Many-body correlations in a multistep variational approach

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We discuss a multistep variational approach for the study of many-body correlations. The approach is developed in a boson formalism (bosons representing particle-hole excitations) and based on an iterative sequence of diagonalizations in subspaces of the full boson space. The purpose of these diagonalizations is that of searching for the best approximation of the ground state of the system. The procedure also leads us to define a set of excited states and, at the same time, of operators which generate these states as a result of their action on the ground state. We examine the cases in which these operators carry one-particle one-hole and up to two-particle two-hole excitations. We also explore the possibility of associating bosons to Tamm-Dancoff excitations and of describing the spectrum in terms of only a selected group of these. Tests within an exactly solvable three-level model are provided. [S0556-2813(99)00512-9]

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I. INTRODUCTION

Developing reliable microscopic approaches for the description of correlations in quantum many-body systems is a field of active research in various branches of physics. A preeminent role in this field has been traditionally played by the random-phase approximation (RPA) [1]. Over the years, however, several attempts [2–16] have also been made to overcome the natural limitations of this theory related, in particular, to its lack of an internal consistency.

In a recent publication [16], with reference to the β-decay physics and working in a quasiparticle formalism, we have discussed an approach aimed at improving the quality of the standard quasiparticle RPA calculations usually made in this field. The basic point of this approach has been that of searching first for the best approximation of the ground state. In order to do this we have started with an initial *ansatz* for this state and we have tried to improve this approximation through a series of minimizations which modified the structure of the state at each step. Excited states have, then, been constructed by acting with an RPA-like phonon on the ground state and fixing the variables of this phonon via the minimization of the energy. Tests of the procedure have proved to be quite encouraging. In the present work, however, we present an evolution of this method which we believe to be more effective and simpler to apply in realistic cases.

The approach is developed in a boson formalism. As a preliminary step, then, a boson space will be defined where bosons identify particle-hole excitations and a mapping procedure will allow the transformation of fermion operators onto their images in this boson space. Similar to the previous work [16], the basic point of the approach will consist in searching first for the best approximation of the ground state. Differently from the mentioned case, however, this will be achieved by means of an iterative sequence of diagonalizations in subspaces of the full boson space. As a further and important difference from the case of Ref. [16], as a result of this sequence of diagonalizations, a set of operators will also be generated which by acting on the ground state of the system will define a set of excited states. We will consider two cases: the case in which these operators carry only one-particle one-hole ($1p$-$1h$) excitations and the case in which they include up to two-particle two-hole ($2p$-$2h$) excitations. In both cases the comparison with exact calculations within a schematic model will allow us to judge the quality of the approximations. As a schematic model we have chosen the SU(3) model [17–19].

In the second part of the work, we will reformulate the fermion-boson correspondence and identify bosons with properly chosen *collective* particle-hole excitations. Then, what is more interesting, we will explore the possibility of describing at least partially the spectrum of the system in terms of only a selected group of these bosons. Once again we will first search for the best approximation of the ground state and we will then construct excited states carrying up to $1p$-$1h$ and $2p$-$2h$ excitations. Tests within the schematic model will be provided also in this case.

The paper is organized as follows. In Sec. II, we will describe the basic points of the procedure limiting ourselves to the case of $1p$-$1h$ excitations. In Sec. III, we will provide some applications within the SU(3) model. In Sec. IV, we will consider an extension of the procedure to include $2p$-$2h$ excitations. In Sec. V, we will examine the case of bosons as collective particle-hole excitations. Finally, in Sec. VI, we will summarize the results and give some conclusions. The Appendix will be reserved to describe some details of the mapping procedure.

II. THE PROCEDURE: $1p$-$1h$ EXCITATIONS

To simplify the notation, we will illustrate the procedure directly within the exactly solvable model which has been used for our tests. This model, the so-called SU(3) model, was first discussed by Li *et al.* [17] and has been used more recently by Matsuo and Matsuyanagi [18] and Takada *et al.* [19] to test some approximation schemes. The model consists of three 2Ω-fold degenerate single-particle shells which are occupied 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 2Ω substates within the shell. The creation and annihilation operators of a fermion in a state (j,m) are defined by $a^{\dagger}_{jm}$ and a_{jm}, respectively.

Let us consider the operators

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

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

$$[K_{ij},K_{kl}]=\delta_{jk}K_{il}-\delta_{il}K_{kj}. \tag{2}$$

It is assumed that 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 [19]

$$\begin{aligned} H_F=&\sum_{i=1,2}\epsilon(i)K_{ii}+\sum_{i,j=1,2}V_x(i,j)K_{i0}K_{0j}\\ &+\frac{1}{2}\sum_{i,j=1,2}V_v(i,j)(K_{i0}K_{j0}+K_{0j}K_{0i})\\ &+\sum_{i,j,k=1,2}V_y(i,j,k)(K_{i0}K_{jk}+K_{kj}K_{0i}), \end{aligned} \tag{3}$$

where the coefficients are real and obey the symmetry conditions $V_x(i,j)=V_x(j,i)$ and $V_v(i,j)=V_v(j,i)$. The eigenstates of H_F are constructed by diagonalizing it in the space

$$F=\left\{ |n_1n_2\rangle=\frac{1}{\sqrt{\mathcal{N}_{n_1n_2}}}(K_{10})^{n_1}(K_{20})^{n_2}|0\rangle \right\}_{0\leqslant n_1+n_2\leqslant 2\Omega}, \tag{4}$$

where $\mathcal{N}_{n_1n_2}$ are normalization factors.

As in Ref. [16], we will work in a boson formalism. To begin, then, we define the boson space

$$B=\left\{ |n_1n_2)=\frac{1}{\sqrt{n_1!n_2!}}(b^{\dagger}_1)^{n_1}(b^{\dagger}_2)^{n_2}|0) \right\}_{0\leqslant n_1+n_2\leqslant 2\Omega}, \tag{5}$$

where the operators $b^{\dagger}_i$ obey the standard boson commutation relations

$$[b_i,b^{\dagger}_j]=\delta_{ij}, \quad [b_i,b_j]=0, \tag{6}$$

and $|0)$ is the boson vacuum. As evident from a glance at Eqs. (4) and (5), a one-to-one correspondence exists between the states of F and B, the boson operators $b^{\dagger}_i$ playing the role of the excitation operators K_{i0}, and the boson vacuum $|0)$ replacing the HF state $|0\rangle$. As anticipated in the Introduction, however, in Sec. V we will also examine a different correspondence and so a different meaning to attribute to these boson operators.

The mapping procedure to construct boson images of fermion operators is the same discussed in previous works [12,16] and it is based on the requirement that corresponding matrix elements in F and B be equal. The procedure is, therefore, of the Marumori-type. We will give further details in the Appendix. Here, we simply say that, in correspondence with the Hamiltonian H_F (3), we introduce a Hermitian boson Hamiltonian H_B which contains up to five-boson terms. This has therefore the general form

$$\begin{aligned} H_B=&\alpha+\sum_i\beta_i(b^{\dagger}_i+\text{H.c.})+\sum_{ij}\gamma_{ij}b^{\dagger}_ib_j+\sum_{i\leqslant j}\phi_{ij}(b^{\dagger}_ib^{\dagger}_j+\text{H.c.})+\sum_{i\leqslant j}\sum_k\epsilon_{ijk}(b^{\dagger}_ib^{\dagger}_jb_k+\text{H.c.})+\sum_{i\leqslant j}\sum_{k\leqslant l}\delta_{ijkl}b^{\dagger}_ib^{\dagger}_jb_kb_l\\ &+\sum_{i\leqslant j\leqslant k}\sum_l\rho_{ijkl}(b^{\dagger}_ib^{\dagger}_jb^{\dagger}_kb_l+\text{H.c.})+\sum_{i\leqslant j\leqslant k}\sum_{l\leqslant m}\tau_{ijklm}(b^{\dagger}_ib^{\dagger}_jb^{\dagger}_kb_lb_m+\text{H.c.}). \end{aligned} \tag{7}$$

To illustrate the iterative sequence of diagonalizations on which our approach is based we start by introducing an arbitrary boson state $|\Psi^{(0)}_0)$. We consider this as a zeroth-order approximation of the ground state and we assume $|\Psi^{(0)}_0)=1/\sqrt{3}[|0)+b^{\dagger}_1|0)+b^{\dagger}_2|0)]$. Let us then consider the space

$$B^{(1)}\equiv\{|\Psi^{(0)}_0),b^{\dagger}_i|\Psi^{(0)}_0),b_i|\Psi^{(0)}_0)\}_{i=1,2} \tag{8}$$

and diagonalize H_B in this space. $B^{(1)}$ is, in general, considerably smaller than the full boson space B. In our calculations, for instance, we have assumed $2\Omega=10$ and this implies that the space B can have up to ten-boson states, while $B^{(1)}$ contains only up to two-boson states. However, if $|\Psi^{(1)}_0)$ denotes the lowest eigenstate resulting from this diagonalization, one can only expect that $|\Psi^{(1)}_0)$ will provide an approximation of the ground state better than (or, at worst, equal to) $|\Psi^{(0)}_0)$. This is due to the fact that we are allowing the new state to have more components than $|\Psi^{(0)}_0)$ and that the coefficients of $|\Psi^{(1)}_0)$ are fixed to guarantee the lowest energy of the state. We define $|\Psi^{(1)}_0)$ as the first-order approximation of the ground state.

As a next step, we consider the space

$$B^{(2)}\equiv\{|\Psi^{(1)}_0),b^{\dagger}_i|\Psi^{(1)}_0),b_i|\Psi^{(1)}_0)\}_{i=1,2} \tag{9}$$

and diagonalize H_B in this space. If $|\Psi^{(2)}_0)$ is the lowest

eigenstate resulting from this diagonalization, the above arguments lead us to expect that also $|\Psi_0^{(2)}\rangle$ will be better than $|\Psi_0^{(1)}\rangle$. We define $|\Psi_0^{(2)}\rangle$ as the second-order approximation of the ground state. The procedure can go on as many times as one wishes. By performing a sequence of diagonalizations in spaces whose dimensionality remains unchanged (and much smaller than that of the full boson space), one can construct approximations of the ground state which improve step by step.

It turns out to be interesting to reformulate the procedure just described as follows. We define the operator

$$(Q_0^\dagger)^{(\nu)} = \sum_i X_i^{(\nu)} b_i^\dagger + \sum_i Y_i^{(\nu)} b_i + Z^{(\nu)}. \tag{10}$$

It is, then,

$$|\Psi_0^{(0)}\rangle = (Q_0^\dagger)^{(0)}|0\rangle, \tag{11}$$

with $X_i^{(0)} = Z^{(0)} = 1/\sqrt{3}$ (the coefficients $Y_i^{(0)}$ remain undetermined in this case). Similarly, one can define an operator $(Q_0^\dagger)^{(1)}$ such that

$$|\Psi_0^{(1)}\rangle = (Q_0^\dagger)^{(1)}|\Psi_0^{(0)}\rangle, \tag{12}$$

and so on for all other approximations. In general, if $|\Psi_0^{(k)}\rangle$ denotes the kth approximation of the ground state, one can write

$$|\Psi_0^{(k)}\rangle = (Q_0^\dagger)^{(k)}|\Psi_0^{(k-1)}\rangle = (Q_0^\dagger)^{(k)}(Q_0^\dagger)^{(k-1)}\cdots(Q_0^\dagger)^{(0)}|0\rangle. \tag{13}$$

Therefore, $|\Psi_0^{(k)}\rangle$ is a product of $k+1$ operators $Q^\dagger$ of the type (10), k corresponding to the k diagonalizations in the $B^{(k)}$ subspaces plus the operator $(Q_0^\dagger)^{(0)}$ corresponding to the starting ansatz $|\Psi_0^{(0)}\rangle$. Concerning this state, some comments are necessary to justify its use. In principle, one could have started with a diagonalization similar to all the other ones, namely in a space of the type (8) where $|\Psi_0^{(0)}\rangle \equiv |0\rangle$. However, the coefficients β_i of the boson Hamiltonian (7) are nothing but the matrix elements of H_F between the HF state $|0\rangle$ and the 1p-1h states $K_{i0}|0\rangle$ (see the Appendix). These coefficients turn out to be zero in our model and the same would happen in a realistic case. In consequence of that no mixing is possible between the states $|0\rangle$ and $b_j^\dagger|0\rangle$ and so a diagonalization in the space $\{|0\rangle, b_j^\dagger|0\rangle\}$ could generate (what indeed happens in our model) the boson vacuum $|0\rangle$ as the lowest eigenstate. This would lead to a crash of the iterative mechanism.

Once a sufficient number of iterations has been performed the procedure is expected to reach convergence. If this is the case, any diagonalization beyond a given one, say the kth one, will have to leave the results unmodified. This necessarily implies that the operator $(Q_0^\dagger)^{(k+1)}$ which will emerge from the $(k+1)$th diagonalization will have coefficients

$$X_i^{(k+1)} = Y_i^{(k+1)} = 0, \quad Z^{(k+1)} = \pm 1. \tag{14}$$

Convergence of the procedure therefore means convergence towards these values of the coefficients X, Y, and Z.

As a result of the same $(k+1)$th diagonalization, besides the operator $(Q_0^\dagger)^{(k+1)}$, one will also obtain the operators $(Q_i^\dagger)^{(k+1)}$ associated to the remaining eigenstates. The number of these eigenstates is (up to) $2N$, where N is the number of the 1p-1h excitations ($N=2$ in our model). If we call $|\text{g.s.}\rangle$ our best approximation for the ground state, i.e., $|\text{g.s.}\rangle \equiv |\Psi_0^{(k)}\rangle$, these further eigenstates can be written as

$$|\Psi_i^{(k+1)}\rangle \equiv (Q_i^\dagger)^{(k+1)}|\text{g.s.}\rangle \quad (i=1,\ldots,2N). \tag{15}$$

Keeping in mind that $(Q_0^\dagger)^{(k+1)} = \pm 1$, one has that

$$(\text{g.s.}|(Q_i^\dagger)^{(k+1)}|\text{g.s.}\rangle = 0 \quad (i=1,\ldots,2N). \tag{16}$$

Moreover, the operators $(Q_i^\dagger)^{(k+1)}$ satisfy the orthogonality conditions

$$(\text{g.s.}|(Q_i)^{(k+1)}(Q_j^\dagger)^{(k+1)}|\text{g.s.}\rangle = \delta_{ij} \quad (i,j=1,\ldots,2N). \tag{17}$$

This procedure, therefore, leads us to define a set of operators $(Q_i^\dagger)^{(k+1)}$ whose action on the ground state gives rise to a set of excited states which, considering the nature of the operators (10), all carry excitations of the type 1p-1h.

This way of representing the excited states shows evident similarities to that of the RPA. The operators $Q^\dagger$ (10) indeed remind us (although in a boson formalism) of the phonon operators of the RPA. However, important differences do appear between the two approaches. While in the RPA the ground state is defined as the vacuum of the operators Q, this is not true in this approach. Here, a sequence of the operations of the variational type leads us to construct both the ground state and the set of operators $Q^\dagger$ which define the excited states. In the RPA, instead, the operators $Q^\dagger$ are first constructed by solving some equations (not of variational type) and an explicit expression for the ground state can be subsequently derived. We also notice that the $Q^\dagger$'s (10), although constructed in terms of bosons, are not real bosons themselves since they do not obey standard commutation relations of the type (6). This is not the case in the RPA where, at least in the standard quasiboson approximation, the operators $Q^\dagger$ are treated as bosons.

Before concluding this section, some comments are necessary about the violation of the Pauli principle, which is always a risk whenever dealing with boson transformations. Although the sequence of diagonalizations described above can be extended as long as one wishes and so one can, in principle, form states of the type (13) which involve any number of operators $Q^\dagger$, not all the components of these states may be ''physical.'' In other words, there could be components, the so-called ''spurious'' components, which have not a counterpart in the fermion space F. In our model, for instance, whenever acting with more than 2Ω operators $Q^\dagger$ on the boson vacuum $|0\rangle$ one would form states having, among the others, components with more than 2Ω operators $b_j^\dagger$ and these are all spurious components.

In order to properly take into account these components, one should, in principle, perform the diagonalizations in spaces of the type

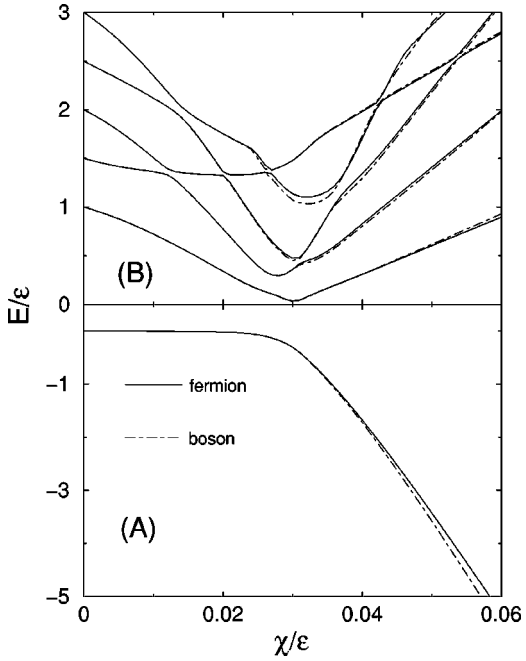

FIG. 1. Ground-state energy (A) and excitation energies of the lowest five states (B) as functions of the strength χ/ϵ. The solid lines are obtained by diagonalizing H_F (3) in F (4), while dot-dashed lines refer to H_B (7) in B (5).

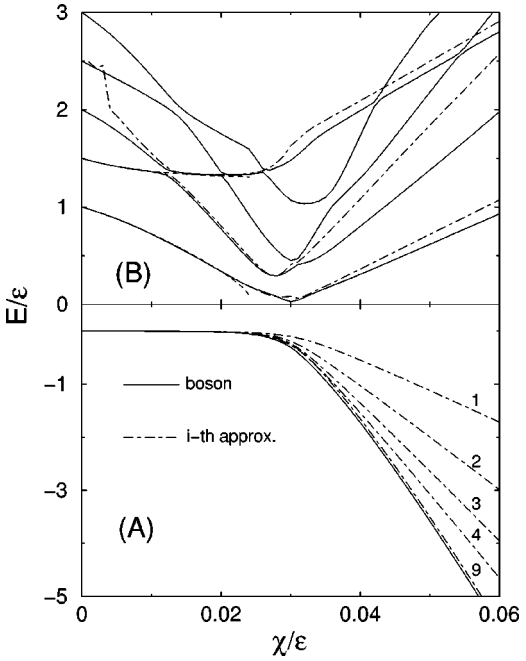

FIG. 2. Ground-state energy (A) and excitation energies of the lowest five states (B) as functions of the strength χ/ϵ. The solid lines are obtained by diagonalizing H_B (3) in B (4) while dot-dashed lines are obtained with the procedure described in Sec. II (only 1*p*-1*h* excitations). The numbers label different orders of approximation. The dashed lines (B) show the RPA one-phonon energies.

$$B^{(k)}=\{|\Psi_0^{(k-1)}),\hat{I}_B b_i^\dagger|\Psi_0^{(k-1)}),b_i|\Psi_0^{(k-1)})\}_{i=1,2}, \quad (18)$$

where we have introduced the identity operator $\hat{I}_B$ of the boson space B. This is rather simple to do in the model under discussion. However, as we will see in the next sections, the rate of convergence of the procedure in the cases examined has always been such as to make the problem associated to the occurrence of these spurious components unimportant in these calculations.

III. RESULTS

The calculations we are going to describe refer to the following choice of the parameters: $2\Omega=10$, $\epsilon(1)=\epsilon$, $\epsilon(2)=1.5\epsilon$, $V_x(i,j)=-2\chi$, $V_v(i,j)=\frac{1}{2}\chi$, and $V_y(i,j,k)=-\frac{3}{4}\chi$ $(i,j,k,=1,2)$. Both ϵ and χ are parameters expressed in units of energy.

In Fig. 1, the solid lines show the ground-state energy (A) and the excitation energies of the lowest five states (B), in units of ϵ, as functions of the strength χ/ϵ. These results are obtained by diagonalizing H_F in F. Dot-dashed lines show the equivalent results for H_B in B. The agreement between the fermion and boson spectra guarantees the very good quality of the boson image H_B.

In Fig. 2, lower part, we show the ground-state energies corresponding to different orders of approximation as indicated by the numbers which label the dot-dashed lines. For comparison, we plot (solid line) the energies which result from the diagonalization of H_B in B since this represents the best one can hope to reproduce in this approach. The same will be done in all the next figures. As seen in Fig. 1, however, fermion and boson energies differ very little from each other. A clear improvement of the quality of the approximation is observed in correspondence with the increasing of its order.

Still in Fig. 2, the upper part, dot-dashed lines show the spectrum obtained within this approach (the spectrum is found in correspondence with the best approximation of the ground state shown in the lower part of the figure). For comparison we also show the energies of the two one-phonon RPA states (dashed lines). The RPA undergoes a collapse as soon as the ground-state energy starts deviating significantly from zero ($\chi/\epsilon\approx 0.024$). The same states, but within the whole range of χ/ϵ, are obtained within our approach and they reproduce well the exact ones. It is worth noting that our approximated spectrum is formed by four excited states (with the only exception of very small values of the strength χ/ϵ where they can become two) as opposed to the two states of RPA. Already for a strength $\chi/\epsilon\gtrsim 0.014$ the second one-phonon RPA state actually corresponds to the third excited state within the present approach. The fourth approximate state lies higher in energy and has not been reported in the figure.

IV. 2*p*-2*h* EXCITATIONS

The same procedure discussed in Sec. II and involving only 1*p*-1*h* excitations can be extended in a natural way to include 2*p*-2*h* excitations as well. The basic difference consists in performing each diagonalization of the iterative sequence in spaces of the type

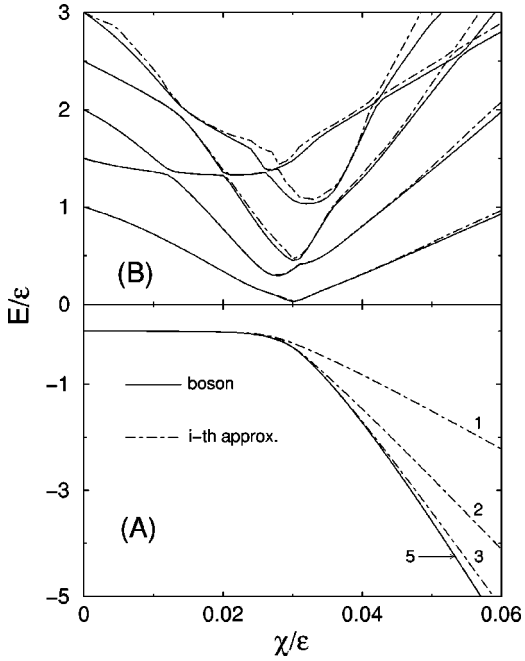

FIG. 3. The same as in Fig. 2 but dot-dashed lines refer now to calculations involving up to 2*p*-2*h* excitations.

$$B^{(k)}=\{|\Psi_0^{(k-1)}),b_i^\dagger|\Psi_0^{(k-1)}),b_i^\dagger b_j^\dagger|\Psi_0^{(k-1)}),\\ b_i|\Psi_0^{(k-1)}),b_ib_j|\Psi_0^{(k-1)})\}_{i\leqslant j=1,2}. \tag{19}$$

Moreover, differently from the case of Sec. II, there is no more need for an initial ansatz for the ground state. The iterative procedure simply begins by performing a diagonalization in a space $B^{(1)}$ of the form (19) where $|\Psi_0^{(0)})\equiv|0)$.

To evaluate the role of these additional excitations in the structure of the spectrum, we have performed calculations similar to those shown in Fig. 2. The new results are reported in Fig. 3. For what concerns the ground-state energy one observes a very good agreement and a faster convergence with respect to the 1*p*-1*h* case. Concerning the spectra of the lowest five excited states, besides the two ''one-phonon'' states discussed in the previous section, also the remaining states are now well reproduced (as for Fig. 2, this spectrum refers to the best approximation of the ground state as indicated in the lower part of the figure). As expected, then, the inclusion of 2*p*-2*h* excitations considerably improves the quality of the approximate spectrum.

V. BOSONS AS COLLECTIVE PARTICLE-HOLE EXCITATIONS

When performing the boson mapping we have established a one-to-one correspondence between the states $|n_1n_2\rangle$ and $|n_1n_2)$ defined in the Eqs. (4) and (5), respectively. In such a correspondence, bosons $b_j^\dagger$ are images of the 1*p*-1*h* operators K_{j0}. However, as already anticipated, this is not the only possibility of correspondence. To show an alternative choice, we proceed as in Takada *et al.* [19] and first define the Tamm-Dancoff (TD) phonon operator

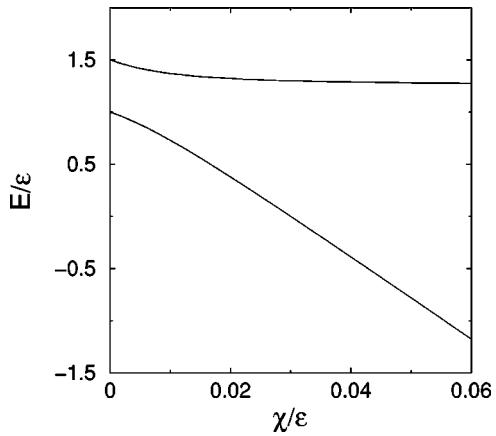

FIG. 4. Tamm-Dancoff energies as functions of the strength χ/ϵ.

$$V_\lambda^\dagger=\frac{1}{\sqrt{2\Omega}}\sum_i v_i^{(\lambda)}K_{i0}. \tag{20}$$

The amplitudes $v_i^{(\lambda)}$ satisfy the orthogonality condition

$$\sum_i v_i^{(\lambda)}v_i^{(\lambda')}=\delta_{\lambda\lambda'} \tag{21}$$

and are obtained by diagonalizing H_F in the basis $\{(1/\sqrt{2\Omega})K_{i0}|0\rangle\}_{i=1,2}$. In terms of these TD operators we construct the space

$$\left\{\overline{|n_1n_2\rangle}=\frac{1}{\sqrt{\mathcal{N}'_{n_1n_2}}}(V_1^\dagger)^{n_1}(V_2^\dagger)^{n_2}|0\rangle\right\}_{0\leqslant n_1+n_2\leqslant 2\Omega}. \tag{22}$$

This space is the same as Eq. (4) but just a different representation. Therefore, if we establish a one-to-one correspondence between states (22) and (5) and we reconstruct the boson image of H_F, the new boson Hamiltonian will have different coefficients [for instance, the matrix γ_{ij} of Eq. (7) will now be forced to be diagonal] but its spectrum will remain unchanged. In this new representation, bosons correspond to *collective* particle-hole excitations and so play a role very similar to that of the standard $s,d,\ldots$ bosons in the interacting boson model picture [20] (where they are meant to represent collective particle-particle excitations). As in this case, then, it is natural to expect that the structure of the low-lying part of the spectrum may be described in terms of only a selected group of collective bosons.

Our model appears particularly suited to illustrate this point. One can form two TD excitations (20) and their energies are shown in Fig. 4. As one sees, while increasing the strength χ/ϵ, one of the energies remains almost constant while the other one shows a regular and sizable decrease. This behavior leads us to believe that the lowest boson may play a preeminent role in the structure of the low-lying spectrum. We have made some calculations involving only this boson and (to start) only 1*p*-1*h* excitations. By denoting $b^\dagger(b)$ the creation (annihilation) boson operator associated

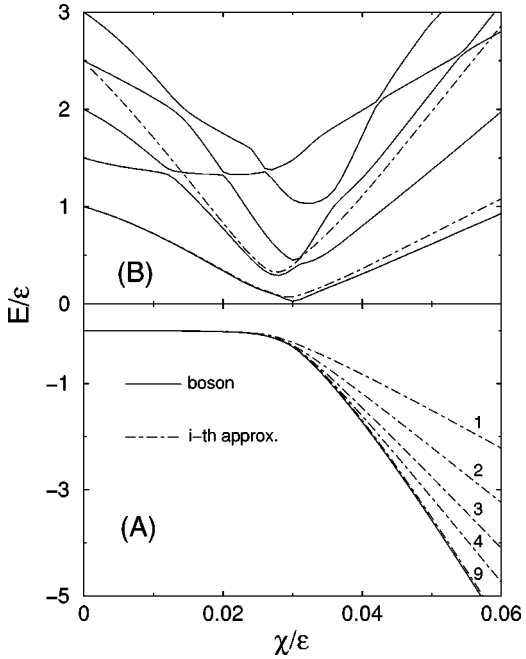

FIG. 5. Ground-state energy (A) and excitation energies of the lowest five states (B) as functions of the strength χ/ϵ. The solid lines are obtained by diagonalizing H_B (3) in B (4), while dot-dashed lines refer to calculations involving only the lowest Tamm-Dancoff boson and 1*p*-1*h* excitations. The numbers label different orders of approximation. Further details in Sec. V.

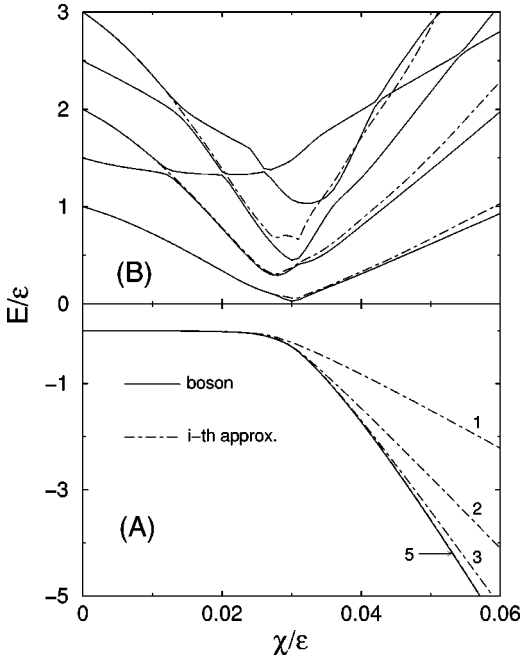

FIG. 6. The same as in Fig. 5 but dot-dashed lines now refer to calculations involving up to 2*p*-2*h* excitations.

to the lowest TD excitation, the procedure consists now in an iterated sequence of diagonalizations in spaces of the type

$$B^{(k)}=\{|\Psi_0^{(k-1)}),b^\dagger|\Psi_0^{(k-1)}),b|\Psi_0^{(k-1)})\}. \tag{23}$$

As the initial ansatz we have assumed the state $|\Psi_0^{(0)})=1/\sqrt{2}[|0)+b^\dagger|0)]$. The new results are shown in Fig. 5. The agreement for the ground state and the first excited state is very good. It is worth stressing that this result has been obtained by working in spaces whose dimensionality is remarkably smaller than that of the full boson space B (3 versus 66 in our model).

In Fig. 6, we show similar calculations which involve up to 2*p*-2*h* excitations. The quality of the agreement for the ground state and the first excited state (already good) remains basically unchanged while also the lowest ''two-phonon'' state (to use an RPA language) is now well described. These calculations therefore confirm the expectation that only the boson associated to the lowest TD excitation plays an active role in the structure of these states.

VI. SUMMARY AND CONCLUSIONS

In this paper we have presented a multistep variational approach for the study of many-body correlations. The approach has been developed in a boson formalism (bosons representing particle-hole excitations) and based on an iterative sequence of diagonalizations in subspaces of the full boson space. The purpose of these diagonalizations has been that of searching for the best approximation of the ground state of the system. The procedure has also led us to define a set of excited states and, at the same time, of operators generating these states as a result of their action on the ground state. We have considered two cases: (a) the case in which these operators carried only 1*p*-1*h* excitations and, (b) the case in which also 2*p*-2*h* excitations were included.

The approach has been tested within an exactly solvable three-level model. The comparison between exact and approximate ground-state energies has allowed us to appreciate the convergence of the procedure in both cases (a) and (b). In the first case, a comparison also with standard RPA calculations has shown that the ''one-phonon'' states that this theory could reproduce up to its crash point were now well reproduced in the whole range of variation of the strength. With the inclusion of 2*p*-2*h* excitations also the remaining low-lying states of the spectrum have been well reproduced.

In the second part of the paper, we have reformulated the fermion-boson correspondence and identified bosons with Tamm-Dancoff phonons. We have then explored the possibility of describing at least partially the spectrum of the system in terms of only a selected group of these bosons. In our model this has implied restricting the set of two possible bosons to the one corresponding to the lowest excitation energy. We have verified that the ground state was still well reproduced and so was the first excited state already at the level of 1*p*-1*h* excitations.

The possibility of selecting a restricted set of collective particle-hole excitations and, therefore, of constructing the boson space only in terms of the corresponding bosons appears to be quite appealing. It may represent, in fact, an effective way to reduce the dimensionalities of the system and so to lead to a much simplified application of the procedure to realistic cases.

APPENDIX

In Sec. II, we established a one-to-one correspondence between a set of fermion states $F \equiv \{|n_1 n_2\rangle\}$, Eq. (4), and a set of boson states $B \equiv \{|n_1 n_2)\}$, Eq. (5), both sets being orthonormal. In correspondence with a given fermion operator $\hat{O}_F$, the mapping procedure which we adopt searches for a boson operator $\hat{O}_B$ such that matrix elements between corresponding states be equal. The operator $\hat{O}_B$ defines the image of $\hat{O}_F$ in B.

The construction of $\hat{O}_B$ proceeds step-by-step involving at each step matrix elements between states which belong to increasingly larger subspaces of F and B [12]. Having in mind to construct boson images with no more than five boson terms, it is sufficient to involve at most the two subspaces

$$F' = \left\{ |0\rangle, \frac{1}{\sqrt{\mathcal{N}_i^F}} K_{i0}|0\rangle, \frac{1}{\sqrt{\mathcal{N}_{ij}^F}} K_{i0}K_{j0}|0\rangle, \frac{1}{\sqrt{\mathcal{N}_{ijk}^F}} K_{i0}K_{j0}K_{k0}|0\rangle \right\}$$

and

$$B' = \left\{ |0), b_i^\dagger|0), \frac{1}{\sqrt{\mathcal{N}_{ij}^B}} b_i^\dagger b_j^\dagger|0), \frac{1}{\sqrt{\mathcal{N}_{ijk}^B}} b_i^\dagger b_j^\dagger b_k^\dagger|0) \right\},$$

where $\mathcal{N}_i^F$, $\mathcal{N}_{ij}^F$, $\mathcal{N}_{ijk}^F$, $\mathcal{N}_{ij}^B$, and $\mathcal{N}_{ijk}^B$ are normalization factors. The boson image $\hat{O}_B$, which one derives, is a Hermitian operator which has the form (7) and coefficients

$$\alpha = \langle 0|\hat{O}_F|0\rangle,$$

$$\beta_i = \frac{\langle 0|\hat{O}_F K_{i0}|\rangle}{\sqrt{\mathcal{N}_i^F}},$$

$$\gamma_{ij} = \frac{\langle 0|K_{0i}\hat{O}_F K_{j0}|\rangle}{\sqrt{\mathcal{N}_i^F \mathcal{N}_j^F}} - \alpha\delta_{ij},$$

$$\phi_{ij} = \frac{\langle 0|\hat{O}_F K_{i0}K_{j0}|\rangle}{\sqrt{\mathcal{N}_{ij}^F \mathcal{N}_{ij}^B}},$$

$$\epsilon_{ijk} = \frac{\langle 0|K_{0k}\hat{O}_F K_{i0}K_{j0}|0\rangle}{\sqrt{\mathcal{N}_k^F \mathcal{N}_{ij}^F \mathcal{N}_{ij}^B}} - \frac{\beta_i\delta_{kj} + \beta_j\delta_{ki}}{\mathcal{N}_{ij}^B},$$

$$\delta_{ijkl} = \frac{\langle 0|K_{0i}K_{0j}\hat{O}_F K_{k0}K_{l0}|0\rangle}{\sqrt{\mathcal{N}_{ij}^F \mathcal{N}_{kl}^F \mathcal{N}_{ij}^B \mathcal{N}_{kl}^B}} - \frac{\alpha\Delta_{ij,kl}^{(2)} + \sum_{i'} (\gamma_{i'k}\Delta_{ij,i'l}^{(2)} + \gamma_{i'l}\Delta_{ij,i'k}^{(2)})}{\mathcal{N}_{kl}^B},$$

$$\rho_{ijkl} = \frac{\langle 0|K_{0i}K_{0j}K_{0k}\hat{O}_F K_{l0}|0\rangle}{\sqrt{\mathcal{N}_{ijk}^F \mathcal{N}_l^F \mathcal{N}_{ijk}^B}} - \sum_{i' \leqslant j'} \phi_{i'j'}\Delta_{ijk,i'j'l}^{(3)},$$

$$\tau_{ijklm} = \frac{\langle 0|K_{0i}K_{0j}K_{0k}\hat{O}_F K_{l0}K_{m0}|0\rangle}{\sqrt{\mathcal{N}_{ijk}^F \mathcal{N}_{lm}^F \mathcal{N}_{ijk}^B \mathcal{N}_{lm}^B}} - \frac{\sum_{i'} \beta_{i'}\Delta_{ijk,i'lm}^{(3)} + \sum_{i' \leqslant j'} \epsilon_{i'j'l}\Delta_{ijk,i'j'm}^{(3)} + \sum_{i' \leqslant j'} \epsilon_{i'j'm}\Delta_{ijk,i'j'l}^{(3)}}{\mathcal{N}_{lm}^B},$$

where

$$\Delta_{ij,i'j'}^{(2)} = (\delta_{ii'}\delta_{jj'} + \delta_{ij'}\delta_{ji'})/\mathcal{N}_{ij}^B$$

and

$$\Delta_{ijk,i'j'k'}^{(3)} = (\delta_{ii'}\delta_{jj'}\delta_{kk'} + \delta_{ii'}\delta_{jk'}\delta_{kj'} + \delta_{ij'}\delta_{jk'}\delta_{ki'} + \delta_{ij'}\delta_{ji'}\delta_{kk'} + \delta_{ik'}\delta_{ji'}\delta_{kj'} + \delta_{ik'}\delta_{jj'}\delta_{ki'})/\mathcal{N}_{ijk}^B.$$

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