Extended random-phase approximation in a boson formalism with Pauli principle

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The random-phase approximation (RPA) is examined in a boson formalism and special attention is focused on the problem of the violation of the Pauli principle affecting this theory. A mapping technique is discussed and the boson image of a two-body fermion Hamiltonian is constructed. Within the boson space so defined, an extension of RPA is proposed where structure and energy of the ground state, as well as those of the one-phonon states, are analyzed with regard to the role of the spurious components associated with a violation of the Pauli principle. A multistep minimization procedure for the determination of a better ground state is also examined. Numerical tests are performed within the Lipkin-Meshkov-Glick model.

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I. INTRODUCTION

The random-phase approximation (RPA) is the simplest theory of excited states of the nucleus which admits the possibility that the ground state is not of purely independent character but may contain correlations [1]. The starting point for this theory involves expressing excited states in terms of an operator that acts on the ground state. After the derivation of exact equations for this operator, two basic approximations are introduced in the RPA [2]: (i) The operator is taken as a linear superposition of creation and annihilation particle-hole (ph) pair operators [taking a Hartree-Fock (HF) basis as a reference] and (ii) the RPA ground state is approximated by the HF state in order to evaluate the expectation values of given operators in this ground state. The latter approximation is usually called the "quasiboson approximation" since, in the case of expectation values of commutators of ph creation and annihilation operators, it is equivalent to neglecting terms in these commutators such that they become the commutators of boson operators. The quasiboson approximation is the basis for the violation of the Pauli principle that affects this theory.

This problem has been treated intensively both in the past [3–9] and recently [10–14]. On the one hand, attempts have been made to avoid it completely by remaining within the fermion space [5–13]. On the other hand, the same problem has also been examined by reformulating the whole theory in a boson formalism by means of mapping techniques [3,4,14]. The latter approach is the one which has been followed in this paper.

In a recent paper [13], a fermion-type approach inspired by the "renormalized RPA" [5,6] has been formulated and applied to the Lipkin-Meshkov-Glick model [15] as well as to realistic forces of the Skyrme type. This approach, sharing similarities also with the "self-consistent RPA" of Ref. [9], was meant to overcome the inconsistency of the RPA described in the above point (ii) by replacing the uncorrelated HF state with the correlated ground state obtained as solution of the equations. However, approximations still persisting in the evaluation of expectation values of some operators in this state have maintained violations of the Pauli principle in the procedure. In this paper, special attention has been focused just on the problem of the violation of this principle within the RPA.

We will begin by examining the problem of transferring the description of a fermion system from a space whose states are built in terms of ph operators acting on the HF state onto a boson space whose building blocks are corresponding boson operators. This will be done by following the general lines of a mapping procedure which has been used in the recent past both in the case of the correspondence between collective pairs of fermions and bosons [16] and in the case of the correspondence between clusters of quarks and elementary baryons [17]. Within the boson space so constructed, we will first reexamine the derivation of the RPA equations and, then, we will take into account the elimination of spurious components associated with a violation of the Pauli principle, both from the ground state and one-phonon states. This analysis will be supported by numerical tests performed within the Lipkin model. Finally, a multistep minimization procedure for the determination of a better ground state will be formulated and tested.

The paper is organized as follows. In Sec. II, we will describe the mapping technique and derive the general expressions for the one-body and two-body parts of the boson image of a fermion operator. In Sec. II A, we will apply these to the case of a two-body fermion Hamiltonian. In Sec. III, within the boson space so constructed, we will discuss the derivation of the RPA equations and illustrate our procedure to go beyond this approximation. In Sec. IV, we will study applications of this procedure to the Lipkin model and we will compare our results with the exact and the RPA ones. In this section also the multistep minimization procedure will be examined. In Sec. V, finally, we will summarize the results and draw some conclusions.

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II. MAPPING TECHNIQUE

The subject of boson mapping for the study of nuclear collective motion is extensively discussed in the literature and for a thorough account we refer to a recent review [18]. In our work, we will follow the notation of Ref. [4], where the problem of ph excitations in closed shell nuclei has been examined on the basis of Marumori's boson expansion method.

We assume a HF-like decomposition of single-particle states into an occupied set $a^\dagger_\alpha$, denoted by Greek subscripts, and an unoccupied set $a^\dagger_m$ with Latin subscripts. We define the fermion-pair operators

$$B^\dagger_{m\alpha} = a^\dagger_m a_\alpha, \tag{1}$$

which satisfy the commutation relations

$$[B^\dagger_{m_1\alpha_1}, B^\dagger_{m_2\alpha_2}] = [B_{m_1\alpha_1}, B_{m_2\alpha_2}] = 0 \ , \tag{2a}$$

$$[B_{m_1\alpha_1}, B^\dagger_{m_2\alpha_2}] = \delta_{m_1m_2}\delta_{\alpha_1\alpha_2} - \delta_{m_1m_2}a_{\alpha_2}a^\dagger_{\alpha_1} - \delta_{\alpha_1\alpha_2}a^\dagger_{m_2}a_{m_1} \ . \tag{2b}$$

They are such that

$$B_{m\alpha}|\mathrm{HF}\rangle = 0 \ , \tag{3}$$

where $|\mathrm{HF}\rangle$ represents the HF ground state.

We now consider the set of fermion states

$$|0\rangle \equiv |\mathrm{HF}\rangle \ , \tag{4a}$$

$$|m_1\alpha_1\rangle = B^\dagger_{m_1\alpha_1}|0\rangle \ , \tag{4b}$$

$$\cdots$$

$$|m_1\alpha_1, m_2\alpha_2, ..., m_N\alpha_N\rangle = \prod_{i=1}^{N} B^\dagger_{m_i\alpha_i}|0\rangle \ , \tag{4c}$$

which we arrange according to a given order, for instance, $m_1 < m_2 < \cdots < m_N$ and $\alpha_1 < \alpha_2 < \cdots < \alpha_N$. The inequality between any two of the particle or hole indices assures these states to be compatible with the Pauli principle. Moreover, they are orthonormal. We call $S^{(N)}$ the space spanned by these basis vectors and define $|i\rangle$ the state among these which carries i ph excitations.

As boson correspondent of the operator (1), we define the operator $b^\dagger_{m\alpha}$ obeying the commutation relations

$$[b^\dagger_{m_1\alpha_1}, b^\dagger_{m_2\alpha_2}] = [b_{m_1\alpha_1}, b_{m_2\alpha_2}] = 0 \ , \tag{5a}$$

$$[b_{m_1\alpha_1}, b^\dagger_{m_2\alpha_2}] = \delta_{m_1m_2}\delta_{\alpha_1\alpha_2}, \tag{5b}$$

and we also introduce a vacuum state $|0)$ such that

$$b_{m\alpha}|0) = 0 \ , \tag{6}$$

in analogy with the fermion case [Eq. (3)].

Let us then define a set of boson states in a one-to-one correspondence with the fermion ones (4):

$$|0) \ , \tag{7a}$$

$$|m_1\alpha_1) = b^\dagger_{m_1\alpha_1}|0) \ , \tag{7b}$$

$$\cdots$$

$$|m_1\alpha_1, m_2\alpha_2, ..., m_N\alpha_N) = \prod_{i=1}^{N} b^\dagger_{m_i\alpha_i}|0) \ . \tag{7c}$$

We call $s^{(N)}$ the space generated by these states and $|i)$ the state corresponding to $|i\rangle$. States (7) form an orthonormal set. We remark that, unlike Marumori's prescription adopted in Ref. [4], no antisymmetrization is introduced here in the definition of these boson states. The states of the space $s^{(N)}$ are simply defined in terms of products of boson operators $b^\dagger_{m\alpha}$ whose indices are arranged as in the fermion space $S^{(N)}$. This guarantees that $s^{(N)}$ spans the whole physical subspace. Compared with the antisymmetrized definition, this has the advantage of making simpler the use of the boson states and, therefore, as we will see later, the use of the operator projecting onto this subspace. Such an operator plays an important role in the procedure discussed in this paper.

The boson image O_b of a given fermion operator O_f can be constructed step by step by examining the correspondence between the spaces $S^{(N)}$ and $s^{(N)}$ for increasing values of N. The fermion and boson spaces being such that

$$(i|i') = \langle i|i'\rangle = \delta_{ii'} \ , \tag{8}$$

the boson image at each N, $O^{(N)}_b$, can be simply defined by the equality

$$(i|O^{(N)}_b|i') = \langle i|O_f|i'\rangle \tag{9}$$

for $0 \le i, i' \le N$.

We notice that the simplicity of this condition as compared to analogous conditions of previous mappings [see, for instance, Eq. (34) of Ref. [17]] is just a consequence of the elementarity of the fermion-pair operators (1) which are mapped.

The simplest correspondence to examine is that at $N = 1$. By assuming O_f to be Hermitian, one finds

$$O_b^{(1)} = a + \sum_{m\alpha} c_{m\alpha}(b_{m\alpha}^\dagger + b_{m\alpha}) + \sum_{m\alpha m'\alpha'} d_{m\alpha m'\alpha'} b_{m\alpha}^\dagger b_{m'\alpha'} \ , \tag{10a}$$

with

$$a = \langle 0|O_f|0\rangle \ , \tag{10b}$$

$$c_{m\alpha} = \langle 0|O_f|m\alpha\rangle \ , \tag{10c}$$

$$d_{m\alpha m'\alpha'} = \langle m\alpha|O_f|m'\alpha'\rangle - \langle 0|O_f|0\rangle \delta_{mm'}\delta_{\alpha\alpha'} \ . \tag{10d}$$

The next case, at $N = 2$, leads to (by denoting for simplicity $i \equiv \{m\alpha\}$)

$$O_b^{(2)} = O_b^{(1)} + \sum_{i_1 i_2} e_{i_1 i_2}(b_{i_1}^\dagger b_{i_2}^\dagger + b_{i_2} b_{i_1}) + \sum_{i_1 i_2 i_3} g_{i_1 i_2 i_3}(b_{i_1}^\dagger b_{i_2}^\dagger b_{i_3} + b_{i_3}^\dagger b_{i_2} b_{i_1}) + \sum_{i_1 i_2 i_3 i_4} f_{i_1 i_2 i_3 i_4} b_{i_1}^\dagger b_{i_2}^\dagger b_{i_3} b_{i_4}, \tag{11a}$$

with

$$e_{i_1 i_2} = \frac{1}{2}\langle 0|O_f|i_1 i_2\rangle \ , \tag{11b}$$

$$g_{i_1 i_2 i_3} = \frac{1}{2}(\langle i_3|O_f|i_1 i_2\rangle - \delta_{i_1 i_3}\langle 0|O_f|i_2\rangle - \delta_{i_2 i_3}\langle 0|O_f|i_1\rangle) \ , \tag{11c}$$

$$\begin{aligned} f_{i_1 i_2 i_3 i_4} = \frac{1}{4}[&\langle i_1 i_2|O_f|i_3 i_4\rangle - \delta_{i_1 i_4}\langle i_2|O_f|i_3\rangle - \delta_{i_2 i_4}\langle i_1|O_f|i_3\rangle - \delta_{i_1 i_3}\langle i_2|O_f|i_4\rangle \\ &-\delta_{i_2 i_3}\langle i_1|O_f|i_4\rangle + \langle 0|O_f|0\rangle(\delta_{i_1 i_4}\delta_{i_2 i_3} + \delta_{i_1 i_3}\delta_{i_2 i_4})]. \end{aligned} \tag{11d}$$

The correspondence can be studied further for any increasing value of N, leading to more complicated expressions of the boson image.

A. Hamiltonian

We consider now explicitly a fermion Hamiltonian of the general form

$$H_f = \sum_{ab} h_{ab} a_a^\dagger a_b + \frac{1}{4}\sum_{abcd} V_{abcd} a_a^\dagger a_b^\dagger a_d a_c \ , \tag{12}$$

where V_{abcd} stands for the antisymmetrized matrix element of the two-body interaction. Within the HF-like decomposition of the single-particle states defined at the beginning of Sec. II, we rewrite this as [4]

$$H_f = E_{\rm HF} + H_{11} + H_{22} + (H_{40} + \text{H.c.}) + H_{22}^{'} + (H_{31} + \text{H.c.}) \ , \tag{13a}$$

where

$$E_{\rm HF} = \langle \text{HF}|H_f|\text{HF}\rangle = \sum_\alpha h_{\alpha\alpha} + \frac{1}{2}\sum_{\alpha\beta} V_{\alpha\beta\alpha\beta} \ , \tag{13b}$$

$$H_{11} = -\sum_\alpha \epsilon_\alpha a_\alpha a_\alpha^\dagger + \sum_m \epsilon_m a_m^\dagger a_m \ , \tag{13c}$$

$$H_{22} = \sum_{\alpha\beta mn} V_{m\beta\alpha n} a_m^\dagger a_\alpha a_\beta^\dagger a_n \ , \tag{13d}$$

$$H_{40} = \frac{1}{4}\sum_{\alpha\beta mn} V_{mn\alpha\beta} a_m^\dagger a_\alpha a_n^\dagger a_\beta \ , \tag{13e}$$

$$H'_{22} = \frac{1}{4}\sum_{mnpq} V_{mnpq} a^\dagger_m a^\dagger_n a_q a_p + \frac{1}{4}\sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} a_\delta a_\gamma a^\dagger_\alpha a^\dagger_\beta \tag{13f}$$

and

$$H_{31} = \frac{1}{2}\sum_{mnp\alpha} V_{mn\alpha p} a^\dagger_m a_\alpha a^\dagger_n a_p + \frac{1}{2}\sum_{m\alpha\beta\gamma} V_{m\alpha\beta\gamma} a^\dagger_m a_\gamma a_\beta a^\dagger_\alpha \ . \tag{13g}$$

In Eq. (13c), ϵ_α and ϵ_m are the single-particle energies of occupied and unoccupied states, respectively. By means of the procedure discussed in the previous section, we find as boson image of H_f (up to terms of second order):

$$H_b = E_{\rm HF} + \sum_{m\alpha}(\epsilon_m - \epsilon_\alpha) b^\dagger_{m\alpha} b_{m\alpha} + \sum_{m_1\alpha_1 m_2\alpha_2} V_{m_1\alpha_2\alpha_1 m_2} b^\dagger_{m_1\alpha_1} b_{m_2\alpha_2}$$
$$+ \frac{1}{2}\sum_{m_1\alpha_1 m_2\alpha_2} V_{m_1 m_2\alpha_1\alpha_2}(b^\dagger_{m_1\alpha_1} b^\dagger_{m_2\alpha_2} + \text{H.c.}) + O(3) \ . \tag{14}$$

This Hamiltonian differs from that of Ref. [4] by a factor of $\frac{1}{\sqrt{2}}$ in the last term.

III. RPA AND PAULI PRINCIPLE: OUR PROCEDURE

The derivation of the RPA equations within the boson formalism just illustrated can be carried out through a few steps. Let us first define $|-)$ and $|\nu)$ as the exact eigenstates of the Hamiltonian H_b corresponding to the ground state and to an excited one, respectively, i.e.,

$$H_b|-) = E_0|-) \tag{15}$$

and

$$H_b|\nu) = E_\nu|\nu) \ . \tag{16}$$

Moreover, let $q^\dagger_\nu$ be an operator such that

$$|\nu) = q^\dagger_\nu|-) \tag{17}$$

and also that

$$q_\nu|-) = 0 \ . \tag{18}$$

By means of the previous equations one easily deduces that

$$E_\nu = (\nu|H_b|\nu) = (-|q_\nu H_b q^\dagger_\nu|-) = (-|[q_\nu,[H_b,q^\dagger_\nu]]|-) + E_0. \tag{19}$$

With reference to the derivation of this expression relating the energy of the one-phonon state $q^\dagger_\nu|-)$, E_ν, with that of the ground state $|-)$, E_0, the RPA equations can be constructed on the basis of two approximations. The first consists in writing the $q^\dagger_\nu$ operator as

$$q^\dagger_\nu = \sum_{m\alpha} X^\nu_{m\alpha} b^\dagger_{m\alpha} + \sum_{m\alpha} Y^\nu_{m\alpha} b_{m\alpha} \ . \tag{20}$$

To this operator one then associates, as an approximate ground state, the state $|\text{RPA})$ defined by

$$q_\nu|\text{RPA}) = 0 \tag{21}$$

and, as an approximate one-phonon state $|\nu)$, the state

$$|\nu)_{\rm RPA} = q^\dagger_\nu|\text{RPA}) \ . \tag{22}$$

The orthonormalization of these states requires

$$[q_\nu, q^\dagger_{\nu'}] = \sum_{m\alpha}(X^\nu_{m\alpha}X^{\nu'}_{m\alpha} - Y^\nu_{m\alpha}Y^{\nu'}_{m\alpha}) = \delta_{\nu\nu'} \ . \tag{23}$$

Making use of the conditions (21) and (23) one finds, in analogy with Eq. (19), that

$$E^{\rm RPA}_\nu = (\text{RPA}|q_\nu H_b q^\dagger_\nu|\text{RPA}) = (\text{RPA}|[q_\nu,[H_b,q^\dagger_\nu]]|\text{RPA}) + E^{\rm RPA}_0 \ , \tag{24}$$

where

$$E^{\rm RPA}_0 = (\text{RPA}|H_b|\text{RPA}) \ . \tag{25}$$

The second approximation consists in inserting in Eq. (24) the boson Hamiltonian truncated at terms of second order only [see Eq. (14)]. In this case, the double commutator at the right-hand side (rhs) of Eq. (24) reduces simply to a number and precisely

$$[q_\nu,[H_b,q_\nu^\dagger]] = \sum_{m\alpha}(\epsilon_m-\epsilon_\alpha)[(X^\nu_{m\alpha})^2+(Y^\nu_{m\alpha})^2] + \sum_{m\alpha p\gamma} V_{m\gamma\alpha p}(X^\nu_{m\alpha}X^\nu_{p\gamma}+Y^\nu_{m\alpha}Y^\nu_{p\gamma}) - \sum_{m\alpha p\gamma} V_{mp\alpha\gamma}(X^\nu_{m\alpha}Y^\nu_{p\gamma}+Y^\nu_{m\alpha}X^\nu_{p\gamma}) \ . \tag{26}$$

By minimizing this expression with respect to $X_{m\alpha}$ and $Y_{m\alpha}$, under the condition (23), and so by minimizing the one-phonon energy (24), one obtains the conventional RPA equations

$$(\epsilon_m-\epsilon_\alpha)X^\nu_{m\alpha}+\sum_{p\gamma}V_{m\gamma\alpha p}X^\nu_{p\gamma}-\sum_{p\gamma}V_{mp\alpha\gamma}Y^\nu_{p\gamma}=(E^{\rm RPA}_\nu-E^{\rm RPA}_0)X^\nu_{m\alpha} \tag{27a}$$

and

$$(\epsilon_m-\epsilon_\alpha)Y^\nu_{m\alpha}+\sum_{p\gamma}V_{p\alpha\gamma m}Y^\nu_{p\gamma}-\sum_{p\gamma}V_{mp\alpha\gamma}X^\nu_{p\gamma}=-(E^{\rm RPA}_\nu-E^{\rm RPA}_0)Y^\nu_{m\alpha} \ . \tag{27b}$$

Besides the two approximations discussed so far, however, there is a further approximation, hidden in the first one, which affects these equations: the neglect in the state (22) [or, similarly, in the condition (21)] of those components which are "spurious" in that they do not correspond to any fermion state allowed by the Pauli principle, on the basis of the correspondence between fermion and boson spaces established in Sec. II. Such components are more directly visible in the state |RPA) when, as result of the condition (21), this state is written as [2]

$$|{\rm RPA}) = \mathcal{N}e^S|0) \ , \tag{28}$$

where $\mathcal{N}$ is a normalization constant, $|0)$ is the state defined by Eq. (6), and

$$S=\frac{1}{2}\sum_{m\alpha}\sum_{n\beta}Z_{m\alpha n\beta}b^\dagger_{m\alpha}b^\dagger_{n\beta} \ , \tag{29}$$

with, in terms of matrices,

$$Z=-(YX^{-1})^* \ . \tag{30}$$

Already in the S operator (29), in fact, terms with equal particle or hole indices are components with no fermion counterpart.

In the following, we will take the state |RPA), Eq. (28), as a starting point and we will examine its structure and its energy, as well as those of the one-phonon energy $q^\dagger_\nu|{\rm RPA})$, by focusing our attention on the problem of the elimination of these spurious components.

As has been stressed in Sec. II, $s^{(N_{\rm max})}$, where $N_{\rm max}$ is the maximum number of ph excitations allowed by the Pauli principle, is a boson space that spans the whole physical subspace. This is the space within which the mapped boson operators are defined. Therefore, in order to project out the above spurious components from ground and excited states, we act on these states with the identity operator $\hat I$ of $s^{(N_{\rm max})}$, giving rise to

$$\widetilde{|{\rm RPA})} = \hat I|{\rm RPA}) \tag{31}$$

and

$$|\widetilde{\nu}) = \hat I q^\dagger_\nu|\widetilde{\rm RPA}) \ . \tag{32}$$

In order to see in detail the results of these operations, let us notice that the most general expression for the operator $\hat I$ is

$$\hat I = |0)(0| + \sum_{m\alpha}|m\alpha)(m\alpha| + \sum_{m_1<m_2,\alpha_1<\alpha_2}|m_1\alpha_1,m_2\alpha_2)(m_1\alpha_1,m_2\alpha_2| + \cdots \ , \tag{33}$$

and, from its action on the state (28), we obtain

$$\hat I|{\rm RPA}) = \hat I\mathcal{N}\left(1+S+\frac{1}{2!}S^2+\cdots\right)|0) \equiv \mathcal{N}(|0)+\widetilde{|2)}+\widetilde{|4)}+\cdots+\widetilde{|N_{\rm max})}) \tag{34a}$$

(assuming that $N_{\rm max}$ is even, for simplicity), where

$$\widetilde{|2)} = \sum_{m_1<m_2,\alpha_1<\alpha_2} G^{(2)}_{m_1\alpha_1m_2\alpha_2}(Z)|m_1\alpha_1,m_2\alpha_2) \ , \tag{34b}$$

$$\widetilde{|4)} = \sum_{m_1<m_2<m_3<m_4,\alpha_1<\alpha_2<\alpha_3<\alpha_4} G^{(4)}_{m_1\alpha_1m_2\alpha_2m_3\alpha_3m_4\alpha_4}(Z)|m_1\alpha_1,m_2\alpha_2,m_3\alpha_3,m_4\alpha_4) \ , \tag{34c}$$

with

$$G^{(2)}_{m_1\alpha_1 m_2\alpha_2}(Z) = \frac{1}{1!}\frac{1}{2^1}\sum_{(i_1,i_2)}^{(1,2)} Z_{m_{i_1}\alpha_{i_1}m_{i_2}\alpha_{i_2}} = Z_{m_1\alpha_1 m_2\alpha_2} \ , \tag{34d}$$

$$G^{(4)}_{m_1\alpha_1 m_2\alpha_2 m_3\alpha_3 m_4\alpha_4}(Z) = \frac{1}{2!}\frac{1}{2^2}\sum_{(i_1,i_2,i_3,i_4)}^{(1,2,3,4)} Z_{m_{i_1}\alpha_{i_1}m_{i_2}\alpha_{i_2}} Z_{m_{i_3}\alpha_{i_3}m_{i_4}\alpha_{i_4}} , \tag{34e}$$

and, in general,

$$G^{(2R)}_{m_1\alpha_1 m_2\alpha_2\cdots m_{2R}\alpha_{2R}}(Z) = \frac{1}{R!}\frac{1}{2^R}\sum_{(i_1,i_2,\ldots,i_{2R})}^{(1,2,\ldots,2R)} Z_{m_{i_1}\alpha_{i_1}m_{i_2}\alpha_{i_2}}\cdots Z_{m_{i_{2R-1}}\alpha_{i_{2R-1}}m_{i_{2R}}\alpha_{i_{2R}}} \ . \tag{34f}$$

In the last expression, the symbol $\sum_{(i_1,i_2,\ldots,i_{2R})}^{(1,2,\ldots,2R)}$ indicates the summation over the $(2R)!$ terms obtained with the sets $(i_1,i_2,\ldots,i_{2R})$ running through all possible permutations of $(1,2,\ldots,2R)$. Moreover, we notice that the definition of these coefficients $G^{(2R)}_{m_1\alpha_1 m_2\alpha_2\cdots m_{2R}\alpha_{2R}}(Z)$ only refer to indices $m_1 < m_2 < \cdots < m_{2R}$ and $\alpha_1 < \alpha_2 < \cdots < \alpha_{2R}$ while, for any other choice of these indices, their value is meant to be zero.

Similarly, for the state (32), we obtain

$$\hat{I}q^\dagger_\nu|\widetilde{RPA}) = \mathcal{N}\hat{I}q^\dagger_\nu(|0) + \widetilde{|2)} + \widetilde{|4)} + \cdots + \widetilde{|N_{\max})}) \equiv \mathcal{N}(\widetilde{|1)} + \widetilde{|3)} + \cdots + \widetilde{|N_{\max}-1)}), \tag{35a}$$

where

$$\widetilde{|1)} = \sum_{m_1,\alpha_1} F^{(1)}_{m_1\alpha_1}(X,Y,Z)|m_1\alpha_1) \ , \tag{35b}$$

$$\widetilde{|3)} = \sum_{m_1<m_2<m_3,\alpha_1<\alpha_2<\alpha_3} F^{(3)}_{m_1\alpha_1 m_2\alpha_2 m_3\alpha_3}(X,Y,Z)|m_1\alpha_1, m_2\alpha_2, m_3\alpha_3) \ , \tag{35c}$$

with

$$F^{(1)}_{m_1\alpha_1}(X,Y,Z) = X^\nu_{m_1\alpha_1} + \sum_{m_0,\alpha_0} Y^\nu_{m_0\alpha_0}\sum_{(i_1,i_2)}^{(0,1)} G^{(2)}_{m_{i_1}\alpha_{i_1}m_{i_2}\alpha_{i_2}}(Z) \ , \tag{35d}$$

$$\begin{aligned} F^{(3)}_{m_1\alpha_1 m_2\alpha_2 m_3\alpha_3}(X,Y,Z) = {} & \sum_{(i_1,i_2,i_3)}^{(1,2,3)} X^\nu_{m_{i_1}\alpha_{i_1}} G^{(2)}_{m_{i_2}\alpha_{i_2}m_{i_3}\alpha_{i_3}}(Z) \\ & + \sum_{m_0,\alpha_0} Y^\nu_{m_0\alpha_0}\sum_{(i_1,i_2,i_3,i_4)}^{(0,1,2,3)} G^{(4)}_{m_{i_1}\alpha_{i_1}m_{i_2}\alpha_{i_2}m_{i_3}\alpha_{i_3}m_{i_4}\alpha_{i_4}}(Z), \end{aligned} \tag{35e}$$

and, in general,

$$\begin{aligned} F^{(R)}_{m_1\alpha_1 m_2\alpha_2\cdots m_R\alpha_R}(X,Y,Z) = {} & \sum_{(i_1,i_2,\ldots,i_R)}^{(1,2,\ldots,R)} X^\nu_{m_{i_1}\alpha_{i_1}} G^{(R-1)}_{m_{i_2}\alpha_{i_2}\cdots m_{i_R}\alpha_{i_R}}(Z) \\ & + \sum_{m_0,\alpha_0} Y^\nu_{m_0\alpha_0}\sum_{(i_1,i_2,\ldots,i_{R+1})}^{(0,1,\ldots,R)} G^{(R+1)}_{m_{i_1}\alpha_{i_1}m_{i_2}\alpha_{i_2}\cdots m_{i_{R+1}}\alpha_{i_{R+1}}}(Z) \ , \end{aligned} \tag{35f}$$

with the definition $G^{(0)}(Z) \equiv 1$.

Expressions (34) and (35) allow one to express the states $\widetilde{|\mathrm{RPA}\rangle}$ and $|\widetilde{\nu}\rangle$ as combinations of the basis states (7) of $s^{(N_{\max})}$. The knowledge of these combinations as well as that of the matrix elements of H_b between these states, as defined in the mapping procedure, makes possible the evaluation of the quantities

$$\widetilde{E}_\nu = \frac{(\widetilde{\nu}|H_b|\widetilde{\nu})}{(\widetilde{\nu}|\widetilde{\nu})} \tag{36}$$

and

$$\widetilde{E}_0 = \frac{(\widetilde{\mathrm{RPA}}|H_b|\widetilde{\mathrm{RPA}})}{(\widetilde{\mathrm{RPA}}|\widetilde{\mathrm{RPA}})} \ . \tag{37}$$

As results of the operations just illustrated, then, $\widetilde{E}_\nu$ and $\widetilde{E}_0$ replace the quantities $E_\nu^{(\mathrm{RPA})}$, (24), and $E_0^{(\mathrm{RPA})}$, Eq. (25), which have been introduced before in the derivation of the RPA equations. Differently from that case, however, no special relation of the type (30) exists now among the X, Y, and Z variables, the condition

$$\hat{I}q_\nu|\widetilde{\mathrm{RPA}}\rangle = 0 \tag{38}$$

being not satisfied, in general. It is worth noticing that, independently of this condition, states $\widetilde{|\mathrm{RPA}\rangle}$ and $|\widetilde{\nu}\rangle$ are always orthogonal due to their particular structures shown in Eqs. (34a) and (35a).

The calculations which will be performed in the following will consist, first, in the minimization of $\widetilde{E}_0$ with respect to the Z variables and, second, in the minimization of $\widetilde{E}_\nu$ with respect to the X and Y variables (the Z variables needed in this case being those derived in the first minimization). These calculations will refer to the Lipkin model. Comparisons will also be shown with the standard RPA and the exact results. Extensions of similar calculations to realistic cases will be discussed, then, in Sec. V.

Of course, the energies $\widetilde{E}_0$ and $\widetilde{E}_\nu$ calculated above closely depend on the form of the state (28) and this state has a very restrictive ph dependence. In general, this form (28) cannot be guaranteed as the most appropriate for the description of the ground state of the system. Therefore, in the second part of this paper, we will examine a procedure aiming at providing a more general parametrization of the ground state.

IV. APPLICATION TO THE LIPKIN MODEL

The model to which we will refer in this section, the Lipkin model [15], serves as a standard test for many-body approximations because of its simplicity and effectiveness. The Hamiltonian of the model is

$$H_f = \epsilon K_0 - \frac{1}{2}V(K_+^2 + K_-^2) \ , \tag{39a}$$

where

$$K_0 = \frac{1}{2}\sum_{m=1}^{\Omega}(a_m^\dagger a_m - a_{-m}^\dagger a_{-m}) \ , \tag{39b}$$

$$K_+ = \sum_{m=1}^{\Omega} a_m^\dagger a_{-m} \ , \tag{39c}$$

$$K_- = (K_+)^\dagger = \sum_{m=1}^{\Omega} a_{-m}^\dagger a_m, \tag{39d}$$

and $a_m^\dagger$ (a_m) are creation (annihilation) fermion operators. This Hamiltonian is associated with a system of two Ω-fold degenerate levels filled by Ω fermions. ϵ can therefore be seen as the difference between the Hartree-Fock energies of these two levels and $a_m^\dagger$ ($1 \le m \le \Omega$) creates a particle in the upper level while $a_{-m}^\dagger$ creates in the lower one. The interaction in H_f scatters pairs of particles between the two levels without changing the value of m which specifies the particular degenerate state within the shell. For the Hamiltonian (39a), the static Schrödinger problem can be solved exactly by using the standard group technique associated with the SU(2) Lie algebra of the operators K_0, K_+, K_-.

A. Boson transformation

Because of the peculiarities of the Hamiltonian (39a), it turns out to be appropriate to introduce the fermion-pair operators

$$B_m^\dagger = a_m^\dagger a_{-m} \ , \tag{40}$$

in correspondence of which we define the boson creation operator $b_m^\dagger$. By following the procedure discussed in Sec. II, we obtain, in correspondence to H_f,

$$H_b^{(1)} = -\frac{\epsilon}{2}\Omega + \epsilon\sum_m b_m^\dagger b_m \tag{41}$$

and

$$H_b^{(2)} = -\frac{\epsilon}{2}\Omega + \epsilon\sum_m b_m^\dagger b_m - \frac{1}{2}V\sum_{m_1 m_2}(b_{m_1}^\dagger b_{m_2}^\dagger + b_{m_1} b_{m_2}) \ . \tag{42}$$

In principle, in order to define the exact boson image of H_f in the full space $s^{(\Omega)}$, one should construct up to $H_b^{(\Omega)}$. However, it is enough to observe that (if $m_1 \neq m_2 \neq m_3$)

$$[H_f, B_m^\dagger]|0\rangle = \epsilon B_m^\dagger|0\rangle, \tag{43}$$

$$[[H_f, B_{m_1}^\dagger], B_{m_2}^\dagger]|0\rangle = -V|0\rangle, \tag{44}$$

$$[[[H_f, B_{m_1}^\dagger], B_{m_2}^\dagger], B_{m_3}^\dagger] = 0, \tag{45}$$

as well as

$$[H_b, b_m^\dagger]|0) = \epsilon b_m^\dagger|0) \ , \tag{46}$$

$$[[H_b, b_{m_1}^\dagger], b_{m_2}^\dagger] = -V \ , \tag{47}$$

$$[[[H_b, b_{m_1}^\dagger], b_{m_2}^\dagger], b_{m_3}^\dagger] = 0, \tag{48}$$

and that corresponding states have equal overlap [Eq. (8)], to conclude that

$$H_b^{(\Omega)} = H_b^{(2)} \equiv H_b \ . \tag{49}$$

Indeed, this boson Hamiltonian diagonalized in the basis

$$|0) \ , \tag{50a}$$

$$|1) = \mathcal{N}_1 \sum_i b_i^\dagger|0) \ , \tag{50b}$$

$$\cdots$$

$$|n) = \mathcal{N}_n \sum_{i_1<i_2<\cdots<i_n} b_{i_1}^\dagger b_{i_2}^\dagger \cdots b_{i_n}^\dagger|0) \ , \tag{50c}$$

up to $n = \Omega$ and where $\mathcal{N}_n = \sqrt{\frac{(\Omega-n)!n!}{\Omega!}}$, gives rise to a spectrum coinciding with that of the Lipkin Hamiltonian (39a) in its largest multiplet [15].

The Lipkin model has been adopted, in the past, as an ideal laboratory for boson mapping theories, because of its simplicity. Two examples of these mappings often quoted in the literature are those discussed in Refs. [9,14,19] and are based on the Marumori [20] and Belyaev-Zelevinskii [21] techniques. The boson Hamiltonians derived in these cases differ from (42) for two basic differences: First, they are written in terms of a "collective" boson $b^\dagger$ and, second, they contain higher-order operators. Concerning the first point, the difference between the $b_m^\dagger$ operators defined in Sec. II and this $b^\dagger$ arises from the latter being associated with the fermion $B^\dagger = \sum_{m=1}^{\Omega} B_m^\dagger$ rather than with the single $B_m^\dagger$. Higher-order terms in these Hamiltonians correct, instead, for the Pauli principle. In the Marumori case, for instance, the origin of these terms can be easily observed by repeating the procedure of Sec. II with the only difference consisting in the use of the $B^\dagger$ and $b^\dagger$ in the definition of the $S^{(N)}$ and $s^{(N)}$ spaces. Terms up to Nth order are now necessary in the boson Hamiltonian in order to guarantee the equality between the corresponding fermion and boson matrix elements of these spaces. This is not the case for the Hamiltonian (42) due to the special choice of the basis (4) and (7) which allows an easier elimination of spurious components associated with a violation of the Pauli principle in the boson space. In the following, we will also refer to some RPA calculations based on these boson Hamiltonians of the literature.

B. Calculations with our procedure

In substitution of the operator (20), we simply introduce here

$$q^\dagger = X \sum_i b_i^\dagger + Y \sum_i b_i \ , \tag{51}$$

with X and Y real and where the index ν has been suppressed since we refer exclusively to the first excited state. Similarly, we rewrite the operator (29) as

$$S = \frac{1}{2} Z \sum_{ij} b_i^\dagger b_j^\dagger \ . \tag{52}$$

By means of the unity operator [special case of (33)]

$$\hat{I} = \sum_{n=0}^{\Omega} |n)(n| \ , \tag{53}$$

where $|n)$ is the state (50c), we construct the ground state

$$|\widetilde{\mathrm{RPA}}) = \hat{I} N e^S|0) = \sum_{n=0}^{\Omega/2} Z^n G(n, Z)|2n) \ , \tag{54a}$$

where

$$G(n, Z) = \frac{F(n)}{\sqrt{\sum_{n=0}^{\Omega/2} Z^{2n} F(n)^2}} \tag{54b}$$

and

$$F(n) = \frac{(2n)!}{n! 2^n \mathcal{N}_{2n}} \ . \tag{54c}$$

Similarly, the excited state is

$$|\widetilde{\nu}) = \hat{I} q^\dagger |\widetilde{\mathrm{RPA}}) = \sum_{n=0}^{\Omega/2} Z^n G(n, Z)[Y a(2n)|2n-1) + X b(2n)|2n+1)] \ , \tag{55a}$$

where

$$a(2n) = (\Omega - 2n + 1)\mathcal{N}_{2n-1}^{-1}\mathcal{N}_{2n} \ , \tag{55b}$$

$$b(2n) = (2n+1)\mathcal{N}_{2n+1}^{-1}\mathcal{N}_{2n} \ . \tag{55c}$$

By noticing that

$$(n|H_b|n') = \delta_{n',n}\left(-\frac{\epsilon}{2}\Omega + \epsilon n\right) + \delta_{n',n+2}\left[-V\mathcal{N}_n^{-1}\mathcal{N}_{n+2}\frac{(\Omega-n)!}{(\Omega-n-2)!2}\right] + \delta_{n,n'+2}\left[-V\mathcal{N}_{n'}^{-1}\mathcal{N}_{n'+2}\frac{(\Omega-n')!}{(\Omega-n'-2)!2}\right] \ , \tag{56}$$

the energies $\widetilde{E}_0$ [Eq. (37)] and $\widetilde{E}_\nu$ [Eq. 36)] are now ready to be evaluated.

The calculations which we are going to discuss consist of, first, the minimization of $\widetilde{E}_0$ with respect to Z and, then, by making use of the values of this variable so derived, the minimization of $\widetilde{E}_\nu$ with respect to X and Y. These energies (in units of ϵ) are shown in Figs. 1, 2, and 3 for the cases $\Omega = 8$, 14, and 30, respectively, as a function of the interaction parameter $F = \Omega V/\epsilon$. In each figure, the solid lines are the exact results while the dashed ones refer to our procedure. In all three cases, the $\widetilde{E}_0$ energy reproduces rather well the exact values, some small differences appearing only with the increasing of the interaction parameter F. A better agreement is found for the $\widetilde{E}_\nu$ energy, such that solid and dashed lines are essentially overlapping in all three cases and for the range of F shown. However, because of the behavior of the exact energies of the ground and excited states which tend to coincide as soon as F increases, $\widetilde{E}_0$ crosses $\widetilde{E}_\nu$ at a critical F. The difference $\widetilde{E}_\nu - \widetilde{E}_0$ is shown, with a dashed line labeled 1 in Figs. 4, 5, and 6 for the cases $\Omega = 8$, 14, and 30, respectively. In the same figures, the solid line refers to the exact result and the long-dashed one to the RPA result. The meaning of the other lines labeled 2 and 3 will be discussed in the next subsection.

With reference to the RPA-like calculations [9,14,19] based on the boson Hamiltonians discussed in the final part of Sec. IV A, we notice that no such crossing occurs in these cases. For increasing Ω, the above energy difference tends torward a rather constant value which, in the case $\Omega = 30$, is around 0.3 in the range $F = 1.6$–4.0. This refers both to the Marumori- and the Belyaev-Zelevinskii-type Hamiltonians truncated at fourth order. However, the absolute values of the energies of ground and first excited states tend to diverge considerably from the exact ones as soon as F grows (still in the $\Omega = 30$ case, for instance, it is $E_{\text{g.s.}}/\epsilon = -16.8$ at F=2.0).

In Ref. [19], a ground state of the form (28) with an exponent S containing an additional term linear in the boson $b^\dagger$ besides the quadratic one has been examined. However, a state of this type will not be considered here due to its clear incompatibility with the Hamiltonian (42) whose exact ground state carries only even powers of $b^\dagger_m$ operators.

With reference to the procedure of Ref. [13], finally, we notice that its results observed in the case of the Lipkin model exhibit a clear difference from those examined so far in this paper. The energy difference relative to first excited and ground states in the case of Ref. [13], in fact, only deviates from the RPA one in the proximity of the critical point $F = 1$ and, then, approaches zero smoothly. In Figs. 4–6, instead, we have already seen that the approximate energy difference is quite close to the exact one up to values of F larger than 1 and, then, approaches a point at which it becomes negative.

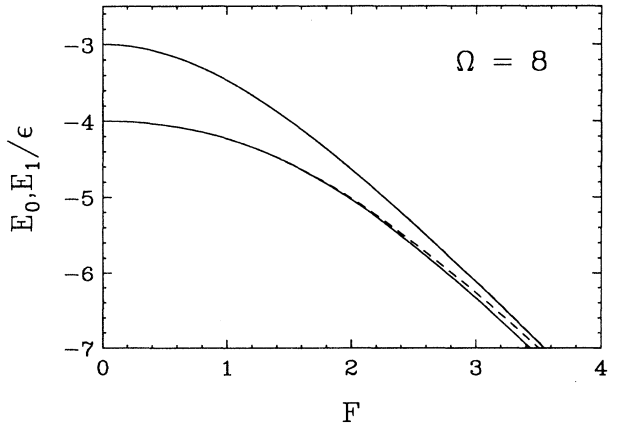

FIG. 1. Energy (in units of ϵ) of ground and first excited states of the Lipkin model, as a function of the interaction parameter $F = \Omega V/\epsilon$. The calculations refer to the case $\Omega = 8$. The solid lines are the exact results and the dashed lines are the results obtained with the procedure illustrated in the text.

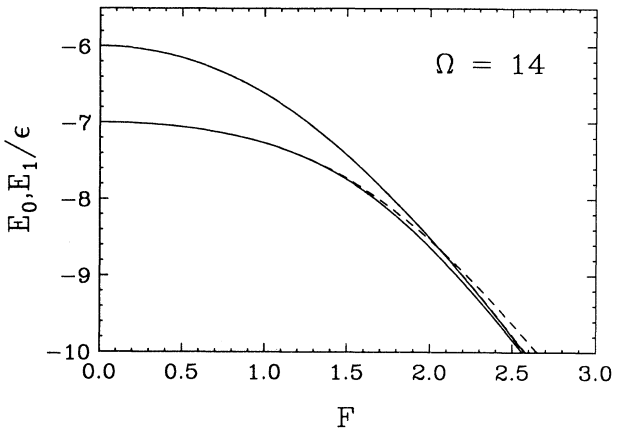

FIG. 2. Same as in Fig. 1 for $\Omega = 14$.

C. Searching for a better ground state

The results discussed so far depend, of course, on the wave function adopted for the ground state. Our choice (28), guided by the condition (21), was shown to be a

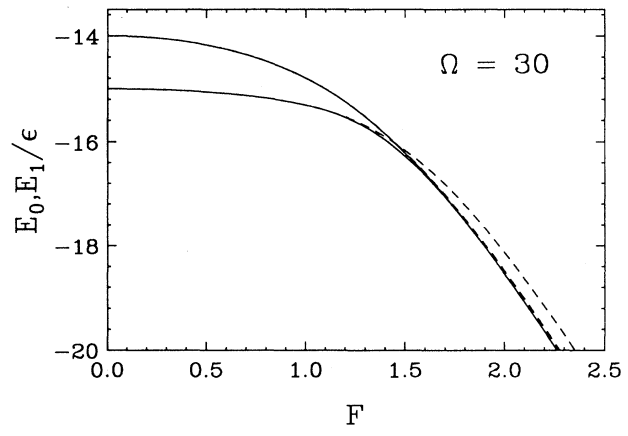

FIG. 3. Same as in Fig. 1 for $\Omega = 30$.

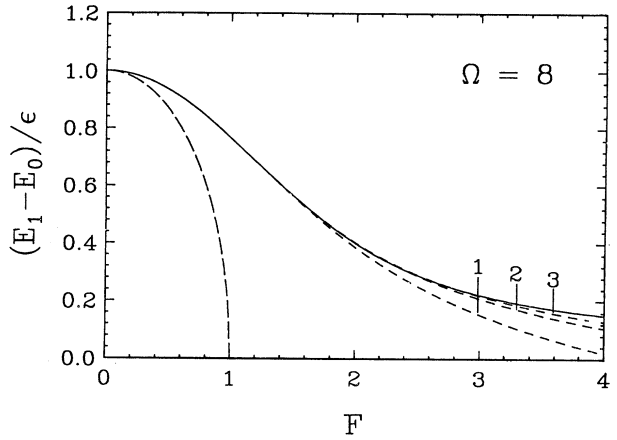

FIG. 4. Energy (in units of ϵ) of the first excited state of the Lipkin model, relative to the ground state, as function of the interaction parameter $F = \Omega V/\epsilon$. The calculations refer to the case $\Omega = 8$. The solid line is the exact result, the long-dashed line is the RPA result, and the dashed lines are the results obtained with our procedure. For the meaning of the symbols 1, 2, and 3, see the text.

rather good one in the cases just treated. However, this form was not always found to be satisfactory. We will investigate now how to search for a better form of this wave function.

In the case of the Lipkin model, the exact ground state of the Hamiltonian (42) is a superposition of $\frac{\Omega}{2}+1$ components carrying from 0 up to Ω particle-hole excitations. The coefficients attached to these components can be determined by minimizing the expectation value of the Hamiltonian in this state by considering the coefficients as independent variational parameters. The decomposition (54a) shows a dependence on only one parameter, Z, of the above $\frac{\Omega}{2}+1$ coefficients in the trial wave function (31) we have used so far. In order to search for a better parametrization of the ground state wave function, let us introduce for it the more general expression

$$|\text{g.s.})_2 = \hat{I} N_2 e^{\frac{1}{2} Z_2 \sum_{ij} b_i b_j} |\text{g.s.})_1 \ , \tag{57}$$

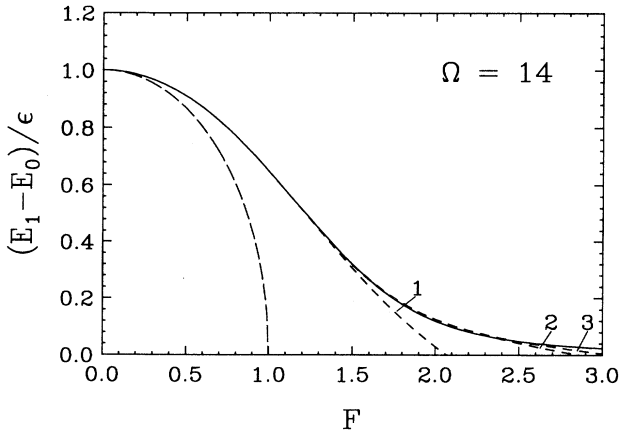

FIG. 5. Same as in Fig. 4 for $\Omega = 14$.

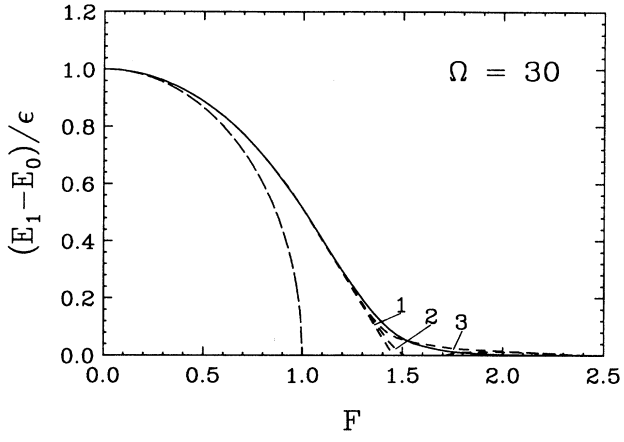

FIG. 6. Same as in Fig. 4 for $\Omega = 30$.

where we have redefined, for convenience,

$$|\widetilde{\text{RPA}}) \equiv |\text{g.s.})_1 = \hat{I} N_1 e^{\frac{1}{2} Z_1 \sum_{ij} b_i^\dagger b_j^\dagger} |0) \ . \tag{58}$$

In these expressions, $\hat{I}$ is the operator (53) and N_1, N_2 are normalization constants. The state $|\text{g.s.})_2$ can be decomposed as

$$|\text{g.s.})_2 = N_2 \sum_{n=0}^{\Omega/2} \sum_{m=0}^{n} Z_1^n Z_2^m G(n, Z_1) H(n, m) |2n - 2m) \ , \tag{59a}$$

with

$$H(n,m) = \frac{\mathcal{N}_{2n-2m}}{\mathcal{N}_{2n}} \frac{(2n)!}{2^m m!(2n-2m)!} \tag{59b}$$

and $G(n, Z)$ given by (54b). This decomposition recalls the previous (54a) with an important difference being that the $\frac{\Omega}{2}+1$ coefficients depend now on two parameters Z_1, Z_2 rather than Z_1 alone. If Z_1 is fixed by the minimization of $\widetilde{E}_0 (\equiv E_0^{(1)})$ discussed in the previous subsection, minimizing $E_0^{(2)} = {}_2(\text{g.s.}|H_b|\text{g.s.})_2$ with respect to Z_2 can only give rise to an energy less or equal to $E_0^{(1)}$ (corresponding to $Z_2 \neq 0$ or $Z_2 = 0$, respectively). Since the evaluation of $E_0^{(2)}$ essentially requires knowledge of the matrix elements

$$(m|e^{\frac{1}{2} Z \sum_{ij} b_i b_j} |m') \ , \tag{60}$$

as well as of the matrix elements (56) of the boson Hamiltonian, it involves a numerical effort of the same level as the evaluation of $E_0^{(1)}$.

Similarly, the state

$$|\text{g.s.})_3 = \hat{I} N_3 e^{\frac{1}{2} Z_3 \sum_{ij} b_i^\dagger b_j^\dagger} |\text{g.s.})_2 \tag{61}$$

depends on the three parameters Z_1, Z_2, Z_3. If Z_1 and Z_2 are taken as those fixed through the minimizations of $E_0^{(1)}$ and $E_0^{(2)}$, respectively, also minimizing $E_0^{(3)} = {}_3(\text{g.s.}|H_b|\text{g.s.})_3$ is as difficult as the previous ones. It only requires complex conjugates of the matrix elements (60)

TABLE I. Ground state energies of the Lipkin model ($\Omega = 30$) for different values of the interaction parameter F and at different levels n of approximation. Also shown are the corresponding exact values. See Sec. IV C for details.

	$F = 1.4$		$F = 2.8$		$F = 4.2$	
n	$E_0^{(n)}$	Z_n	$E_0^{(n)}$	Z_n	$E_0^{(n)}$	Z_n
1	-15.90561	0.337×10^{-1}	-22.64610	0.519×10^{-1}	-31.80271	0.575×10^{-1}
2	-15.92705	0.762×10^{-2}	-23.22068	0.203×10^{-1}	-32.38418	0.130×10^{-1}
3	-15.94548	-0.238×10^{-2}	-23.22879	0.985×10^{-3}	-32.43203	0.201×10^{-2}
4	-15.95648	0.609×10^{-2}	-23.23309	0.234×10^{-2}	-32.45374	0.299×10^{-2}
5	-15.96254	-0.145×10^{-2}	-23.23566	0.559×10^{-3}	-32.46634	0.105×10^{-2}
6	-15.96493	0.310×10^{-2}	-23.23738	0.150×10^{-2}	-32.47466	0.188×10^{-2}
7	-15.96577	-0.561×10^{-3}	-23.23858	0.382×10^{-3}	-32.48054	0.725×10^{-3}
8	-15.96601	0.104×10^{-2}	-23.23946	0.108×10^{-2}	-32.48496	0.138×10^{-2}
9	-15.96608	-0.161×10^{-3}	-23.24012	0.285×10^{-3}	-32.48836	0.555×10^{-3}
10	-15.96610	0.280×10^{-3}	-23.24064	0.832×10^{-3}	-32.49111	0.109×10^{-2}
$E_0^{(\text{exact})}$	-15.96636		-23.24366		-32.51377	

in addition to (56). Moreover, it is also in this case $E_0^{(3)} \leq E_0^{(2)}$. The procedure can go on similarly for $|\text{g.s.})_n$ with $n = 4, 5, ...$, being, in general, true that

$$|\text{g.s.})_n = \hat{I} N_n e^{\frac{1}{2} Z_n \sum_{ij} b_i^\dagger b_j^\dagger} |\text{g.s.})_{n-1} , \tag{62}$$

if n is odd [and $|\text{g.s.})_0 \equiv |0)$], while

$$|\text{g.s.})_n = \hat{I} N_n e^{\frac{1}{2} Z_n \sum_{ij} b_i b_j} |\text{g.s.})_{n-1} , \tag{63}$$

if n is even ($n \geq 2$). By minimizing $E_0^{(n)}$ with respect to Z_n alone and taking the remaining parameters $Z_1, Z_2, ..., Z_{n-1}$ as those which result from the previous minimizations, one repeates an operation, as n grows, always at the same level of difficulty of the initial one ($n = 1$), improving at each step the degree of approximation of the ground state.

We have performed some applications of the procedure just described. In Table I, we show the ground state energies $E_0^{(n)}$, with n ranging from 1 up to 10, which are calculated in the case $\Omega = 30$ and for F=1.4, 2.8, and 4.2. In correspondence to each n value, we also show the values of the Z_n parameters calculated for each F. The values $E_0^{(n)}$ exhibit, as n increases, a clear convergence torward the exact value accompanied by a progressive reduction of the parameter Z_n (to be read for n even and odd, separately). This is more evident as the interaction parameter F gets smaller.

With reference to Figs. 1–3, it is clear from Table I that, after a few iterations, exact and approximate ground state energies become indistinguishable. This was already the case for the energies of the first excited state evaluated in the previous subsection and the small improvement found by minimizing $E_1^{(n)} \propto {}_n(\text{g.s.}|q\hat{I}H_b\hat{I}q^\dagger|\text{g.s.})_n$ with respect to X and Y, for $n > 1$, cannot be appreciated in these figures. In Figs. 4–6, we show the difference $E_1^{(n)} - E_0^{(n)}$ for $n = 2$ and 3. The improvement is visible in these cases. Values of F, F_{cr} still occur at which this difference becomes negative but they are now larger as compared to those found at $n = 1$ and, moreover, this negative difference gets smaller as n increases. As a numerical example, at $\Omega = 30$, it is $F_{\text{cr}} \sim 2.4$ for $n = 3$ while $F_{\text{cr}} \sim 1.4$ for $n = 1$. Still at $\Omega = 30$, $n = 10$, and $F = 4.0$, it is $\frac{E_1 - E_0}{\epsilon} = -0.56 \times 10^{-1}$, that is, $\frac{E_1 - E_0}{E_0} = 0.18 \times 10^{-2}$, while the same quantities for $n = 1$ are about 10 times larger.

V. SUMMARY AND CONCLUSIONS

In this paper we have examined the derivation of the RPA equations in a boson formalism and addressed special attention to the problem of the violation of the Pauli principle which is inherent in this theory.

We have started by establishing a correspondence between a fermion space built in terms of ph operators $B_{m\alpha}^\dagger$ acting on the HF state and a boson space built in terms of $b_{m\alpha}^\dagger$ operators acting on their vacuum. This correspondence has been conceived to guarantee each boson state as a correspondent of a fermion state allowed by the Pauli principle. We have then constructed the boson image of a general fermion operator and focused, in particular, on a two-body Hamiltonian.

The derivation of the RPA equations within this formalism has required, first, constructing an expression for the energy of the one-phonon state $q_\nu^\dagger|-)$ and, second, introducing two approximations: (a) a special form for the $q_\nu^\dagger$ operator as a linear combination of $b_{m\alpha}^\dagger$, $b_{m\alpha}$ and (b) a truncation of the boson Hamiltonian at terms of second order. Besides these approximations, however, the presence of a further approximation has been pointed out, consisting in the neglect, in the boson states involved, of components not corresponding to any fermion state allowed by the Pauli principle on the basis of the correspondence between fermion and boson spaces discussed above.

The first problem which has been faced in this paper has been that of the elimination of these components from both the RPA ground state and the associated one-phonon states. A projection operator has been introduced with this aim and its action on the above states

has been studied. New expressions for the ground state and one-phonon energies have been, then, obtained.

In order to test our procedure we have applied it to the Lipkin model. These quantities have been calculated and compared with exact and RPA results. With respect to the last ones, a clear improvement of the quality of the results has been observed. Comparisons with previous approaches have also been examined.

As a second problem, we have faced the search of a better ground state. Having the vacuum of the q_ν operator as a starting point, we have shown the possibility of constructing new forms of the ground state characterized by a wider parametrization. These forms have been obtained via a multistep minimization procedure and their energies tested at different stages. A rapid convergence toward the exact ground state energy has been observed.

Besides the spuriosity discussed in this paper and associated with a violation of the Pauli principle, other spuriosities can occur which are associated with the breaking of continuous symmetries of the Hamiltonian. An interesting feature of RPA is that such spuriosities separate out exactly and emerge as solutions of the equations of motion with zero energy [1,2]. In the approach followed in this paper, instead, this property does not appear to hold. This problem is common also to other extensions of the RPA such as a second RPA [1] or a generalized RPA [22] and for a wide discussion of this point we refer to Ref. [23].

The quality of the numerical tests carried out within the Lipkin model encourages the extension of similar calculations to more realistic cases. Compared with the calculations performed in this paper, however, some modifications appear necessary in such situations. In the Lipkin model, for instance, it has been possible to express the exponential of the ground state (28) by its full power series expansion projected onto the physical subspace $s^{(\Omega)}$ [Eq. (46)], even for large values of Ω ($\Omega = 30$). In a realistic case, instead, the complexity of all expressions involved makes it unavoidable to introduce a truncation in such an expansion at a value N of particle-hole excitations smaller than the maximum allowed. This is meant to make simpler both the application of the operator projecting onto $s^{(N)}$ and the evaluation of matrix elements of the boson Hamiltonian.

Also the boson Hamiltonian constructed as an image of a general fermion Hamiltonian is not expected to truncate exactly at second order as in the Lipkin case. As a result of the above approximate form of the ground state, terms up to N body are now expected to play a role when evaluating the expectation value of the boson Hamiltonian in this state. Therefore, being able to take into account such terms, no further approximation is introduced. However, a truncation of this operator at some lower order could be required for values of N not adequate.

Calculations similar to the previous ones, but working entirely in the fermion space, could also be attempted. The problems connected with the truncation of the Hamiltonian would not be present in this case. On the other hand, the difficulty inherent in the use of fermion operators $B^+_{m\alpha}$ in place of $b^+_{m\alpha}$ would imply a truncation in the exponential of the ground state definitively more severe than in the boson case. This appears as a drawback especially in relation with the multistep minimization procedure discussed in Sec. IV C. In fact, this procedure gives a better description of the ground state wave function when a larger number of particle-hole components is involved. Work is in progress within some simple realistic cases in order to perform a detailed comparison between fermionic and bosonic approaches.

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