Extension of the second random-phase approximation

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The second random-phase approximation (SRPA) is the simplest and most natural extension of the RPA. It enlarges the space of the elementary modes introduced to describe the collective states by adding 2 particle - 2 hole excitations to the 1 particle - 1 hole ones of the RPA. In deriving the SRPA equations, use is made, as in the RPA, of the so-called quasi-boson approximation (QBA) where expectation values in the ground state of the system are approximated by their values in the uncorrelated reference state. This, however, has been shown to imply a degree of approximation worse than that in the RPA. It is, therefore, necessary to improve the QBA by considering a reference state which contains some correlations. Having in mind to perform such calculations for realistic systems, we consider a simple extension of the SRPA in which the reference state contains 2 particle - 2 hole correlations. The quality of such an extension is tested by applying it to a solvable three-level model and found to be good.

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I. INTRODUCTION

Collective excitations are one of the most common and interesting features of many-body systems. Of particular interest are the collective modes which can be interpreted in terms of vibrations. Nuclei show a large variety of such vibrations, both low lying and high lying [1]. In particular, the giant dipole resonance is due to the coherent motion of protons against neutrons. The analog of the giant dipole resonance in metal clusters is the dipole plasmon excitation which is well known [2,3] and is interpreted as the collective vibration of the electrons against the ions. The random-phase approximation (RPA) has been extensively used as a microscopic theory to study the basic properties of these collective excitations. In this framework, one introduces a set of phonon operators $Q_\nu^\dagger$ whose action on the ground state $|0\rangle$, defined as the vacuum of the Q_ν operators, creates the collective states $|\nu\rangle$. The excitation energies E_ν are solutions of a system of equations which can be derived by using the equations of motion method [4,5]. In the derivation of the standard RPA, use is made of the quasi-boson approximation (QBA), which entails replacing the expectation value in the ground state $|0\rangle$ of any operators with the corresponding value in the uncorrelated reference state. Strictly related to the QBA is the RPA property of predicting a harmonic spectrum with regularly spaced multiphonon states. On the other hand, the existence of anharmonicities in the multiphonon spectra of nuclei and their influence on various physical processes are well established [1,6–8]. Overcoming the QBA has been the starting point of many attempts aimed at improving the RPA.

One line of investigation in such a direction has been based on the reformulation of the whole theory in a boson formalism [9,10]. Along this line, an extension of RPA was presented in Ref. [10] within a three-level Lipkin model [11]. The phonon operators $Q_\nu^\dagger$ were defined from the beginning in terms of true boson operators, and all the fermion operators of interest were replaced by their boson images via a mapping procedure. The RPA-type equations that one constructs in this formalism depend on the degree of the expansion of the boson Hamiltonian. Standard RPA is obtained when the expansion of the boson image of the Hamiltonian is truncated at the lowest order, i.e., at the two boson terms only. Considering higher-order terms provides a natural way to reach a higher level of approximation and so go beyond the standard RPA. In Ref. [10], the boson Hamiltonian was diagonalized within the space containing up to two, three, and four phonon excitations. An important conclusion of such a study was that in order to reproduce the energies of states which in the harmonic limit correspond to two quanta excitations, it is necessary to diagonalize the Hamiltonian in the space of the states including up to four phonons. Such a calculation would not be feasible for a realistic system. Therefore, one has to look for a more affordable approach.

A natural extension of the RPA for the study of two-phonon states is the second RPA (SRPA). However, in its derivation, QBA is still used [12]; and as shown in Refs. [13,14], this is an even more severe approximation than that in the RPA. In the present paper, we introduce an extension of the RPA and SRPA obtained by improving the QBA along the lines indicated in Refs. [13–15]. The quality of the corresponding results is studied by performing calculations within the three-level Lipkin model. We calculate several physical quantities such as excitation and ground state correlation energies, occupation numbers, strength functions, and sum rules. From the comparison of our results with the exact ones, we conclude that the present approach gives a good description of the ground state and of those excited states which in the harmonic limit would correspond to one and two phonon excitations. This approach does not require a very heavy computational effort, and we plan to apply it to the study of realistic systems. Work in this direction is in progress.

The paper is organized as follows. In Sec. II, the formalism associated with the RPA and SRPA is shortly reviewed and the extensions of the two approaches are presented. In Sec. III, the exact and approximate results are compared

and in Sec. IV, our conclusions are drawn. In Appendix A, we show the explicit form of some matrices used in the calculations.

II. FORMALISM

In this section, we present the derivation of the extensions of the RPA and SRPA mentioned in the Introduction and obtained by improving on the QBA. Let us define the operators $Q_\nu^\dagger$ and Q_ν such that

$$Q_\nu|0\rangle = 0, \tag{1}$$

$$|\nu\rangle = Q_\nu^\dagger|0\rangle, \tag{2}$$

where $|0\rangle$ and $|\nu\rangle$ are, respectively, the ground state and a generic excited state of the Hamiltonian H. It is easy to show [4,5] that the following equations hold for an arbitrary operator δQ

$$\langle 0|[\delta Q, [H, Q_\nu^\dagger]]|0\rangle = \omega_\nu \langle 0|[\delta Q, Q_\nu^\dagger]|0\rangle, \tag{3}$$

with $\omega_\nu = E_\nu - E_0$.

Let $|\mathrm{HF}\rangle$ be the Hartree-Fock (HF) ground state of the system where the hole states below the Fermi energy are filled and the particle states above are empty. In the following, we use the indices m, n, p, q and i, j, k, l to indicate, respectively, particle and hole states. To derive the RPA equations, two approximations are made. The first one restrics the operators $Q_\nu^\dagger$ to the space of 1 particle - 1 hole (1p1h) operators, i.e.,

$$Q_\nu^\dagger = \sum_{pi} \left(X_{pi}^{(\nu)} a_p^\dagger a_i - Y_{pi}^{(\nu)} a_i^\dagger a_p\right). \tag{4}$$

The second one is the QBA which amounts to substituting the ground state $|0\rangle$ in Eq. (3) with the uncorrelated state $|\mathrm{HF}\rangle$. An evident inconsistency is introduced since Eq. (3) is obtained assuming that $|0\rangle$ is the vacuum of Q_ν. By using the QBA, the system of Eq. (3), with the elementary excitations $\delta Q \epsilon \{a_i^\dagger a_p, a_p^\dagger a_i\}$, becomes

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^{(\nu)} \\ Y^{(\nu)} \end{pmatrix} = \omega_\nu \begin{pmatrix} G & 0 \\ 0 & -G^* \end{pmatrix} \begin{pmatrix} X^{(\nu)} \\ Y^{(\nu)} \end{pmatrix}, \tag{5}$$

where $X^{(\nu)}$ and $Y^{(\nu)}$ is a short-hand notation for the vectors $X_{pi}^{(\nu)}$ and $Y_{pi}^{(\nu)}$; the RPA matrices are

$$A_{mi,pk} = \langle \mathrm{HF}|[a_i^\dagger a_m, [H, a_p^\dagger a_k]]|\mathrm{HF}\rangle, \tag{6}$$

$$B_{mi,pk} = -\langle \mathrm{HF}|[a_i^\dagger a_m, [H, a_k^\dagger a_p]]|\mathrm{HF}\rangle, \tag{7}$$

and the elements of the norm matrix G are

$$G_{mi,pk} = \langle \mathrm{HF}|[a_i^\dagger a_m, a_p^\dagger a_k]|\mathrm{HF}\rangle = \delta_{ik}\delta_{mp}. \tag{8}$$

A well-known feature of the RPA is that it predicts a harmonic spectrum. It is therefore clear that the RPA is not able to explain the existence of anharmonicities in multiphonon spectra.

One way to obtain a better description of the double excitations of the system is to use the SRPA, where the excitation operators also contain 2p2h terms

$$Q_\nu^\dagger = \sum_{pi} \left(X_{pi}^{(\nu)} a_p^\dagger a_i - Y_{pi}^{(\nu)} a_i^\dagger a_p\right) + \sum_{pimj} \left(X_{pimj}^{(\nu)} a_p^\dagger a_i a_m^\dagger a_j - Y_{pimj}^{(\nu)} a_i^\dagger a_p a_j^\dagger a_m\right). \tag{9}$$

Starting from the equations of motion (3) and using the QBA, one gets in this case

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B}^* & \mathcal{A}^* \end{pmatrix} \begin{pmatrix} \mathcal{X}^{(\nu)} \\ \mathcal{Y}^{(\nu)} \end{pmatrix} = \omega_\nu \begin{pmatrix} \mathcal{G} & 0 \\ 0 & -\mathcal{G}^* \end{pmatrix} \begin{pmatrix} \mathcal{X}^{(\nu)} \\ \mathcal{Y}^{(\nu)} \end{pmatrix}, \tag{10}$$

where

$$\mathcal{A} = \begin{pmatrix} A_{mi,pk} & A_{mi,pqkl} \\ A_{mnij,pk} & A_{mnij,pqkl} \end{pmatrix},$$
$$\mathcal{B} = \begin{pmatrix} B_{mi,pk} & B_{mi,pqkl} \\ B_{mnij,pk} & B_{mnij,pqkl} \end{pmatrix},$$
$$\mathcal{G} = \begin{pmatrix} G_{mi,pk} & 0 \\ 0 & G_{mnij,pqkl} \end{pmatrix},$$

and

$$\mathcal{X}^{(\nu)} = \begin{pmatrix} X_{mi}^{(\nu)} \\ X_{mnij}^{(\nu)} \end{pmatrix}, \qquad \mathcal{Y}^{(\nu)} = \begin{pmatrix} Y_{mi}^{(\nu)} \\ Y_{mnij}^{(\nu)} \end{pmatrix}.$$

The elements $A_{mi,pk}$, $B_{mi,pk}$, and $G_{mi,pk}$ of $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{G}$ are equal to those defined in Eqs. (6), (7), and (8), while the others are

$$A_{mi,pqkl} = \langle \mathrm{HF}|[a_i^\dagger a_m, [H, a_p^\dagger a_q^\dagger a_l a_k]]|\mathrm{HF}\rangle, \tag{11}$$

$$A_{mnij,pk} = \langle \mathrm{HF}|[a_i^\dagger a_j^\dagger a_n a_m, [H, a_p^\dagger a_k]]|\mathrm{HF}\rangle, \tag{12}$$

$$A_{mnij,pqkl} = \langle \mathrm{HF}|[a_i^\dagger a_j^\dagger a_n a_m, [H, a_p^\dagger a_q^\dagger a_l a_k]]|\mathrm{HF}\rangle, \tag{13}$$

$$B_{mi,pqkl} = -\langle \mathrm{HF}|[a_i^\dagger a_m, [H, a_k^\dagger a_l^\dagger a_q a_p]]|\mathrm{HF}\rangle, \tag{14}$$

$$B_{mnij,pk} = -\langle \mathrm{HF}|[a_i^\dagger a_j^\dagger a_n a_m, [H, a_k^\dagger a_p]]|\mathrm{HF}\rangle, \tag{15}$$

$$B_{mnij,pqkl} = -\langle \mathrm{HF}|[a_i^\dagger a_j^\dagger a_n a_m, [H, a_k^\dagger a_l^\dagger a_q a_p]]|\mathrm{HF}\rangle, \tag{16}$$

$$G_{mnij,pqkl} = \langle \mathrm{HF}|[a_i^\dagger a_j^\dagger a_n a_m, a_p^\dagger a_q^\dagger a_l a_k]|\mathrm{HF}\rangle. \tag{17}$$

One can show that

$$G_{mnij,pqkl} = \mathcal{A}(ij)\mathcal{A}(mn)\delta_{ik}\delta_{jl}\delta_{mp}\delta_{nq}, \tag{18}$$

where $\mathcal{A}(ij)$ is the antisymmetrizer for the indices i, j and

$$B_{mi,pqkl} = B_{mnij,pk} = B_{mnij,pqkl} = 0. \tag{19}$$

It has been shown in Refs. [13,14] that QBA is even more severe in SRPA than in RPA. In this work, in order to improve on QBA, we have searched for a correlated state to replace $|\mathrm{HF}\rangle$ in Eqs. (6), (7), and (11)–(16).

In order to get indications on how to improve the QBA, we notice that the standard form of the RPA ground state [i.e., the vacuum of the operators Q_ν of Eq. (4)] is derived under the

approximation that the particle-hole operators $a_m^\dagger a_i$ behave as ideal boson operators, namely,

$$[a_i^\dagger a_p, a_n^\dagger a_j] \approx \delta_{ij}\delta_{pn}, \tag{20}$$

and has the form

$$|\mathrm{RPA}\rangle \propto \exp\left(\frac{1}{2}\sum_{minj} Z_{minj} a_m^\dagger a_i a_n^\dagger a_j\right)|\mathrm{HF}\rangle, \tag{21}$$

where the coefficients Z are determined by

$$\sum_{mi} X_{mi}^{(\nu)*} Z_{minj} = Y_{nj}^{(\nu)*}. \tag{22}$$

An explicit expression of the vacuum $|\mathrm{RPA}\rangle$ cannot be found without resorting to Eq. (20). Wishing to avoid such a bosonic approximation while keeping the correlated state simple enough to be used in realistic calculations, we consider the approximation

$$|\mathrm{RPA}\rangle \approx \mathcal{N}\left(1 + \frac{1}{2}\sum_{minj} Z_{minj} a_m^\dagger a_i a_n^\dagger a_j\right)|\mathrm{HF}\rangle, \tag{23}$$

where $\mathcal{N}$ is a normalization factor, and the operators $a_m^\dagger a_i$ are treated without any bosonic approximation of the type (20). Equation (23) can be viewed as a truncation of Eq. (21). In such a spirit, we make the ansatz that the coefficients Z in Eq. (23) are still determined by Eq. (22). The matrices A, B, and G of both the RPA equations (5) and the SRPA ones (10) are evaluated, in this approximation, by replacing the $|\mathrm{HF}\rangle$ state with the $|\mathrm{RPA}\rangle$ state (23) in Eqs. (6)–(8) and (11)–(17). We notice that when this is done, Eq. (19) is no longer valid. Furthermore, since the matrices A, B, and G depend on Z, i.e., on X and Y, the problem is nonlinear. The procedure we adopt entails solving self-consistently the RPA equations (5) and (22), and keeping the so obtained Z coefficients when we solve the SRPA equations (10).

The present extension of the SRPA shares some similarities with those discussed in Refs. [13,15]. However, in Ref. [13] the Z-coefficients were calculated using the X and Y solutions of the standard RPA, and the matrix elements of A and B connecting 1p1h and 2p2h configurations were neglected. Furthermore, bosonic-type approximations were made when evaluating the matrices A, B, and G. The main difference with respect to Ref. [15] is, that there the Z coefficients were evaluated in first-order Rayleigh-Schrödinger perturbation theory, i.e.,

$$Z_{minj}^{(\mathrm{per})} = \frac{\langle \mathrm{HF}|\hat{V} a_m^\dagger a_i a_n^\dagger a_j|\mathrm{HF}\rangle}{-E_{minj}}, \tag{24}$$

where E_{minj} are the unperturbed energies of the 2p2h excitations and $\hat{V}$ is the residual interaction.

III. MODEL AND RESULTS

In this section, we apply the extensions of the RPA and SRPA discussed in the previous section to an exactly solvable three-level model [11,16]. We check the quality of the results obtained within such extensions by comparing them with the exact ones. Our main aim is to judge to what extent the extended SRPA is adequate to reproduce the anharmonicities present in the two-phonon spectrum. The model consists of three levels of energy ϵ_0, ϵ_1, and ϵ_2. Each of them is 2Ω-fold degenerate, and $N = 2\Omega$ is the total number of fermions in the system. Therefore, in the absence of interaction, the lowest level is fully occupied while the others are empty. This lowest level represents the HF ground state of the system $|\mathrm{HF}\rangle$. A single-particle state is denoted by two quantum numbers j and m, where j labels the shells ($j = 0, 1, 2$) and m specifies the 2Ω substates within each shell. Let us define the operators

$$K_{ij} = \sum_{m=1}^{2\Omega} a_{im}^\dagger a_{jm} \quad (i, j = 0, 1, 2), \tag{25}$$

where $a_{jm}^\dagger$ and a_{jm} are, respectively, the creation and annihilation operators of a fermion in the state (jm).

The operators K satisfy the relations

$$[K_{ij}, K_{kl}] = \delta_{jk}K_{il} - \delta_{il}K_{kj}, \tag{26}$$

$$N = \sum_i K_{ii}, \tag{27}$$

thus forming an SU(3) algebra.

We introduce the Hamiltonian of the system as

$$\begin{aligned} H_f = {} & \sum_{i\neq 0} \epsilon_i K_{ii} + V_0 \sum_{i,j\neq 0} K_{i0}K_{0j} \\ & + V_1 \sum_{i,j\neq 0} (K_{i0}K_{j0} + K_{0j}K_{0i}) \\ & + V_2 \sum_{i,j,k\neq 0} (K_{i0}K_{jk} + K_{kj}K_{0i}) \\ & + V_3 \sum_{i,j,k,l\neq 0} K_{ij}K_{kl}. \end{aligned} \tag{28}$$

The eigenstates and the eigenvalues of the system can be obtained either by using the properties of the SU(3) algebra or by diagonalizing H in the space

$$\left\{|n_1 n_2\rangle = \frac{1}{\sqrt{\mathcal{N}_{n_1 n_2}}}(K_{10})^{n_1}(K_{20})^{n_2}|\mathrm{HF}\rangle\right\}_{0\leqslant n_1+n_2\leqslant 2\Omega}, \tag{29}$$

where $\mathcal{N}_{n_1 n_2}$ are normalization factors.

The results presented in this paper refer to the same set of parameters used in Ref. [16], that is,

$$\begin{aligned} &\epsilon_0 = 0 && \epsilon_1 = \epsilon && \epsilon_2 = 2.5\epsilon \\ &V_0 = -\chi && V_1 = \chi && V_2 = -\chi/2 \\ &V_3 = \chi/10 && 2\Omega = 10. \end{aligned} \tag{30}$$

In this model, the excitation operators of the RPA and SRPA are, respectively (in all formulas below, i and j are greater than zero),

$$Q_\nu^\dagger = \sum_i \left(X_i^{(\nu)}K_{i0} - Y_i^{(\nu)}K_{0i}\right), \tag{31}$$

$$\begin{aligned} Q_\nu^\dagger = {} & \sum_i \left(X_i^{(\nu)}K_{i0} - Y_i^{(\nu)}K_{0i}\right) \\ & + \sum_{i\leqslant j} \left(X_{ij}^{(\nu)}K_{i0}K_{j0} - Y_{ij}^{(\nu)}K_{0i}K_{0j}\right). \end{aligned} \tag{32}$$

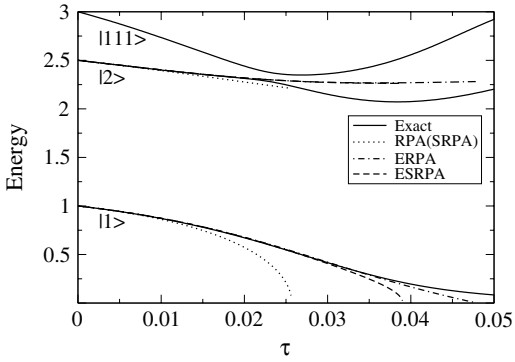

FIG. 1. Excitation energies of the states $|\nu\rangle$ as functions of the strength τ for the set of parameters (30). The results obtained within RPA-SRPA, ERPA, and ESRPA are compared with the exact ones. Energies are expressed in units of ϵ. Also shown are the energies of the state $|111\rangle$ discussed in the text.

In the following, we indicate with the RPA and SRPA the results obtained by using the QBA, namely, by evaluating the matrices in Eqs. (5) and (10) in the $|\mathrm{HF}\rangle$ state. In the present approximation, these matrices are calculated instead in the state

$$|\mathrm{RPA}\rangle = \mathcal{N}\left(1 + \frac{1}{2}\sum_{ij} Z_{ij} K_{i0} K_{j0}\right)|\mathrm{HF}\rangle. \qquad (33)$$

The corresponding extensions of the RPA and SRPA that we introduce in this way will be denoted in the following by ERPA and ESRPA, respectively.

In Figs. 1 and 2 we show the excitation energies as functions of the parameter $\tau = \chi/\epsilon$, calculated within RPA, ERPA, SRPA, and ESRPA. They are compared with the exact excitation energies. It is worth noticing that the exact excitation spectrum in the range of energy considered in Figs. 1 and 2 is actually richer than that shown in these figures. For simplicity, however, with the exception of the state $|111\rangle$ defined below, we only show those states which at $\tau = 0$ are pure 1p1h ($|1\rangle$ and $|2\rangle$) and 2p2h ($|11\rangle$, $|12\rangle$, and $|22\rangle$). In the following, we will refer to them just as 1p1h and 2p2h states. The state $|111\rangle$ of Fig. 1 is instead a state which, at $\tau = 0$, is a pure 3p3h state. For increasing values of τ, this state gets closer and closer to the 1p1h state $|2\rangle$ up to almost crossing it at $\tau \sim 0.025$. Although not shown in Fig. 2 in order not to make the figure too confusing, several other states lie quite close in energy to the 2p2h states $|11\rangle$, $|12\rangle$, and $|22\rangle$. The presence of these extra states of a more complex nature "perturbs" these 2p2h states by leading, for large values of τ, to a more relevant contribution of higher-order ph components. This makes the theoretical description of these states in a RPA-like or SRPA-like formalism more difficult.

As a first result, we notice that going from RPA to SRPA, the energies of the 1p1h states change very little. In Fig. 2, these energies are indistinguishable, and we have plotted them by using the same symbol. Both RPA and SRPA, therefore, are seen to collapse at $\tau \sim 0.026$; but already for $\tau > 0.02$, the energies predicted for the lowest 1p1h state $|1\rangle$ start to deviate significantly from the exact values. A better agreement is found instead in the case of the state $|2\rangle$. As far as the 2p2h states are concerned, we have evaluated the RPA energies of the states $|\nu_1\nu_2\rangle$ as the sum of the energies of the states $|\nu_1\rangle$ and $|\nu_2\rangle$, namely $E_{\nu_1\nu_2} = E_{\nu_1} + E_{\nu_2}$. In these cases, RPA and SRPA show marked differences, the latter approximation leading to a better agreement with the exact results.

Turning now to the extended versions of RPA and SRPA discussed in Sec. II, we notice that both ERPA and ESRPA improve significantly the quality of the approximated results. In particular, the collapse point 16 now shifted to a considerably larger value of τ (0.047 for ERPA and 0.039 for ESRPA), and the energy of the first excited state is reproduced much better than in RPA (SRPA). With reference to this state, we show in Fig. 3 a comparison with the results obtained by the perturbative approach of Ref. [15], both in the case of RPA-like (ERPA-PER) and SRPA-like (ESRPA-PER) calculations. In this approximation, the Z coefficients are evaluated using (24). Similar to what was found in the case of standard RPA and SRPA calculations, the difference between ERPA-PER and ESRPA-PER results for the state $|1\rangle$ is very small and cannot be appreciated in the figure (where we explicitly show only the ERPA-PER results). One observes in this case that the perturbative calculation improves upon RPA (SRPA) by

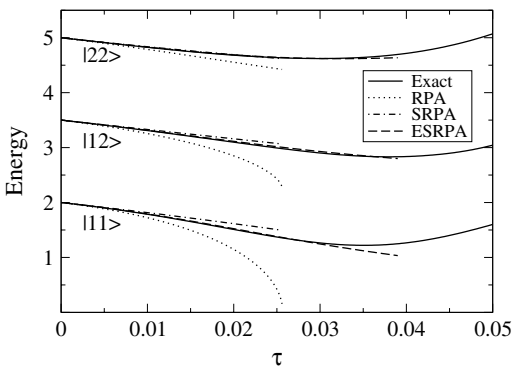

FIG. 2. Same as Fig. 1, but for the states $|\nu_1\nu_2\rangle$. RPA energies are calculated as the sum of the energies of the states $|\nu_1\rangle$ and $|\nu_2\rangle$, namely $E_{\nu_1\nu_2} = E_{\nu_1} + E_{\nu_2}$.

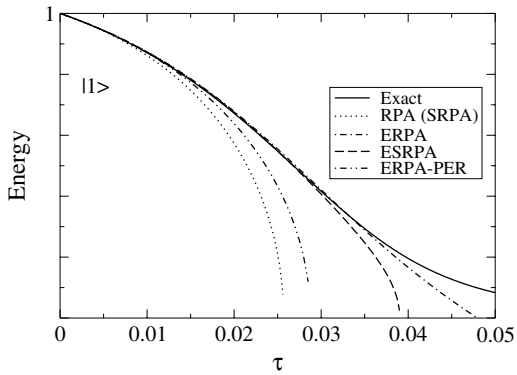

FIG. 3. Excitation energies of the $|1\rangle$ state as functions of the strength τ for the set of parameters (30). The results obtained within RPA (SRPA), ERPA, ESRPA, and ERPA-PER are compared with the exact ones. Energies are expressed in units of ϵ.

exhibiting, in particular, a collapse point at $\tau \sim 0.028$ without reaching, however, the quality of our results. As far as the remaining 1p1h and 2p2h states are concerned, the difference between our approach and the perturbative one is less evident (it is well understood that our calculations extend over a wider range of τ).

It is of interest to look also at the energy weighted sum rules (EWSR). Let us recall that if $|\nu\rangle$ and $|0\rangle$ are exact eigenstates of the Hamiltonian H with energies E_ν and E_0, then for any one-body operator F the following identity holds:

$$\sum_\nu (E_\nu - E_0)|\langle\nu|F|0\rangle|^2 = \frac{1}{2}\langle 0|[F^\dagger,[H,F]]|0\rangle. \qquad (34)$$

The well-known Thouless theorem [17] states that the above equality is satisfied if one evaluates the l.h.s. within the RPA and the mean value of the double commutator in the r.h.s. in the $|\mathrm{HF}\rangle$ state. In this sense, the RPA preserves the EWSR. The same is true for the SRPA (Ref. [12]). One can easily show that the identity (34) is exactly satisfied in our approximation if one keeps only the particle-hole components of the operator F. Vice versa, when one uses its complete expression

$$F = \sum_{\alpha\beta} f_{\alpha\beta} K_{\alpha\beta} \qquad (35)$$

with α and β running over all single-particle states (below and above the Fermi level), some violations are present. In Fig. 4, we show, as a function of τ, the r.h.s. of Eq. (34) calculated in the correlated state (33) and the l.h.s. in ERPA and ESRPA. The calculations are done by assuming that all $f_{\alpha\beta} = 1$.

One sees that the violations increase with τ. At the ERPA level, they reach quite large values, for instance, $\sim$35% at $\tau = 0.035$. A significant improvement is obtained within the ESRPA, the violation being $\sim$10% at the same interaction strength. This is very satisfactory in view of the fact that within other extensions of the RPA, the violations are more severe [16]. The large violations of the EWSR found in the ERPA can be traced back to the fact that, as discussed in Ref. [16], all components of F enter in the r.h.s. of Eq. (34), while when the excitation operators $Q_\nu^\dagger$ are of the RPA type, only 1p1h terms of F contribute to the l.h.s. This is no longer true when $Q_\nu^\dagger$ is of the SRPA type. The approach proposed in Ref. [16] entailed considering RPA-type operators $Q_\nu^\dagger$ which also included $K_{\alpha\beta}$

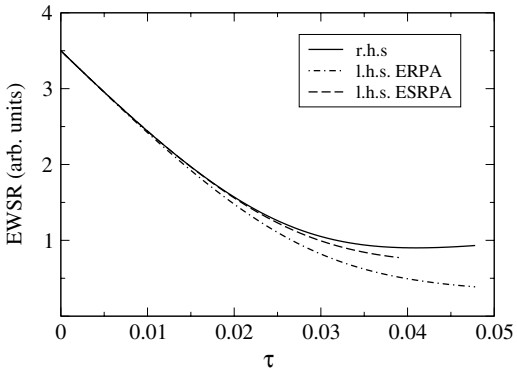

FIG. 4. R.h.s. of Eq. (34) calculated in the correlated state (33) and the l.h.s. evaluated in ERPA and ESRPA.

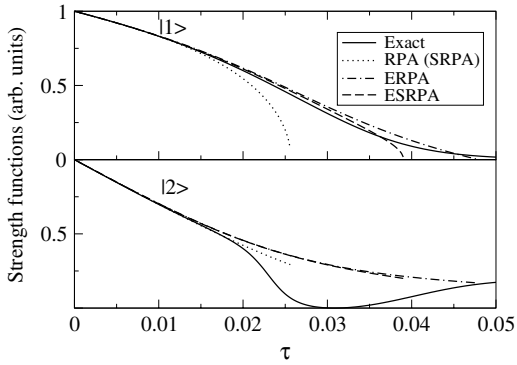

FIG. 5. Strength functions, as functions of the strength τ for the set of parameters (30), for the states $|1\rangle$ and $|2\rangle$. Results obtained within the RPA-SRPA, ERPA, and ESRPA are compared with the exact ones.

terms. It was found that the EWSR were exactly satisfied, but one could not avoid the appearance of a spurious state.

In Figs. 5 and 6, we show the strength functions $|\langle\nu|F|0\rangle|^2$. As far as the 1p1h states are concerned (Fig. 5), the RPA (SRPA) results show large deviations from the exact ones only for τ approaching the collapse point. In the case of 2p2h states (Fig. 6), the SRPA predictions are instead very poor already for values of τ well below the collapse point. The agreement within the ERPA and ESRPA is considerably better although significant deviations are observed also in this case for large τ. As already noticed, however, in this region the structure of these 1p1h and 2p2h states is influenced by the presence of other states of a more complex nature which lie quite close in energy. This could also explain the "odd" behavior exhibited by the exact results relative to the states $|2\rangle$, $|12\rangle$, and $|22\rangle$ for large τ. A more appropriate treatment of these high-lying states would involve diagonalizing the Hamiltonian in a multiphonon space. In Ref. [10], an approach of this kind was attempted, although in a bosonic formalism, within the same model. The conclusion was that in order to reproduce the energies of states which in the harmonic limit would correspond to two quanta excitations, it was necessary to perform a diagonalization in a space which included up to four phonons. Calculations of this kind would be quite difficult in a realistic case, so we did not perform them in the present work.

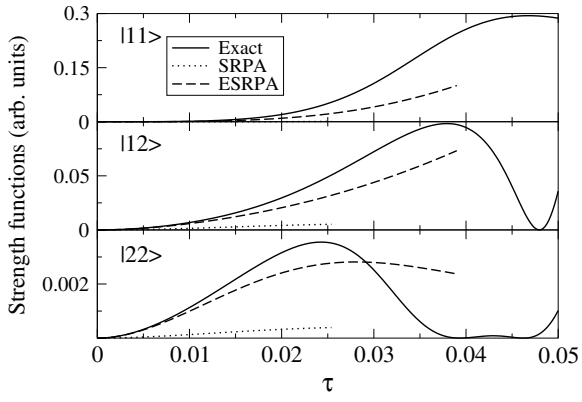

FIG. 6. Same as Fig. 5, but for states $|11\rangle$, $|12\rangle$, and $|22\rangle$.

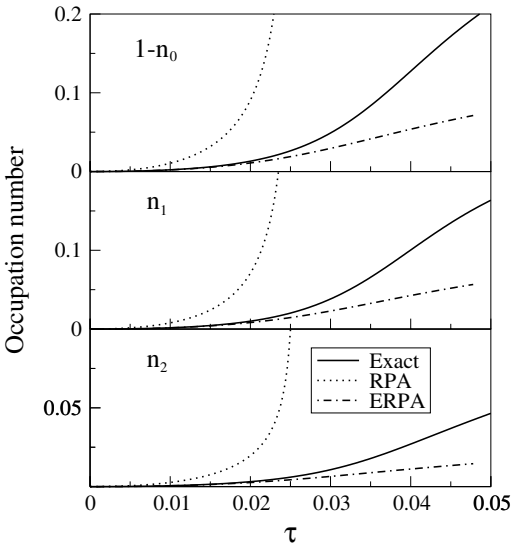

FIG. 7. Exact occupation numbers compared with the RPA and ERPA ones.

Further information on the quality of our approach can be obtained by looking at the occupation numbers. In Fig. 7, we compare the exact values with the RPA and ERPA ones. For the RPA occupation numbers, we used the expressions

$$n_0 = 1 - \frac{1}{2}\sum_{\nu,i} \left|Y_i^{(\nu)}\right|^2 \tag{36}$$

and

$$n_i = \frac{1}{2}\sum_{\nu} \left|Y_i^{(\nu)}\right|^2, \tag{37}$$

where the factor $\frac{1}{2}$, not present in the standard RPA expression, has been introduced following the suggestion of Refs. [18,19]. Within the ERPA, they have been evaluated as the expectation values of $K_{\alpha\alpha}$ in the ground state (33) with the Z coefficients determined using Eq. (22). We notice that the RPA results deviate greatly from the exact ones already for τ well below the collapse point. Within the ERPA, the quality of the agreement improves considerably. It is worthy remarking that while the RPA strongly overestimates the correlations in the ground state, the ERPA underestimates them but to a much less extent.

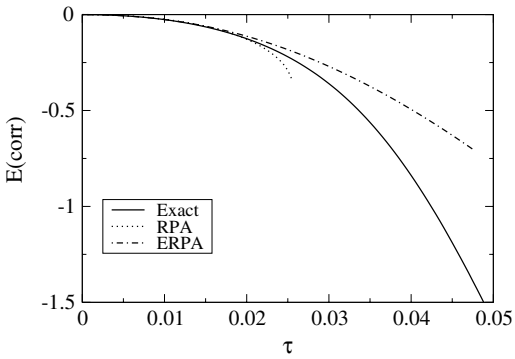

FIG. 8. Exact ground state correlation energy compared with the RPA and the ERPA ones. Energies are in units of ϵ.

This is also evident in Fig. 8, where we plot the RPA ground state correlation energy [4] together with the ERPA and exact ones.

IV. SUMMARY AND CONCLUSIONS

In this work, we have discussed an extension of the RPA and SRPA. The key point of such an extension has been the overcoming of the QBA by replacing the (uncorrelated) $|\mathrm{HF}\rangle$ state with a correlated one in the derivation of the RPA and SRPA equations. The latter state has been assumed to contain up to 2p-2h configurations, whose amplitudes have been determined by self-consistently solving new extended RPA-type equations. In this sense, the correlated state so introduced can be viewed as a truncation of the RPA ground state. Unlike the RPA case, however, no bosonic-type approximations have been introduced when handling particle-hole operators. We have investigated, both in the RPA and SRPA, the effects of releasing the QBA in the way just described. As a testing ground, we have taken the three-level Lipkin model and compared exact calculations with those performed within the RPA, SRPA, and their extensions ERPA and ESRPA, respectively. The comparison has concerned ground state correlation energies, excitation energies, strength functions, and occupation numbers.

Furthermore, we have also examined sum rules. As a general result, we have observed that the ERPA considerably improves the RPA by leading, in particular, to a relevant shift of the collapse point to higher values of the interaction strength as well as to a better description of the spectrum. ESRPA calculations are characterized by a collapse point close to the ERPA one but exhibit a much richer spectrum, being able, in particular, to reproduce also those states which, in the standard RPA formalism, would correspond to double phonon excitations. A significant improvement of the ESRPA over the ERPA has also been observed at the level of the EWSR. As far as the ground state (identical by construction in the ERPA and ESRPA) is concerned, the exact occupation numbers are much better reproduced in the ERPA than in the RPA. One observes, in particular, a tendency of the present approximation to underestimate the ground state correlations (differently from the RPA, which severely overestimates them). This is also evidenced in the behavior of the correlation energies. In conclusion, all the results emerging from the present analysis testify to the good quality of the extension of the SRPA that we have discussed and, thanks to the not very heavy computational effort that it requires, encourage its application to more realistic systems.

APPENDIX A

As discussed in Sec. II, the extension proposed in this paper entails the evaluation of the matrices A, B, and G in the $|\mathrm{RPA}\rangle$ state (33). Of course, the new expressions of these matrices become more involved. As an example, in the following we report the explicit expression of the norm matrix G in the case of the three-level Lipkin model. In the standard RPA and

SRPA, we have

$$G_{i,j} = \frac{1}{2\Omega}\langle \mathrm{HF}|[K_{0i}, K_{j0}]|\mathrm{HF}\rangle = \delta_{ij}, \tag{A1}$$

and

$$\begin{aligned} G_{ij,kl} &= \frac{1}{2\Omega(2\Omega-1)}\langle \mathrm{HF}|[K_{0i}K_{0j}, K_{k0}K_{l0}]|\mathrm{HF}\rangle \\ &= \mathcal{J}(ij)\delta_{lj}\delta_{ik}, \end{aligned} \tag{A2}$$

where $\mathcal{J}(ij)$ is the symmetrizer for the indices i, j.

In the ERPA and ESRPA, we evaluate the above matrices by replacing $|\mathrm{HF}\rangle$ with the $|\mathrm{RPA}\rangle$ state (33)and obtain

$$\begin{aligned} G_{i,j} &= \frac{1}{2\Omega}\langle \mathrm{RPA}|[K_{0i}, K_{j0}]|\mathrm{RPA}\rangle \\ &= \frac{1}{2\Omega}(\delta_{ij}N_{00} - N_{ij}), \end{aligned} \tag{A3}$$

and

$$\begin{aligned} G_{ij,kl} &= \frac{1}{2\Omega(2\Omega-1)}\langle \mathrm{RPA}|[K_{0i}K_{0j}, K_{k0}K_{l0}]|\mathrm{RPA}\rangle \\ &= \frac{1}{2\Omega(2\Omega-1)}\mathcal{J}(ij)\mathcal{J}(kl)(\delta_{lj}(N_{0ik000} + N_{ki00}) - N_{0ik0lj} \\ &\quad - \frac{1}{2}(\delta_{li}\delta_{kj}(N_{0000} + N_{00}) + N_{kjli} - \delta_{li}N_{kj})), \end{aligned} \tag{A4}$$

where

$$N_{\alpha\beta} = \langle \mathrm{RPA}|K_{\alpha\beta}|\mathrm{RPA}\rangle,$$

$$N_{\alpha\beta\gamma\delta} = \langle \mathrm{RPA}|K_{\alpha\beta}K_{\gamma\delta}|\mathrm{RPA}\rangle,$$

$$N_{\alpha\beta\gamma\delta\sigma\nu} = \langle \mathrm{RPA}|K_{\alpha\beta}K_{\gamma\delta}K_{\sigma\nu}|\mathrm{RPA}\rangle,$$

with $\alpha, \beta, \gamma, \delta, \sigma, \nu = 0, 1, 2, \ldots$.

For example, we have

$$\begin{aligned} N_{00} &= \langle \mathrm{RPA}|K_{00}|\mathrm{RPA}\rangle \\ &= 2\Omega\mathcal{N}^2\left(1 + \frac{\Omega}{2\Omega-1}\sum_{kl}|Z_{kl}|^2\right), \end{aligned}$$

$$\begin{aligned} N_{ij} &= \langle \mathrm{RPA}|K_{ij}|\mathrm{RPA}\rangle \\ &= \frac{2\Omega}{2\Omega-1}\mathcal{N}^2\sum_{kl}Z^*_{il}Z_{kj}, \end{aligned}$$

$$\begin{aligned} N_{ij00} &= \langle \mathrm{RPA}|K_{ij}K_{00}|\mathrm{RPA}\rangle \\ &= \frac{4\Omega(\Omega-1)}{2\Omega-1}\mathcal{N}^2\sum_{k}Z^*_{ik}Z_{kj}, \end{aligned}$$

where $i, j = 1, 2$.

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