diagonalization in a m-phonon space are therefore superpositions of zero-,
one-, ..., m-phonon states. Such a diagonalization is expected to lead to a further improved degree of approximation as well as to cause anharmonicities in the spectrum.

Calculations in this boson formalism have been performed in the recent past for atomic nuclei [19, 20] considering a Hamiltonian truncated at four-boson terms and diagonalizing it in the space of one- and two-phonon states. The resulting anharmonicities have not been found large, especially in $^{208}$Pb. In particular, the anharmonicity associated with states whose main component is a Double Giant Resonance has been found of the order of a few hundred $K\text{eV}$. This is certainly related to the fact that RPA gives a good description of Giant Resonances, especially in heavy closed shell nuclei.

In metallic clusters, a strongly collective state is known to exist, the dipole plasmon, which corresponds to the oscillation of the delocalized electrons of the cluster against the positively charged ions. The experimental evidence for states corresponding to the double excitation of the plasmon has not been confirmed [23]. From the theoretical point of view the situation is also quite unclear. From one hand, in [24] a purely harmonic spectrum for the multiple excitation of the plasmon has been predicted. On the other hand, by using the same approach as in [19, 20] huge anharmonicities in the two-plasmon states have been found [25]. An important difference with respect to the case of atomic nuclei is that in metallic clusters the two-body interaction is very long ranged. This is probably the main reason why the RPA ground state is very different from the Hartree-Fock one and the RPA backward amplitudes are quite large. Of course, this may cause that the same level of truncation in the boson expansion is not adequate both in the case of nuclei and of metal clusters.

In principle, configuration mixing calculations can give a clear, model independent, indication on the existence of such two-phonon states and on their degree of anharmonicity. Unfortunately, since the states one looks for are quite high in energy, the number of configurations required to get stable results is huge. In [26] such a study has been performed for a very simple case: two interacting electrons moving in a uniform positive charge distribution. This is a kind of precursor of a metal cluster in the jellium approximation and allows for a numerically exact calculation. Important deviations from the harmonic limit have been
found. More specifically, in addition to an almost perfectly harmonic vibrational band based
on the ground state, the other states can be classified in other bands with a much less degree
of harmonicity.

Aim of this paper is to shed some light on the limits of the approach adopted in [20] and
[25] by applying it to a 3-level solvable model [27]. The analysis we are going to present
is very similar to that in [21] where a 2-level model was considered and the parameters
were adjusted in such a way to mimic the multiple excitation of a Giant Resonance. The
3-level model is, of course, richer. In particular, since there are two single particle states
above the Fermi surface (particle states) and one below (hole), two different elementary p-h
configurations and, correspondingly, two different phonons can be excited. Therefore, one
can better simulate the situation encountered in nuclei which generally present one high-
lying and one low-lying collective modes for each multipolarity. Also, matrix elements of
the interaction connecting a particle-hole state with a two-particle one can be included in
a natural way. These terms are present in a generic two-body interaction and are very
important since they couple states having numbers of phonons differing by one.

The paper is organized as follows. In Sec. II, we will describe the model and the
formalism. In Sec. III, we will analyse the results. Finally, in Sec. IV, we will review the
content of the paper and draw some conclusions.

II. THE MODEL AND THE FORMALISM

The model [27] consists of three 2Ω-fold degenerate single-particle shells which are oc-
cupied by 2Ω particles. In the absence of interaction, then, the lowest level is completely
filled while the others are empty. This state, the “Hartree-Fock” (HF) state of the system,
is denoted by $|0\rangle$. A single-particle state is specified by a set of quantum numbers $(j, m)$,
where $j$ stands for the shell $(j=0,1,2)$ and $m$ specifies the $2\Omega$ substates within the shell. The
creation and annihilation operators of a fermion in a state $(j, m)$ are defined by $a_{jm}^\dagger$ and
$a_{jm}$, respectively.
Let us consider the operators

\[ K_{ij} = \sum_{m=1}^{2\Omega} a^\dagger_{im} a_{jm} \quad (i, j = 0, 1, 2). \]  

These operators satisfy the Lie algebra of the group SU(3)

\[ [K_{ij}, K_{kl}] = \delta_{jk} K_{il} - \delta_{il} K_{kj}. \]  

The Hamiltonian of the model is written in terms of the generators \( K_{ij} \) only and contains up to two-body interactions. Its form is

\[
H_F = \sum_{i=1,2} \epsilon(i) K_{ii} + \sum_{i,j=1,2} V_x(i, j) K_{i0} K_{j0} \\
+ \frac{1}{2} \sum_{i,j=1,2} V_v(i, j) (K_{i0} K_{j0} + K_{0j} K_{0i}) \\
+ \sum_{i,j,k=1,2} V_y(i, j, k) (K_{i0} K_{jk} + K_{kj} K_{0i}),
\]

with real coefficients. The eigenstates of \( H_F \) can be constructed either by using the properties of the SU(3) algebra or by diagonalizing it in the space

\[
F = \left\{ |n_1 n_2\rangle = \frac{1}{\sqrt{N_{n_1 n_2}}} (K_{10})^{n_1} (K_{20})^{n_2} |0\rangle \right\}_{0 \leq n_1 + n_2 \leq 2\Omega},
\]

where \( N_{n_1 n_2} \) are normalization factors.

In order to introduce the boson formalism, let’s define the space

\[
B = \left\{ |n_1 n_2\rangle = \frac{1}{\sqrt{n_1! n_2!}} (b_1^\dagger)^{n_1} (b_2^\dagger)^{n_2} |0\rangle \right\}_{0 \leq n_1 + n_2 \leq 2\Omega},
\]

where the operators \( b_i^\dagger \) obey the standard boson commutation relations

\[
[b_i, b_j^\dagger] = \delta_{ij}, \quad [b_i, b_j] = 0
\]

and \( |0\rangle \) is the vacuum of the \( b_i \)’s operators. A one-to-one correspondence exists between the states of \( F \) and \( B \), the boson operators \( b_i^\dagger \) playing the role of the excitation operators \( K_{i0} \) and the boson vacuum \( |0\rangle \) replacing the HF state \( |0\rangle \).

The mapping procedure to construct boson images of fermion operators is the same discussed in previous works (see, for instance, Ref. [28]) and, due to the orthonormality of both
sets of states $|n_1, n_2\rangle$ and $|n_1, n_2\rangle$, it is simply based on the requirement that corresponding matrix elements in $F$ and $B$ be equal. The procedure is, therefore, of Marumori-type. We refer to Ref. [28] for more details. Here, we simply say that, in correspondence with the Hamiltonian $H_F$ (2.3), we introduce a hermitian boson Hamiltonian $H_B$ which, in the most extended version, has the form

$$H_B = \alpha + \sum_i \beta_i (b_i^\dagger + \text{h.c.}) + \sum_{ij} \gamma_{ij} b_i^\dagger b_j + \sum_{i \leq j} \phi_{ij} (b_i^\dagger b_j^\dagger + \text{h.c.})$$

$$+ \sum_{i \leq j} \sum_k \epsilon_{ijk} (b_i^\dagger b_j^\dagger b_k + \text{h.c.}) + \sum_{i \leq j} \sum_{k \leq l} \delta_{ijkl} b_i^\dagger b_j^\dagger b_k b_l. \quad (2.7)$$

with the coefficients depending on the parameters $\epsilon(i), V_x, V_v, V_y$ of Eq.(2.3).

Let us now introduce the operators

$$Q_{\nu}^\dagger = \sum_i X^{(\nu)}_i b_i^\dagger - \sum_i Y^{(\nu)}_i b_i. \quad (2.8)$$

and let the state $|\Psi_0\rangle$ satisfy the condition

$$Q_{\nu}|\Psi_0\rangle = 0. \quad (2.9)$$

By using the equations of motion method [29] one finds that the amplitudes $X$ and $Y$ are solutions of

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^{(\nu)} \\ Y^{(\nu)} \end{pmatrix} = \omega^{(\nu)} \begin{pmatrix} X^{(\nu)} \\ Y^{(\nu)} \end{pmatrix}. \quad (2.10)$$

where

$$A_{ij} = (\Psi_0|[b_i, [H_B, b_j^\dagger]]|\Psi_0), \quad (2.11)$$

$$B_{ij} = -(\Psi_0|[b_i, [H_B, b_j]]|\Psi_0) \quad (2.12)$$

and $\omega^{(\nu)}$ are the energies of the excited states

$$|\nu\rangle = Q_{\nu}^\dagger |\Psi_0\rangle. \quad (2.13)$$

As anticipated in the Introduction, the form of Eqs. (2.10) is strictly related to the degree of truncation of the boson Hamiltonian. In the hypothesis that $H_B$ contains up to two-boson
terms, the double commutators in Eqs. (2.11) and (2.12) are just numbers which, therefore, are also the values of the matrices $A$ and $B$. This is the simplest case which can be realized in this formalism and represents the boson counterpart of the standard RPA. This degree of approximation can be improved by introducing a Hamiltonian with higher-order terms like, for instance, (2.7). In this case the double commutators are operators. In order to calculate their expectation values in $|\Psi_0\rangle$, as required in Eqs. (2.11) and (2.12), one can express the $b$ and $b^\dagger$ operators in terms of $Q$ and $Q^\dagger$ by reversing Eq. (2.8) (and its conjugate) and use the fact that the ground state $|\Psi_0\rangle$ is defined as the vacuum of the Q’s. This procedure gives, however, matrices $A$ and $B$ which depend on the X and Y amplitudes and, consequently, equations of motion (2.10) which are nonlinear. In what follows this nonlinear extension of RPA will be called ERPA.

Having determined the X and Y amplitudes within RPA or ERPA, one can express the Hamiltonian $H_B$ in terms of the operators Q and $Q^\dagger$. In the case of RPA, namely when the boson Hamiltonian (2.7) is truncated at two-boson terms only, $H_B$ can be rewritten simply as

$$H_B = E_0 + \sum_\nu \omega^{(\nu)} Q^\dagger_\nu Q_\nu,$$

(2.14)

where $\omega^{(\nu)}$ are the energies solutions of the RPA equations (2.10). This Hamiltonian obviously doesn’t mix states with different phonon numbers and so its eigenstates are pure zero-, one-, ..., m-phonon states. For a higher-level truncation in the boson Hamiltonian, like for instance that of Eq. (2.7), $H_B$ acquires instead the more general form

$$H_B = E_0 + H_{10}(Q^\dagger + h.c.) + H_{11}Q^\dagger Q + H_{20}(Q^\dagger Q^\dagger + h.c.) +$$

$$H_{21}(Q^\dagger Q^\dagger Q + h.c.) + H_{30}(Q^\dagger Q^\dagger Q^\dagger + h.c.) +$$

$$H_{22}Q^\dagger Q^\dagger QQ + H_{31}(Q^\dagger Q^\dagger Q^\dagger Q + h.c.) + H_{40}(Q^\dagger Q^\dagger Q^\dagger Q^\dagger Q^\dagger + h.c.),$$

(2.15)

(for simplicity, we have dropped all the indices) where the $H_{ij}$ coefficients are functions of X and Y. Also in this case, as in RPA, the term $H_{20}$ as well as the non-diagonal terms $H_{11}$ vanish, as can be easily shown using the fact that the X and Y amplitudes are solutions of the
ERPA equations (2.10). The remaining terms of (2.15), however, mix states with different phonon numbers so that the eigenstates of the full Hamiltonian become combinations of these states. This fact introduces an evident difference with RPA since the energies which result from the ERPA equations are not eigenvalues of the boson Hamiltonian in the phonon space as it is in the case of RPA (where they provide the excitation energies of the one-phonon eigenstates). In the next section, we will show the results obtained by diagonalizing (2.15) in different bases, containing up to two-, three- and four-phonon states, and compare them with the RPA and the exact ones.

III. RESULTS AND DISCUSSION

Let us first of all fix the parameters entering in the Hamiltonian (2.3). The energies $\epsilon(1)$ and $\epsilon(2)$ have been chosen equal to $\epsilon$ and 2.5$\epsilon$, respectively. In order to simplify the analysis, the coefficients $V_x(i, j)$, $V_v(i, j)$, $V_y(i, j, k)$ have been assumed independent of the indices $i, j, k$ and proportional to one parameter, $\chi$. More precisely, we have fixed $V_x = -\chi$, $V_v = \frac{1}{4}\chi$, $V_y = -\frac{3}{8}\chi$ as in Ref. [14]. Both $\epsilon$ and $\chi$ are parameter expressed in units of energy. All calculations have been performed for a system of $2\Omega = 10$ particles.

We begin our analysis by examining the limits of validity of the truncation in the boson Hamiltonian (2.7). To do that we compare the exact spectrum of the fermion Hamiltonian (2.3) with that obtained by diagonalizing $H_B$ (2.7) in the full boson space. The results are shown in Fig. 1 where we report, as functions of the strength $\tau = \frac{2\Omega \chi}{\epsilon}$, the energies of those states which, at zero strength, are pure 1p-1h or 2p-2h states. For later use we also label these states with the symbols $|\nu\rangle$ and $|\nu_1\nu_2\rangle$ meaning by that the states which, in the limit $\tau \to 0$, are the one-phonon ($|\nu\rangle \equiv Q_\nu \Psi_0$) and two-phonon ($|\nu_1\nu_2\rangle \equiv Q_{\nu_1}^\dagger Q_{\nu_2}^\dagger \Psi_0$) states of the RPA formalism. The eigenvalues of the boson hamiltonian (dashed lines) are found in good agreement with the exact ones in the whole range of variation of $\tau$. In the following we will take the spectrum of the truncated hamiltonian as the reference one.

In Fig. 2, we show the energies resulting from the RPA and ERPA equations together
with the reference spectrum. For small values of the strength, RPA and ERPA give almost identical results, in good agreement with the reference ones. Differences become really visible around \( \tau = 0.28 \), where RPA undergoes a collapse. In this region ERPA solutions remain instead stable and close to the reference ones. On the basis of the comments at the end of Sec. II, however, we notice that these ERPA energies can be considered excitation energies of one-phonon states only in the hypothesis that all the terms of (2.15) but \( E_0 \) and \( H_{11} \) play a minor role.

Although not clearly visible at a first glance, the spectrum of Fig. 1 shows marked anharmonicities. In order to quantify these, in Fig. 3 we plot the ratios

\[
R_{\nu_1\nu_2} = \frac{E_{\nu_1\nu_2} - (E_{\nu_1} + E_{\nu_2})}{E_{\nu_1} + E_{\nu_2}},
\]

where by \( E_\nu \) and \( E_{\nu_1\nu_2} \) we mean the exact energies of the states \( |\nu\rangle \) and \( |\nu_1\nu_2\rangle \) defined in Fig. 1. One notices a well different behaviour of the three ratios plotted. In the case of the state \( |11\rangle \) the ratio is seen to grow rapidly for increasing \( \tau \). In the case of the state \( |22\rangle \), \( R_{\nu_1\nu_2} \) remains instead almost exactly zero therefore showing that the corresponding exact state can be fairly well described as a pure two-phonon state. The remaining “mixed” state \( |12\rangle \) exhibits only a moderate anharmonicity. These results resembles that of Ref. [26] where a realistic two-electron system was examined. Indeed, in both cases, the spectrum is found to exhibit some levels with a clear harmonic nature mixed, however, to other levels which do not display at all this nature. This mix of states makes of course complicate to provide a clear cut answer to the question of how much harmonic is the spectrum of these many-body systems, the answer strongly depending on which levels one is looking at.

The existence of the anharmonicities evidenced in Fig. 3 represents an evident limit to the harmonic picture of RPA and points to the need of diagonalizing the full Hamiltonian (2.15) in a multiphonon space in order to reproduce the exact spectrum properly. We have performed three separate calculations by diagonalizing \( H_B \) in spaces including up to two-, three- and four-phonon configurations. The results are shown in Fig. 4 together with the reference ones. The internal structure of the collective phonons entering in the basis states
is the one obtained in ERPA, i.e. the $X$ and $Y$ amplitudes are solutions of Eqs. (2.10) where the full Hamiltonian (2.7) has been used. Keeping for simplicity the same labelling of states used in Fig. 1, we can say that, as expected from the previous discussion, for the states $|1\rangle$, $|2\rangle$ and $|22\rangle$ the results are almost independent of the basis and in very good agreement with the exact ones. For the state $|11\rangle$ we find instead a marked dependence on the basis, the results approaching more and more the reference ones when the space is enlarged. Going from the smaller space to that including up to three phonons the agreement is quite good for $\tau \lesssim 0.25$. For a higher strength the space needs to be further enlarged up to four phonons. A somewhat similar behaviour, although less pronounced, is seen for the state $|12\rangle$.

As a final result, in Fig. 5 we show the ground state energies calculated within RPA and as they result by diagonalizing the Hamiltonian (2.15) in multiphonon spaces. All these results are compared with the exact ones and with those obtained by diagonalizing the boson Hamiltonian (2.7). It is interesting to see that the good agreement between fermion and boson results already found in Fig. 1 for the excitation energies is confirmed also in this case. As expected, RPA overestimates the exact values. All the diagonalizations in multiphonon spaces lead instead to an underestimation of these values showing, however, a rapid convergence to the exact values with increasing the size of the spaces.

IV. CONCLUSIONS

In this paper we have analysed some of the lowest excited states of the spectrum of a solvable 3-level model, namely those that in RPA would be described as one and two-phonon states. We have worked in a boson formalism. As a preliminary step, then, we have constructed a boson image of the fermion Hamiltonian whose expansion has been truncated at four-boson terms. The procedure followed in such a derivation has been of Marumori-type. The quality of the boson Hamiltonian has been tested by comparing its eigenvalues with the exact ones. Within the considered range of variation of the interaction strength the agreement between fermion and boson energies has always been found quite good.
By making use of this boson Hamiltonian we have constructed RPA-type equations and solved them iteratively. The new solutions have gained in stability with respect to the RPA ones and, in particular, around the RPA collapse point the new energies have exhibited a good agreement with the exact ones. This extension of RPA, while introducing corrections to the Pauli Principle violations present in RPA, naturally leads to a Hamiltonian which mixes states with a different number of phonons. We have performed diagonalizations in spaces containing up to two-, three- and four-phonon states and observed an improved quality of the approximate spectra with increasing the size of the spaces.

Special attention has also been addressed to the problem of the anharmonicity of the spectrum. This has been found relevant for the state which, in RPA, is described as the double excitation of the lowest one-phonon state. On the contrary, for the other states, a less pronounced anharmonicity has been found. These findings agree with those of Ref. [26] and point to the necessity of considering together all the possible elementary excitations of a many-body system when discussing the anharmonicity of its spectrum.
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FIGURES

FIG. 1. Excitation energies of the states $|\nu >$ and $|\nu_1 \nu_2 >$ which, at zero interaction strength, are pure 1p-1h and 2p-2h states respectively. The exact energies (full lines) are compared with the energies obtained diagonalizing the hamiltonian $H_B$ in the full boson space (dashed lines). The energies are shown as functions of the parameter $\tau$.

FIG. 2. Excitation energies, as functions of $\tau$, calculated within RPA (dotted lines) and ERPA (dashed lines) compared with the corresponding reference energies (full lines).

FIG. 3. The ratios $R_{\nu_1 \nu_2}$ (Eq. (3.1)) calculated for the states $|11 >$, $|12 >$ and $|22 >$ as functions of $\tau$.

FIG. 4. Excitation energies, as functions of $\tau$, obtained diagonalizing $H_B$ in spaces including up to two- (dotted lines), three- (dot-dashed lines) and four- (dashed lines) phonon configurations compared with the reference excitation energies (full lines).

FIG. 5. Ground states energies, as functions of $\tau$, obtained in the exact fermionic calculation (full line), in the reference calculation (dashed line), in RPA (+ symbols), in the diagonalizations up to two phonons (left triangles), up to three phonons (diamonds) and up to four phonons (circles).
