Collective excitations in Random Phase Approximation and beyond

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Abstract. Collective excitations are one of the most common and interesting features of many-body systems. Of particular interest are those collective modes which can be interpreted in terms of vibrations. Nuclei show a large variety of such modes, both low-lying and high-lying. In particular the giant dipole resonance is due to the coherent motion of protons against neutrons. Its analogue in metal clusters is the dipole plasmon excitation, due to the oscillation of electrons against the positive ions. The Random Phase Approximation (RPA) is extensively used as a microscopic theory to study the basic properties of these collective excitations. In the derivation of RPA use is made of the Quasi Boson Approximation (QBA). It consists in replacing the expectation values in the correlated ground state with those in the uncorrelated (Hartree-Fock) one. Strictly related to QBA is the feature of RPA of predicting a harmonic spectrum. On the other hand, the existence of anharmonicities in the multiphonon spectra of nuclei and their relevance in various physical processes are well established. Overcoming QBA has represented the starting point of many attempts aiming at improving RPA. A recently developed approach in this line will be presented and discussed. A very nice property of RPA is to satisfy Energy Weighted Sum Rules (EWSR). However, some violations are present in several extensions of RPA. We will show how to cure this shortcoming.

1. Introduction
A common feature of finite-size many-body systems is the existence of collective excitations. The Random Phase Approximation (RPA) is the microscopic approach most currently used to study such modes, described as superpositions of particle-hole and hole-particle elementary configurations [1]. To derive RPA in its standard form, use is made of the Quasi Boson Approximation (QBA) which amounts to consider the Hartree-Fock ground state, rather than the correlated one, as reference state. This is justified only if ground state correlations are not too strong. Otherwise a better and, if possible self-consistent, treatment of these correlations becomes necessary. For example, it has been shown in the context of metal clusters that correlations in the ground state can be quite strong and induce important deviations from 1 and 0 in the occupation numbers [2]. One possible way to explicitly introduce correlations in the ground state consists in constructing a RPA-like formalism where the violations of the Pauli principle related to QBA are cured. This has been done along two main lines, by using...
either boson expansion methods [3] or remaining in the fermionic space [4]. The so-called
renormalized RPA (RRPA) method, starting from the early works of Hara and Rowe in the
1960’s [5] belongs to the latter. In RRPA the one body density matrix is assumed diagonal
but, due to the g.s. correlations, its eigenvalues are different from 0 and 1 and are calculated
self consistently. In the derivation of the equations of motion no use is made of QBA. A very
important feature of standard RPA is that it preserves the energy weighted sum rules (EWSR)
[1]. This property is lost within all the above approaches since only particle-hole excitations
are considered. An attempt to overcome this problem has been discussed in Ref. [6], where
an extended RRPA approach has been introduced, including particle-particle and hole-hole
configurations in addition to the standard p-h ones. The method has been applied to a three-
level Lipkin model, with one single particle level below the Fermi energy and two above, and it
has been shown that the EWSR are exactly satisfied. However, a new problem arises related
to the existence of a non physical mode that does not correspond to any level in the exact
excitation spectrum of the model. This unpleasant problem makes unfeasible the application of
this method to a realistic case because it would be impossible to reveal the existence of such
mode and to identify it. A way to overcome this difficulty has been recently proposed and tested
within the Lipkin model [7]. It is based on a generalization of the approach introduced in Ref.
[8] in the context of metal clusters, which has been shown to be self-consistent within the p-h
space. The generalization with respect to [8] consists in enlarging the space following the line
suggested in Ref. [6]. Similarly to what is done in Ref. [8], no renormalization is introduced
and the one-body density matrix (OBDM) is not assumed to be diagonal.

2. Formalism and Results
Let us now sketch the derivation of the main equations and show the most relevant results. After
the single particle basis is fixed by solving the HF equations, we introduce phonon operators $Q$
having the same form as the RP A ones,

$$Q_{\nu}^\dagger = \sum_{\nu,h} (X_{\nu,h}^\dagger a_{\nu,h}^\dagger - Y_{\nu,h}^\dagger a_{\nu,h}^\dagger)$$

(1)

avoiding thus the use of renormalized operators. The $X$ and $Y$ amplitudes are solutions of

$$
\begin{pmatrix}
A & B \\
B^* & A^*
\end{pmatrix}
\begin{pmatrix}
X^{(\nu)} \\
Y^{(\nu)}
\end{pmatrix} = \omega_{\nu}
\begin{pmatrix}
G & 0 \\
0 & -G^*
\end{pmatrix}
\begin{pmatrix}
X^{(\nu)} \\
Y^{(\nu)}
\end{pmatrix},
$$

(2)

where

$$
A_{\nu,h,p,h'} = \langle 0 | [a_{\nu,h}^\dagger a_{\nu,p}, H, a_{\nu,p'}^\dagger a_{\nu,h'}] | 0 \rangle, \quad B_{\nu,h,p,p'} = -\langle 0 | [a_{\nu,h}^\dagger a_{\nu,p}, H, a_{\nu,p'}^\dagger a_{\nu,h'}] | 0 \rangle
$$

(3)

and satisfy the orthonormality conditions

$$\sum_{\nu,h,h'} (X_{\nu,h}^\dagger X_{\nu,h'}^\dagger - Y_{\nu,h}^\dagger Y_{\nu,h'}^\dagger)G_{\nu,h,h'} = \delta_{\nu\nu'}.$$  

(4)

In Eq. (3) the symmetrized double commutators are defined as

$$[A, B, C] = \frac{1}{2} \{[A, [B, C]] + [[A, B], C]\}.$$  

(6)

The standard RPA equations can be obtained by replacing the state $| 0 \rangle$ with the uncorrelated
HF one in the matrices $A$, $B$ and $G$. This substitution introduces a visible inconsistency since, on
one hand, the definition of the ground state as the vacuum of the Q operators is used to derive the Eqs. (2), while, on the other hand, the HF state is used in calculating the expectation values appearing in those equations. Furthermore, it introduces some violations of the Pauli principle.

In general, one and two-body density matrices appear in the double commutators. By using the method of the linearization of the equations of motion, one gets the matrices A, B and G expressed in terms of the OBDM only (see ref. [8]). Its matrix elements can be evaluated by using the number operator method [9] in terms of the X and Y amplitudes. Therefore the equations of motion (2) are nonlinear. In order to solve them, we use an iterative procedure. At the n-th iterative step, we compute A, B and G by using the X and Y amplitudes of the (n-1)-th step. As starting point we take the solutions of the standard RPA equations. This iterative procedure is carried on until convergence is reached. The above described method is quite general and can be applied to any finite Fermi system. In order to analyze how well it works, an application has been done to study metallic clusters which, besides being realistic systems having some similarities with nuclei, have the great advantage that the basic interaction is well known, the Coulomb one. In Fig. 1 we show the $S = 0$ dipole strength distribution in several Na clusters. As it is apparent, the method works quite well in improving over standard RPA.

![Dipole Strength Distribution Na](image)

**Figure 1.** (Color online) Spin=0 dipole strength for $Na_N$ metal cluster with $N = 8, 20, 40$ and $58$. Solid line refers to calculations performed within the present approach, while the dashed line refers to standard RPA calculations.

As it is well known, if $|0\rangle$ and $|\nu\rangle$ are a complete set of exact eigenstates of the Hamiltonian with eigenvalues $E_0$ and $E_\nu$, the following identity holds:

$$\sum_\nu \omega_\nu |\langle \nu | F | 0 \rangle|^2 = \frac{1}{2} \langle 0 | [F, [H, F]] | 0 \rangle,$$

(7)

where $\omega_\nu = E_\nu - E_0$.
The above equality is in general violated to some extent when \(|0\rangle, |\nu\rangle\), and \(\omega_{\nu}\) are calculated with some approximation. To which extent it is satisfied is a measure of the adequacy of the approximation. Let us examine the transition amplitudes induced by a one-body operator,

\[ F = \sum_{\alpha, \beta} \langle \alpha | F | \beta \rangle a^\dagger_{\alpha} a_{\beta} \]  

between the ground and excited states. By using the definition (1) and the vacuum property of \(|0\rangle\), one gets

\[ \langle \nu | F | 0 \rangle = \langle 0 | [Q_{\nu}, F] | 0 \rangle. \]  

The above expression is general and it is valid independently of the explicit form of the \(Q\) operators. When the latter have the form (1), only the p-h components of the transition operator \(F\) are selected. A very important feature of RPA, known as Thouless theorem [10] can be described as follows. If in both sides of Eq. (7), the HF state is used, from Eq. (9) one gets

\[ \langle \nu | F | 0 \rangle = \sum_{p h} \left\{ X_{ph}^{\nu*} \langle p | F | h \rangle + Y_{ph}^{\nu*} \langle h | F | p \rangle \right\}. \]  

i.e., the standard RPA expression. The right-hand side can be completely expressed in terms of the \(A\) and \(B\) matrices of RPA. It is then easy to show that equality (7) is exactly satisfied. This result is very important also because it guarantees that spurious excitations corresponding to broken symmetries as, for example, the translational invariance, separate out and are orthogonal to the physical states. We remark that, when the right-hand side is evaluated in the HF state, only the p-h components of the transition operator \(F\) appear in it. The same happens in the l.h.s. but it is essentially related to the p-h nature of the \(Q\) operators. In fact, when the correlated \(|0\rangle\) is maintained, it is still true that only the p-h components of the transition operator \(F\) appear in the l.h.s. and one has

\[ \langle \nu | F | 0 \rangle = \sum_{p h'} \left\{ X_{ph}^{\nu*} \langle p | F | h' \rangle + Y_{ph}^{\nu*} \langle h' | F | p \rangle \right\} G_{ph,p'h'}, \]  

while this is no more the case in the r.h.s., where the whole structure of \(F\) appears. This is the reason why all extension of RPA, with only p-h excitations, violate Eq. (7).

We thus introduce more general \(Q\) operators

\[ Q_{\nu}^\dagger = \sum_{\alpha > \beta} (X_{\alpha \beta}^{\nu} a^\dagger_{\alpha} a_{\beta} - Y_{\alpha \beta}^{\nu} a^\dagger_{\beta} a_{\alpha}), \]  

where \(\alpha\) and \(\beta\) are single-particle states and \(\alpha > \beta\) means that \(n_\alpha < n_\beta\) (\(n\) being the occupation number of the state).

The new \(A\), \(B\) and \(G\) matrices have the same expressions of the so far discussed approach but the \(p'\)s and \(h'\)s indices are replaced now by the \(\alpha'\)s and \(\beta'\)s ones, respectively (see Ref. [7]). The strong advantage of this method with respect to that of Ref. [6] is that, by diagonalizing the norm matrix and by looking at the overlaps of the excited states with the ground state the non-physical states can be isolated and eliminated from the spectrum. In order to analyze the advantages of this procedure we have applied it to a 3-level Lipkin model and the results are shown in Fig. 2 where the excitation spectrum (panel (a)) and the eigenvalues of the norm matrix (panel(b)) are displayed as a function of the strength parameter. The present calculation is denoted in the figure with the acronym EERPA (extended and enlarged RPA). EERPA results (solid lines) are compared with the exact corresponding values (dashed lines) and with the standard RPA.
energies (dotted lines). The first two RPA excited states are indicated with (1) and (3). A much better agreement with the exact results is found for EERPA with respect to RPA. This is mostly evident for the first RPA excited state already before the RPA collapse point, \( \tau = 0.026 \). With EERPA the collapse point is located much further and the good agreement with the exact values is kept in the whole region where the EERPA results exist. The state (2), whose energy is equal to \( \epsilon_2 - \epsilon_1 \) when \( \tau \) approaches 0, does not correspond to any exact solution. Thus it is non-physical. This straightforward identification would not be possible when the EERPA is applied to the study of realistic systems since exact results are not available in that case. In general, however, one can proceed as follows. In the panel (b) of the same figure we plot the eigenvalues of the norm matrix. One can observe that even beyond the RPA collapse point one eigenvalue is much smaller than the others, its value being equal to 0.03 at the RPA collapse. At \( \tau = 0.035 \), that is far beyond the collapse, the three eigenvalues are still well separated: 0.09, 0.69 and 0.84, respectively. This tells us that one of the three solutions is non-physical. In order to identify it we look at the overlap of the ground state with the three excited ones, which are shown in the panel (c) of Fig. 2. As it is very clearly visible, such overlap for the state labelled as (2) is strongly different from zero, while for the others it is much smaller. Thus we can conclude that indeed such state is the non-physical one. Of course, in the case of a schematic, exactly solvable model such identification can be done directly by looking at the exact energy spectrum while this is not possible in realistic cases. On the other hand, the appearance of a (almost) zero eigenvalue of the norm matrix together with a large overlap with g.s. is an unambiguous criterion to single out the states to be eliminated and it is viable also in realistic systems. The fact that the overlaps of the physical states with the ground state are not exactly zero, especially for large values of the strength, is related to the approximations present in the approach. For example, the OBDM is evaluated by using the number operator method truncated at a certain order, which probably is not enough for values of the strength well beyond the RPA collapse point. However, in physical cases we expect to be in situations corresponding to smaller values of the strength or, in worst cases, around the RPA collapse point. We remark that the above discussed criterion, to disentangle physical from non-physical states, could not be applied in the previous approach [6] since there the OBDM is assumed diagonal.

3. Conclusions and Perspectives

In conclusion, we have presented an extension of RPA in which ground state correlations are treated in a self-consistent way and no use of the quasiboson approximation is made. An application to metallic clusters shows that an important improvement with respect to standard RPA is achieved. However, a drawback of that approach, common to all extensions of RPA, is that EWSR are violated. In order to overcome this difficulties we have further generalized the approach by enlarging the configuration space beyond the p-h excitations, including also the particle-particle and hole-hole ones. The method has been applied to a three-level Lipkin model and we have shown that possible non-physical states can be isolated and eliminated from the spectrum by diagonalizing the norm matrix and by looking at the overlaps with the ground state. The obtained results strongly encourage the application of the present approach to more realistic systems. Work in this direction is in progress.
Figure 2. (Color online) Panel (a): Excitation energies of the states (1), (2) and (3) and the eigenvalues of the norm matrix (panel (b)) as a function of the strength parameter $\tau = \chi/\epsilon$. The energies in the Y axis are expressed in units of $\epsilon$. In the panel (c) the corresponding overlaps of the three states with the ground state are shown. See Ref. [7] for more details.

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