Extension of random-phase approximation preserving energy weighted sum rules: An application to a 3-level Lipkin model

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A limitation common to all extensions of random-phase approximation including only particle-hole configurations is that they violate to some extent the energy weighted sum rules. Considering one such extension, the improved RPA (IRPA), already used to study the electronic properties of metallic clusters, we show how it can be generalized in order to eliminate this drawback. This is achieved by enlarging the configuration space, including also elementary excitations corresponding to the annihilation of a particle (hole) and the creation of another particle (hole) on the correlated ground state. The approach is tested within a solvable 3-level model.

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I. INTRODUCTION

Collective excitations are a common feature of a large variety of many body systems. Their properties are intimately related to the structure of the ground state upon which they are built. The simplest theory of excited states of a quantum system where correlations are taken into account to some extent is the random-phase approximation (RPA). In this theory one introduces a set of operators $Q_\nu^\dagger$, whose action on the ground state $|\Psi_0\rangle$ creates the collective excitations, while the ground state itself is the vacuum for the Q_ν operators. The latters are defined as linear superpositions of particle-hole (ph) creation and annihilation operators, occupied (h) and unoccupied (p) single particle states being defined with respect to the Hartree-Fock ground state $|\mathrm{HF}\rangle$. The X and Y coefficients of these linear forms are solutions of equations which can be derived by using the equations of motion method [1,2]. If the Hamiltonian contains one- and two-body terms, the solution of these equations would imply the evaluation of one- and two-body density matrices. Standard RPA is obtained by replacing them by those calculated in the uncorrelated ground state $|\mathrm{HF}\rangle$. This approximation introduces a visible inconsistency since, on one hand, the definition of $|\Psi_0\rangle$ as the vacuum of the Q_ν operators is used to derive the formal equations determining the X and Y amplitudes; while, on the other hand, $|\mathrm{HF}\rangle$ is used instead of $|\Psi_0\rangle$ in calculating the expectation values appearing in those equations.

Various attempts have been made to eliminate this inconsistency. We quote the pioneering works [3,4] where the renormalized RPA (RRPA) was introduced. The RRPA was applied to study the low-lying spectrum and the transition densities of vibrational nuclei [5] and the double beta decay [6–8] more recently. A very important contribution to the solution of this problem has been given in Ref. [9], where a general scheme, the self-consistent RPA (SCRPA), was developed (see also Ref. [10] and references therein). In Ref. [8] a fully renormalized RPA (fully RRPA) has been proposed, which shares some similarities with the approach we are going to present in this paper. In Refs. [11] and [12] it was shown that by using the number operator method [13] it is possible to get for the X and Y coefficients a closed set of equations having the same form as in RPA, where the density matrices in the correlated ground state are expressed in terms of the X and Y coefficients themselves. Thus the equations to solve are non linear and their solution requires a big computational effort. In order to appreciate how much a better treatment of correlations modifies the RPA results, in the same paper a simplified version of the approach was proposed, the IRPA, based on the linearization of the equations of motion. The simplification consists in contracting the two-body terms appearing in the commutator of the Hamiltonian with a one-body ph operator with respect to the correlated ground state. In this way only one-body density matrices have to be evaluated: the so obtained equations are still nonlinear, but they are much easier to be solved, since only the one-body density matrix appears. When the latter is calculated in $|\mathrm{HF}\rangle$ rather than in the correlated $|\Psi_0\rangle$, RPA is again obtained [14]. This approach was applied in Refs. [11] and [12] to the study of the electronic properties of some simple metal clusters, obtaining a better description than RPA. However, the formulation is quite general and its applicability is by no means limited to such systems.

A limitation common to all extensions of RPA including only ph configurations is that they violate to some extent the energy weighted sum rules (EWSR's). In the present paper we will show that this drawback can be eliminated by enlarging the configuration space, including also those configurations corresponding to the annihilation of a particle (hole) and the creation of another particle (hole) on the ground state. This is in the same spirit of Refs. [15] and [16], where, for the first time, the particle-particle and hole-hole configurations were included within the SCRPA approximation.

Very recently a paper [17] came to our knowledge, where the same problem is tackled and studied within a solvable 4-level model with a separable residual interaction. As we will show below, there are several differences with the present paper:

(i) We explicitly show that the EWSR is exactly satisfied when the configuration space is enlarged;

(ii) By comparison with the exact solutions of the model we can judge the quality of the results obtained in IRPA and its enlarged version, with respect to the RPA ones;

(iii) This comparison allows us to point out that, besides the merit of solving the EWSR problem, the approach has the shortcoming that spurious solutions appear. This problem is not discussed in Ref. [17] where, indeed, probably because a separable residual interaction is used, only one collective state is found despite the fact that three elementary excitation modes are present in the model. In this context, it is worth mentioning that spurious solutions are also found in Ref. [8], where they are interpreted as ''new excitation modes.''

The paper is organized as follows. In Sec. II we shortly recall the main IRPA equations, pointing to the origin of the EWSR violations. Then we show how this problem is solved when the enlarged space is considered. In Sec. III we illustrate the approach by applying it to a solvable 3-level model [19–21] and comparing the different approximations among themselves and with the exact results.

II. FORMULATION OF THE APPROACH

In this section we recall the main steps leading to the IRPA equations, presented in detail in Refs. [11] and [12], and illustrate why, being limited to ph excitations, the IRPA approximation violates the EWSR [2]. Then we show that, enlarging the space by including also pp and hh configurations, this difficulty is overcome. In this respect, our approach is similar to the fully RRPA [8].

A. IRPA and the EWSR problem

Let $|\Psi_0\rangle$ be the ground state of the system and $|\Psi_\nu\rangle$ its excited states. Assuming that the latters are linear combinations of ph and hp configurations built upon $|\Psi_0\rangle$ one writes

$$|\Psi_\nu\rangle \equiv Q_\nu^\dagger |\Psi_0\rangle \equiv \sum_{ph} [X_{ph}^\nu B_{ph}^\dagger - Y_{ph}^\nu B_{ph}] |\Psi_0\rangle, \tag{1}$$

where p (h) denotes the quantum numbers of an unoccupied (p) and occupied (h) single particle state in the uncorrelated Hartree-Fock reference state $|\mathrm{HF}\rangle$. In Eq. (1) we have introduced renormalized ph creation ($B^\dagger$) and annihilation (B) operators. In Refs. [11] and [12] it is shown that in the basis diagonalizing the one-body density matrix they can be written as

$$B_{ph}^\dagger = D_{ph}^{-1/2} a_p^\dagger a_h, \tag{2}$$

with

$$D_{ph} \equiv n_h - n_p, \tag{3}$$

where n_h and n_p are, respectively, the hole and particle occupation numbers in the correlated ground state $|\Psi_0\rangle$. Assuming that $|\Psi_0\rangle$ is the vacuum of the Q_ν operators,

$$Q_\nu |\Psi_0\rangle = 0, \tag{4}$$

the ortonormality conditions for the excited states leads to

$$\delta_{\nu\nu'} = \langle \Psi_\nu | \Psi_{\nu'} \rangle = \sum_{ph} [X_{ph}^{\nu *} X_{ph}^{\nu'} - Y_{ph}^{\nu *} Y_{ph}^{\nu'}]. \tag{5}$$

The equations determining the X^ν and Y^ν amplitudes and the excitation energies E_ν of the states $|\Psi_\nu\rangle$ are obtained by using the equations of motion method [1,2]. They read

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = E_\nu \begin{pmatrix} X^\nu \\ -Y^\nu \end{pmatrix}, \tag{6}$$

with the A and B matrices given by

$$A_{ph,p'h'} = \langle \Psi_0 | [B_{ph}, H, B_{p'h'}^\dagger | \Psi_0 \rangle \tag{7}$$

and

$$B_{ph,p'h'} = -\langle \Psi_0 | [B_{ph}^\dagger, H, B_{p'h'}^\dagger] | \Psi_0 \rangle. \tag{8}$$

In Eqs. (7) and (8) H is the Hamiltonian of the system and

$$[A,B,C] \equiv \frac{1}{2}([A,[B,C]] + [[A,B],C]). \tag{9}$$

The standard RPA equations can be obtained by putting $n_h = 1$, $n_p = 0$ in the expressions for the operators B and $B^\dagger$ (2) and by replacing the correlated ground state $|\Psi_0\rangle$ appearing in Eqs. (7) and (8) with the Hartree-Fock one $|\mathrm{HF}\rangle$. In Ref. [14] it is shown that the RPA equations can equivalently be obtained by linearizing the commutator $[H, B_{p'h'}^\dagger]$ in Eqs. (7) and (8), i.e., by contracting it with respect to $|\mathrm{HF}\rangle$. A better approximation is done in IRPA, where the linearization is made by contraction in $|\Psi_0\rangle$. In a loose notation, this means

$$[H, a_p^\dagger a_h] \to a^\dagger a + a^\dagger a^\dagger a a \sim a^\dagger a + \langle \Psi_0 | a^\dagger a | \Psi_0 \rangle a^\dagger a. \tag{10}$$

Therefore the occupation numbers in the correlated ground state appear in the IRPA expressions, while those in $|\mathrm{HF}\rangle$ (i.e., 0 or 1) appear in standard RPA. This procedure leads to

$$A_{ph,p'h'} = \frac{1}{2}(D_{ph}^{1/2} D_{p'h'}^{-1/2} + D_{p'h'}^{1/2} D_{ph}^{-1/2})(\epsilon_{p'p}\delta_{hh'} - \epsilon_{hh'}\delta_{pp'}) + D_{ph}^{1/2} D_{p'h'}^{1/2} (hp'|H_2|ph'), \tag{11}$$

where

$$\epsilon_{p'p} \equiv (p'|H_1|p) + \sum_\alpha n_\alpha (p'\alpha|H_2|p\alpha) \tag{12}$$

and

$$\epsilon_{hh'} \equiv (h|H_1|h') + \sum_\alpha n_\alpha (\alpha h|H_2|\alpha h'). \tag{13}$$

For the matrix B one gets

$$B_{ph,p'h'} = D_{ph}^{1/2} D_{p'h'}^{1/2} (hh'|H_2|pp'). \tag{14}$$

In the above equations H_1 is the one-body term of the Hamiltonian and H_2 its two-body part. We denote by α a generic single particle state (occupied or unoccupied in $|\mathrm{HF}\rangle$). As shown in Appendix A of Ref. [11], using the

number operator method [13] the occupation numbers appearing in the A and B matrices can be expressed in terms of the X and Y amplitudes as

$$n_p=\sum_{h\nu\nu'}\left(\delta_{\nu\nu'}-\frac{1}{2}\sum_{p_1h_1}D_{p_1h_1}X^{\nu'}_{p_1h_1}X^{\nu *}_{p_1h_1}\right)D_{ph}Y^{\nu}_{ph}Y^{\nu' *}_{ph}, \tag{15}$$

$$n_h=1-\sum_{p\nu\nu'}\left(\delta_{\nu\nu'}-\frac{1}{2}\sum_{p_1h_1}D_{p_1h_1}X^{\nu'}_{p_1h_1}X^{\nu *}_{p_1h_1}\right)D_{ph}Y^{\nu}_{ph}Y^{\nu' *}_{ph}. \tag{16}$$

Therefore Eqs. (6) are nonlinear. They have been solved iteratively in the case of metallic clusters [11,12]. It is, however, apparent that the approach is quite general and can be applied to any many body system. The matrices A and B in IRPA, Eqs. (11) and (14), are different from those in standard RPA. On one side the Hartree-Fock single particle energies appearing in the A matrix of RPA are replaced by the quantities appearing in the first line of Eq. (11). On the other side, the residual interaction in the expressions for A and B is now renormalized by the factors $D^{1/2}$'s. In RRPA only the latter modification is present. This latter modification is present also in RRPA.

A serious problem arises with respect to the EWSR. As is well known, if $|\Psi_0\rangle$ and $|\Psi_\nu\rangle$ are a complete set of exact eigenstates of the Hamiltonian, with eigenvalues E_0 and E_ν, the following identity holds:

$$\sum_\nu (E_\nu-E_0)|\langle\Psi_\nu|F|\Psi_0\rangle|^2=\frac{1}{2}\langle\Psi_0|[F,[H,F]]|\Psi_0\rangle, \tag{17}$$

where F is any Hermitian single particle operator. The equality (17) is in general violated to some extent when $|\Psi_0\rangle$, $|\Psi_\nu\rangle$ and E_ν are calculated within some approximation. To which extent it is satisfied is a measure of the adequacy of the approximation. A very important feature of RPA is that Eq. (17) is satisfied for any one-body operator if, in calculating its two sides, one considers $|\mathrm{HF}\rangle$ instead of $|\Psi_0\rangle$ and the solutions of RPA for $|\Psi_\nu\rangle$ and $(E_\nu-E_0)$ [18]. This feature follows from the fact that, when $|\mathrm{HF}\rangle$ is used in Eq. (17) instead of $|\Psi_0\rangle$ only particle-hole matrix elements remain in the right-hand side. It is easy to show [11] that, if the transition operator F has only p-h matrix elements, the two sides of Eq. (17) are equal also within IRPA. However, this is not the case in general.

Let us consider separately the two sides of Eq. (17) in IRPA, with a general one-body Hermitian operator F:

$$F=\sum_{\alpha\beta}f_{\alpha\beta}a^\dagger_\alpha a_\beta. \tag{18}$$

The left-hand side is easily calculated and gives

$$\begin{aligned}\sum_\nu (E_\nu-E_0)|\langle\Psi_\nu|F|\Psi_0\rangle|^2&=\sum_\nu (E_\nu-E_0)|\langle\Psi_0|Q_\nu F|\Psi_0\rangle|^2\\&=\sum_\nu (E_\nu-E_0)|\langle\Psi_0|[Q_\nu,F]|\Psi_0\rangle|^2\\&=\sum_\nu (E_\nu-E_0)\left|\sum_{ph}f_{ph}D^{1/2}_{ph}(X^\nu_{ph}+Y^\nu_{ph})\right|^2,\end{aligned} \tag{19}$$

which is formally equal to the RPA result, apart from the factor $D^{1/2}_{ph}$. Therefore only the ph components of F enter. This is due to the fact that the excited states are described as superpositions of ph configurations only. Starting from Eqs. (6) and using the properties of the X and Y amplitudes, Eq. (19) can be written as

$$\sum_\nu (E_\nu-E_0)|\langle\Psi_\nu|F|\Psi_0\rangle|^2=\sum_{ph}D^{1/2}_{ph}f_{ph}\sum_{p'h'}D^{1/2}_{p'h'}f_{p'h'}(A_{ph,p'h'}-B_{ph,p'h'}). \tag{20}$$

In order to evaluate the right-hand side of Eq. (17) one can use for the commutator $[H,F]$ the same linearization procedure already used in deriving Eqs. (11) and (14). It is easy to realize that the result of such calculation cannot be equal to Eq. (20) since not only the ph matrix elements of the residual interaction will appear in it, but also other terms if they are present in the one-body operator F. This happens because the expectation value of the double commutator is taken in the correlated ground state $|\Psi_0\rangle$. We will show this in the next subsection, where an enlarged configuration space, including also pp and hh components, will be used to express the excited states. Of course, if the correlations present in $|\Psi_0\rangle$ are small and the occupation numbers do not differ too much from 0 and 1, the violations of the EWSR are small. But, in general, this is not the case. For example, for Na clusters, the discrepancy was found [11,12] to be about 25%.

B. The enlarged space

As shown in the previous subsection, the problem of violations of the EWSR arises because also in IRPA, as in RPA, the excited states are expressed as superpositions of ph configurations. Let us then consider the more general expansion

$$|\overline{\Psi}_\nu\rangle=\overline{Q}^\dagger_\nu|\overline{\Psi}_0\rangle=\sum_{\alpha>\beta}(\overline{X}^\nu_{\alpha\beta}B^\dagger_{\alpha\beta}-\overline{Y}^\nu_{\alpha\beta}B_{\alpha\beta})|\overline{\Psi}_0\rangle, \tag{21}$$

where α and β stand for any single particle state and $\alpha>\beta$ means that we order these states according to decreasing occupation numbers, i.e. $n_\alpha<n_\beta$. The operators $B^\dagger_{\alpha\beta}$ and

$B_{\alpha\beta}$ are an obvious generalization of Eqs. (2) and (3). As before we define $|\overline{\Psi}_0\rangle$ as the vacuum of the $\overline{Q}_\nu$ operators:

$$\overline{Q}_\nu|\overline{\Psi}_0\rangle=0. \tag{22}$$

In order to make the notation simpler, we will omit the bars in the collective operators and in the states, which, of course, are different from those considered in IRPA since now pp and hh configurations are included, in addition to the ph ones. The derivation of the equations of motion can be done by following the same linearization procedure as before. They have the same form as in Eq. (6), the matrices A and B being now

$$A_{\alpha\beta,\gamma\delta}=\frac{1}{2}(D^{1/2}_{\alpha\beta}D^{-1/2}_{\gamma\delta}+D^{1/2}_{\gamma\delta}D^{-1/2}_{\alpha\beta})(\epsilon_{\alpha\gamma}\delta_{\beta\delta}-\epsilon_{\beta\delta}\delta_{\alpha\gamma}) + D^{1/2}_{\alpha\beta}D^{1/2}_{\gamma\delta}(\beta\gamma|H_2|\alpha\delta) \tag{23}$$

and

$$B_{\alpha\beta,\gamma\delta}=\frac{1}{2}(D^{1/2}_{\alpha\beta}D^{-1/2}_{\gamma\delta}-D^{1/2}_{\gamma\delta}D^{-1/2}_{\alpha\beta})(\epsilon_{\alpha\delta}\delta_{\beta\gamma}-\epsilon_{\beta\gamma}\delta_{\alpha\delta}) + D^{1/2}_{\alpha\beta}D^{1/2}_{\gamma\delta}(\delta\beta|H_2|\gamma\alpha), \tag{24}$$

where

$$\epsilon_{\alpha\beta}=(\alpha|H_1|\beta)+\sum_\gamma n_\gamma(\alpha\gamma|H_2|\beta\gamma). \tag{25}$$

Apart from the fact that in Eqs. (23) and (24) the indices run over all single particle states, the main difference with Eqs. (11) and (14) is the presence of the ϵ terms also in the B matrix.

Coming back to the EWSR problem, Eq. (20) is easily generalized to

$$\sum_\nu (E_\nu-E_0)|\langle\Psi_\nu|F|\Psi_0\rangle|^2 = \sum_{\alpha>\beta} f_{\alpha\beta}D^{1/2}_{\alpha\beta}\sum_{\gamma>\delta} f_{\gamma\delta}D^{1/2}_{\gamma\delta}(A_{\alpha\beta,\gamma\delta}-B_{\alpha\beta,\gamma\delta}), \tag{26}$$

which, after some tedious manipulations, can be written as

$$\sum_\nu (E_\nu-E_0)|\langle\Psi_\nu|F|\Psi_0\rangle|^2 = \frac{1}{2}\sum_{\alpha\beta} f_{\alpha\beta}D_{\alpha\beta}\sum_{\gamma\delta} f_{\gamma\delta}[\epsilon_{\alpha\gamma}\delta_{\beta\delta}-\epsilon_{\beta\delta}\delta_{\alpha\gamma} + (\beta\gamma|H_2|\alpha\delta)D_{\gamma\delta}]. \tag{27}$$

The double commutator is easily calculated by using the same linearization procedure adopted to derive the equations of motion. Doing that one realizes that Eq. (17) is indeed satisfied. Thus one obtains a kind of generalization of the Thouless theorem. Namely, Eq. (17) is satisfied if one calculates its two sides by using the solutions of the equations of motion and by making the same approximations introduced in the derivation of the latters.

In principle the new approach does not appear to be more difficult than IRPA and its equations can be solved in realistic cases by the same iterative procedure used there. In practice, however, the computational effort is much heavier since the configuration space is much larger. For this reason we have decided to apply it to a solvable 3-level model [19–21].

We show this application in the next section, where we compare the results of IRPA and of its enlarged version with the exact solutions of the model.

III. THE MODEL AND THE RESULTS

Let us first of all illustrate the solvable model to which we applied the enlarged version of IRPA.

It consists of three levels, 0, 1, and 2, with energies ϵ_0, ϵ_1, and ϵ_2, respectively. Let 2Ω be the degeneracy of each level and $N=2\Omega$ the total number of fermions in the system.

We define the operators

$$K_{ij}\equiv\sum_m a^\dagger_{im}a_{jm}, \tag{28}$$

where the indices i and j denote one of the three levels and the index m runs over the 2Ω substates of each of them. The operators K satisfy the following commutation relations:

$$[K_{ij},K_{kl}]=\delta_{jk}K_{il}-\delta_{il}K_{kj}. \tag{29}$$

They are therefore the generators of the U(3) algebra. The algebra becomes SU(3) if we consider the additional relation

$$N=\sum_i K_{ii}, \tag{30}$$

that fixes the total number of particles.

We introduce the Hamiltonian for our system as follows:

$$H=\sum_{i\neq0}\epsilon_iK_{ii}+V_0\sum_{i,j\neq0}K_{i0}K_{0j}+V_1\sum_{i,j\neq0}(K_{i0}K_{j0}+K_{0j}K_{0i}) + V_2\sum_{i,j,k\neq0}(K_{i0}K_{jk}+K_{kj}K_{0i})+V_3\sum_{i,j,k,l\neq0}K_{ij}K_{kl}. \tag{31}$$

The terms with the V_0 and V_1 strengths describe, respectively, the $phph$ and $pphh$ parts of the interaction. The term with the V_2 strength is related to the $ppph$ part, while the last term represents the $pppp$ part. In standard RPA the only two-body terms of H that enter in the expressions for the matrices A and B of the equations of motion (6) are those with the strengths V_0 and V_1, i.e., the ph two-body terms. In the IRPA approach [11,12] the ground state that is actually used in the calculations is correlated; so the single particle occupation numbers are not strictly 1 for hole states and 0 for particle states, as in $|\mathrm{HF}\rangle$. In this case also the $pppp$ term enters in the expressions for the matrices (actually only in the matrix A). In the IRPA approach with the enlarged configuration space all the terms contribute.

The exact results for the system can be obtained either by using the SU(3) symmetry of the model or by diagonalizing the Hamiltonian (31) in the complete set of states

$$|n_1 n_2\rangle \equiv C(K_{10})^{n_1}(K_{20})^{n_2}|0\rangle, \tag{32}$$

where $|0\rangle$ denotes the state in which all the particles are in the level 0, n_1 and n_2 are the numbers of particles in the levels 1 and 2, respectively, and C represents a normalization factor.

With the same set of parameters chosen for the exact calculation, after having performed a standard RPA calculation, we solved the equations of motion both in the IRPA approach of Refs. [11] and [12] and in the new approach, with the enlarged configuration space. In the IRPA case the operators $Q^{\dagger}_{\nu}$ are defined as linear combinations of ph ($i0$, with: $i \neq 0$) and hp ($0i$, with $i \neq 0$) configurations, as in Eq. (1),

$$Q^{\dagger}_{\nu} \equiv \sum_i \left(X^{\nu}_i \tilde{K}_{i0} - Y^{\nu}_i \tilde{K}_{0i}\right), \tag{33}$$

while in the enlarged calculation they are defined as in Eq. (21),

$$Q^{\dagger}_{\nu} \equiv \sum_{i>j} \left(X^{\nu}_{ij} \tilde{K}_{ij} - Y^{\nu}_{ij} \tilde{K}_{ji}\right), \tag{34}$$

where

$$\tilde{K}_{ij} \equiv \frac{1}{(2\Omega)^{1/2}} D_{ij}^{-1/2} K_{ij}\,. \tag{35}$$

With the definition (35) we get, for the excited states of the system, the same orthonormality conditions as given in Eq. (5).

Note that in Eq. (34) the indices i and j run over all the three single particle levels of the model. In both cases (33) and (34) we have solved the non linear problem of Eqs. (6) by means of an iterative procedure. We fixed the number of particles N equal to 10. In this case the number of exact eigenstates of the Hamiltonian is 66. The RPA and IRPA calculations will give two excited states, since their configuration space is composed only by the two configurations (1,0) and (2,0). The enlarged IRPA will give three states, since its configuration space is made by the three configurations (1,0), (2,1), and (2,0).

We tested various values for the four parameters V_0, V_1, V_2, and V_3 and for the energies of the levels, the results being qualitatively the same. In Fig. 1 we show one case, where

$$\epsilon_0 = 0, \quad \epsilon_1 = \epsilon, \quad \epsilon_2 = 2.5\epsilon, \tag{36}$$

$$V_0 = -\chi, \quad V_1 = \chi, \quad V_2 = \frac{-\chi}{2}, \quad V_3 = \frac{\chi}{10}. \tag{37}$$

Both the ϵ and χ parameters have the units of an energy. In the figure the excitation energies are represented versus the increasing values of the strength χ. Dashed lines refer to exact values of energies. Among all the 66 exact eigenvalues the two represented ones are those with energies equal to 1 and 2.5 at $\chi = 0$; i.e. those which correspond to the two RPA and IRPA excited states. Dotted lines refer to RPA and dot-dashed lines to IRPA values. The three values corresponding to the enlarged IRPA approach are represented by full lines.

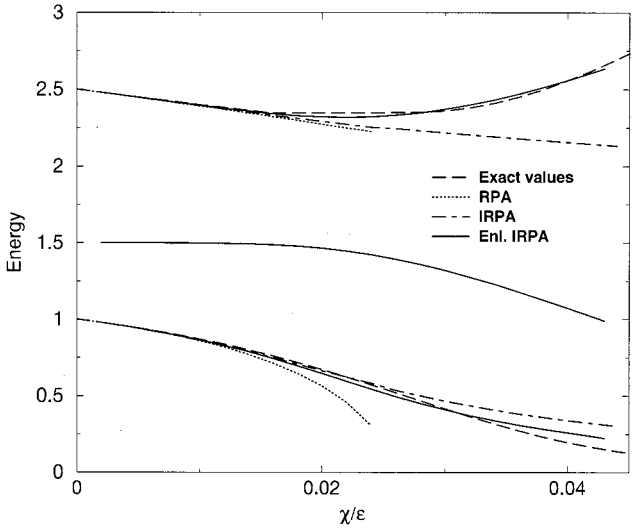

FIG. 1. Excitation energies versus χ/ϵ, with the parameters of Eqs. (36) and (37). The energies in the Y axis are expressed in units of ϵ.

The collapse point of RPA, where its first excitation energy becomes imaginary, appears at $\chi = 0.024$. We observe that both the IRPA and the enlarged IRPA calculations push the collapse point towards greater values of the strength parameter χ; so, in this regard, both methods improve the RPA results. Moreover it can be seen that the two exact values are better approximated by the first and the third states obtained in the enlarged IRPA approach, than by the two IRPA states. This is especially evident for the higher state.

It is interesting to focus the attention on the presence of the additional state that the enlarged IRPA gives, with respect to RPA and IRPA. Actually this state does not correspond to any of the found exact states. This fact seems to indicate that it is a spurious state. On the other hand its energy is not zero or very small, as it happens normally for spurious states. Its energy always starts, when χ starts from zero, from the energy difference between the levels 1 and 2, and so it depends on how we fix the values ϵ_1 and ϵ_2. This would mean that, if we applied our approach in a realistic calculation, the spurious states that would appear would not be easily recognized and eliminated, not having in principle zero or very small energies. This could cause problems in the interpretation of the calculated spectrum of excitations. A similar situation is encountered in RPA at finite temperature and was also found in Ref. [8]. Let us look at the transition probabilities related to this state. Figure 2 shows the transition probabilities related to the obtained states, for RPA and EIRPA calculations, for different χ strengths. Let us observe in the figure the transition probability related to the spurious state,

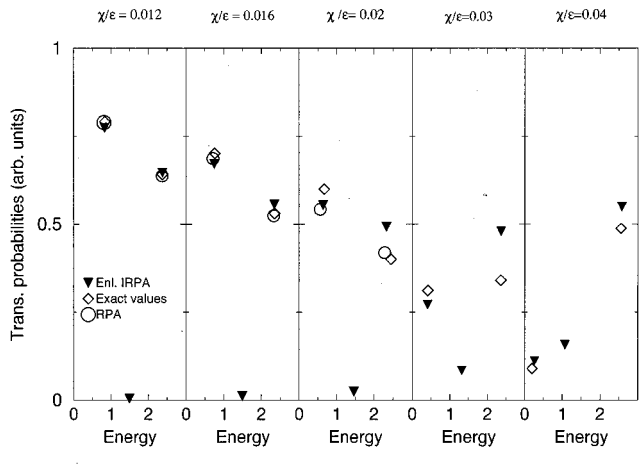

FIG. 2. Transition probabilities for four values of χ/ϵ, with the parameters of Eqs. (36) and (37). The energies in the X axis are expressed in units of ϵ.

$$P_{sp}=|\langle\Psi_{\nu_{sp}}|F|\Psi_0\rangle|^2, \tag{38}$$

where $|\Psi_0\rangle$ is the ground state, $|\Psi_{\nu_{sp}}\rangle$ is the spurious state, and F the one-body operator (18) with all the $f_{\alpha\beta}$'s equal to 1. We can see that P_{sp} is very small, with respect to the other two transition probabilities, only when χ is far from the collapse point; when χ approaches the collapse point the transition probability (38) becomes appreciable (see the case $\chi=0.04$ in the figure). The same trend is found for other sets of parameters.

This means that in the evaluation of any physical quantity, in a realistic calculation, the existence of spurious states would have some influence and it would be important to recognize and eliminate them from the calculation. The problem of how to recognize them is still open, as they do not have in general small energies and/or small transition probabilities.

TABLE I. The left-hand side (lhs) of EWSR in the IRPA and in the enlarged IRPA cases, together with the right-hand side (rhs), for different values of χ/ϵ and with the parameters (33) and (34).

χ/ϵ	lhs IRPA	lhs enl. IRPA	rhs
0.012	1.84957	2.1877893606	2.1877893605
0.03	0.89411	1.3607871867	1.3607871868
0.04	0.67858	1.5861229231	1.5861229230

We present now, in Table I, the results obtained for the EWSR, in IRPA, and in enlarged IRPA cases. These results refer again to the choice (36) and (37) for the parameters. The violation of the EWSR, in the IRPA case, increases with the increasing values of the χ parameter and is about of 30% for $\chi=0.03$. In the enlarged IRPA case the EWSR is always exactly satisfied, as expected.

This is an important achievement of the present method, because, as stressed in Sec. I, all the methods that have been proposed so far in order to go beyond the RPA, by avoiding the inconsistency of the quasiboson approximation, always violate the EWSR identity.

IV. CONCLUSIONS

In conclusion, we have presented an extension of RPA which avoids the use of the quasiboson approximation and, at variance with many other attempts made in the same direction, preserves exactly the EWSR. This is obtained as a generalization of a previously studied approach by enlarging the configuration space with respect to that commonly used, which contains only particle-hole elementary excitations. The approach has been tested on a 3-level solvable model.

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