

Variational approach to collective excitations

M. Sambataro^{1,*} and N. Dinh Dang^{2,†}

¹*Istituto Nazionale di Fisica Nucleare, Sezione di Catania, Corso Italia 57, I-95129 Catania, Italy*

²*RI-beam Factory Project Office, The Institute of Physical and Chemical Research, 2-1 Hirosawa, Wako City, 351-0198 Saitama, Japan*

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We discuss a variational approach to collective excitations in a boson formalism based on quasiparticles. Bosons are defined in correspondence with pairs of quasiparticles and boson images of fermion operators are constructed by means of a mapping procedure of Marumori-type. Phonons of the type used within the random phase approximation (RPA) are introduced as Bogoliubov transformations of these bosons. The variables entering into the definition of these phonons as well as of the quasiparticle operators are fixed simultaneously by minimizing the expectation value of the boson Hamiltonian in the vacuum of the phonons. The approach is tested within an exactly solvable two-level model which is characterized by a pairing Hamiltonian. A quite good agreement is found for the energies of the ground state and of the first 0^+ excited state. The comparison with the Bardeen-Cooper-Schrieffer method and the quasiparticle RPA as well as with some recent self-consistent RPA-type approaches is discussed. [S0556-2813(99)01103-6]

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I. INTRODUCTION

The study of correlations in quantum many-body systems is a subject of great interest among the physicists of various fields. Such an interest is testified to by the continuous development of new methods which aim at improving the treatment of these correlations and so at making the microscopic description of collective excitations as reliable as possible.

Among the approaches which have attracted more attention in this field, a preeminent role is certainly played by the random phase approximation (RPA). This represents, in fact, the simplest theory of excited states which admits the possibility that the ground state is not of purely independent-particle character but may contain correlations [1]. As is well known, however, this theory suffers from an internal inconsistency due to the replacement, during the derivation of its equations, of the expectation values in the correlated ground state by the corresponding values in the uncorrelated or Hartree-Fock (HF) one. This is usually known as the quasiboson approximation (QBA). This important drawback has provided the starting point for the elaboration of several approaches attempting to restore the self-consistency of the theory. Among the first who have dealt with this problem we quote Hara [2] and Rowe [3]. Since then, several other approaches have appeared within the same subject both in nuclear physics [4–18] and in other fields [19]. Also the present work has to be set in this context.

These approaches can be essentially divided into two groups: (a) those formulated in a fermion formalism [2–13,19] and (b) those in which one has instead turned to a boson formalism [14–18]. For what concerns the first group, searching for the self-consistency and therefore avoiding the QBA ultimately implies evaluating expectation values of one- and two-body operators in the (unknown) correlated ground state. Various approximation schemes have been de-

veloped for the best determination of these quantities. They usually lead to the construction of a set of nonlinear equations which are solved iteratively. Difficulties inherent in the practical realization of this scheme are discussed in Ref. [13].

For what concerns group (b), the main idea of these approaches consists of transferring first the whole problem onto an appropriate boson space. This space is built by means of boson operators which are the “images” of the fermion operators defining the standard RPA phonons. These boson operators also allow to define new boson phonons. By means of an appropriate procedure, any fermion operator is mapped onto its boson image so that all calculations can be performed in this space.

A clear advantage of the boson approach over the fermion one is that the internal inconsistency typical of RPA is fully overcome. Evaluating the expectation value of a boson operator in the correlated ground state does not cause indeed any difficulty since it can now be done without an explicit knowledge of the wave function of this state. Moreover, the phonon operators are ideal bosons and so also the problems related to the definition of the ground state of the system as vacuum of non-commuting fermion phonons [10] are overcome. The standard RPA equations can be easily derived in correspondence with the use of a “zeroth-order” boson Hamiltonian. Therefore, this boson formalism offers an efficient way of going beyond RPA which consists of making use of higher-order boson images of the Hamiltonian [18]. Similarly to what happens in the self-consistent fermion approaches to RPA, this leads to a set of nonlinear equations. Of course, using this boson formalism also leads to a violation of the Pauli principle and this problem has been the subject of a recent investigation [17].

The purpose of the present work is that of further developing an RPA-type approach to collective excitations within a boson formalism. Differently from previous works on this subject [17,18] we will base this formalism on quasiparticles. This will allow a simultaneous treatment of particle-hole and particle-particle (hole-hole) correlations. In short, we will

*Electronic address: samba@ct.infn.it

†Electronic address: dang@rikaxp.riken.go.jp

first perform a standard Bogoliubov transformation and define a set of boson operators in correspondence with quasiparticle pair operators. A boson space will be defined in terms of these bosons and a mapping procedure will allow us to transform all fermion operators of interest into equivalent operators acting in this boson space. As a further step, RPA-type phonons will be constructed as Bogoliubov transformations of these bosons and the structure of both the quasiparticles and the phonons will be simultaneously fixed by minimizing the expectation value of the boson Hamiltonian in the vacuum of these phonons under some constraints. These constraints are related to the conservation of the particle number (otherwise violated in this quasiparticle formalism) and to the fermion and boson nature of the quasiparticle and phonon operators, respectively. Of course, performing this minimization is equivalent to solving a set of nonlinear equations, which is formally similar to what is already seen in the case of fermion self-consistent approaches.

This way of proceeding shares some common points with well known approaches like the Bardeen-Cooper-Schrieffer (BCS) method [or, more in general, the Hartree-Fock-Bogoliubov (HFB) one] and the quasiparticle RPA (QRPA). For what concerns the similarity with the first one, one notices already at this stage (but it will be clearer in the following) that the present way of proceeding reminds a kind of ‘‘higher order’’ BCS. The step forward with respect to BCS originates from the second Bogoliubov transformation which leads to a new vacuum, used to evaluate the expectation values of the Hamiltonian and of the number operator, which is richer in structure than the standard quasiparticle vacuum.

A similarity with the QRPA is also evident due to the introduction of an RPA-like phonon which, although an ideal boson, closely reminds the standard QRPA one. However, important differences between the two approaches can be seen since, in the present case, (i) both the quasiparticles and the phonons are fixed simultaneously, (ii) the ground state energy (rather than the excitation energy as in QRPA) is the basic objective of the procedure and (iii) this is a variational procedure. Point (ii) also represents a further point of difference with the work of Ref. [18] which was instead focused on the excitation energy of the system. Last but not least, we mention the fact that the boson Hamiltonian which is used in this calculation and which is truncated at four-boson terms is considerably more refined than the one which would be sufficient to obtain the standard RPA equations working in a boson formalism.

The paper is organized as follows. In Sec. II, we will describe the procedure. In Sec. III, we will show several applications of this procedure in the case of an exactly solvable two-level model. In the same section, we will also compare this approach with others like BCS, QRPA and some recently developed fermion self-consistent approaches. Finally, in Sec. IV, we will summarize the results and draw some conclusions.

II. THE FORMALISM

In order to avoid a notation otherwise rather cumbersome, we will illustrate the formalism directly in the case of the exactly solvable model which has been chosen as a test for our calculations. This model, although rather simple, offers

all the basic features of a realistic calculation and so also the extension of the formalism to any other case does not give cause for special concerns.

The model has been first employed by Högaasen-Feldman [20] and refers to a system of nucleons interacting in an average potential via a pairing force. The Hamiltonian is therefore of the type

$$\hat{H} = \sum_j \epsilon_j \hat{N}_j - G \sum_{j,j'} \sqrt{\Omega_j} \sqrt{\Omega_{j'}} A_j^\dagger A_{j'}, \quad (1)$$

with

$$\hat{N}_j = \sum_m a_{jm}^\dagger a_{jm}, \quad (2)$$

$$A_j^\dagger = \frac{1}{\sqrt{2}} [a_j^\dagger a_j^\dagger]^0, \quad (3)$$

where $\Omega_j = j + \frac{1}{2}$ and a_{jm}^\dagger creates a particle with angular momentum j and projection m . The simplifying hypothesis is that there are only two single-particle levels with the same angular momentum. Hence, the index j of a_{jm}^\dagger will be used thereafter to distinguish lower and upper level, while the angular momentum remains unchanged. We will also replace Ω_j by Ω , for simplicity.

The operators \hat{N}_j , A_j^\dagger , and the Hermitian conjugate A_j obey the commutation relations

$$[A_j, A_{j'}^\dagger] = \delta_{jj'} \left(1 - \frac{\hat{N}_j}{\Omega} \right), \quad (4)$$

$$[\hat{N}_j, A_{j'}^\dagger] = \delta_{jj'} 2A_j^\dagger. \quad (5)$$

These commutators define an SU(2) algebra for each level and the two-level model satisfies an SU(2) \otimes SU(2) algebra. Thanks to this special group structure, the derivation of the exact eigenvalues of the Hamiltonian only requires some simple angular-momentum algebra for the construction of the matrix to be diagonalized. The calculations are performed within a space whose basic configurations are characterized by distributions of particles in seniority-zero states in both lower and upper levels.

In this work we shall limit ourselves to the study of the ground state and of the first 0^+ excited state of the system. Differently from Ref. [20], however, we will not only consider a system with a particle number $N = 2\Omega$ but we will rather leave N free to vary in the whole interval $(0, 4\Omega)$.

As has been anticipated in the Introduction, we will make use of a quasiparticle formalism and so we introduce the Bogoliubov-Valatin transformation

$$\alpha_{jm}^\dagger = u_j a_{jm}^\dagger - v_j \tilde{a}_{jm}, \quad (6)$$

where $\tilde{a}_{jm} = (-1)^{j-m} a_{j-m}$ and

$$u_j^2 + v_j^2 = 1. \quad (7)$$

We also define the state $|\rangle$ as the quasiparticle vacuum, i.e.,

$$\alpha_{jm}| \rangle = 0. \quad (8)$$

Inverting Eq. (6) (and its Hermitian conjugate) we can now rewrite any fermion operator in this quasiparticle formalism. The Hamiltonian (1) becomes

$$\begin{aligned} \hat{H} = & c_0 + \sum_i (c_1)_i \hat{N}_i + \sum_i (c_2)_i (\mathcal{A}_i^\dagger + \mathcal{A}_i) + \sum_{ij} (c_3)_{ij} \mathcal{A}_i^\dagger \mathcal{A}_j \\ & + \sum_{ij} (c_4)_{ij} (\mathcal{A}_i^\dagger \hat{N}_j + \hat{N}_j \mathcal{A}_i) + \sum_{ij} (c_5)_{ij} (\mathcal{A}_i^\dagger \mathcal{A}_j^\dagger + \mathcal{A}_j \mathcal{A}_i) \\ & + \sum_{ij} (c_6)_{ij} \hat{N}_i \hat{N}_j, \end{aligned} \quad (9)$$

with

$$\mathcal{A}_j^\dagger = \frac{1}{\sqrt{2}} [\alpha_j^\dagger \alpha_j^\dagger]^0, \quad (10)$$

$$\hat{N}_j = \sum_m \alpha_{jm}^\dagger \alpha_{jm}, \quad (11)$$

and whose coefficients can be found in Ref. [21]. Similarly, the particle number operator $\hat{N} = \sum_j \hat{N}_j$ becomes

$$\hat{N} = 2\Omega \sum_j v_j^2 + \sum_j (u_j^2 - v_j^2) \hat{N}_j + 2\sqrt{\Omega} \sum_j u_j v_j (\mathcal{A}_j^\dagger + \mathcal{A}_j). \quad (12)$$

As is well known, the minimization of the expectation value

$$\langle |\hat{H}| \rangle = c_0 = \Omega \sum_i v_i^2 (2\epsilon_i - Gv_i^2) - G\Omega^2 \left(\sum_i u_i v_i \right)^2, \quad (13)$$

with respect to the variables u_j, v_j and under the constraint

$$\langle |\hat{N}| \rangle = 2\Omega \sum_j v_j^2 = N \quad (14)$$

which guarantees the conservation of the particle number in average, gives rise to the BCS equations. In particular, it can be shown by making use of the Thouless theorem [25] that a necessary (although not sufficient [22]) condition for this minimum to occur is that

$$\langle |(\hat{H} - \lambda \hat{N}) \alpha_{jm}^\dagger \alpha_{j'm'}^\dagger | \rangle = 0, \quad (15)$$

where λ is the Lagrange multiplier. Equations (7), (14), and (15) define the well-known BCS equations for the variables u_j, v_j , and λ .

The variational procedure that we are going to study in this work draws inspiration from that just mentioned for BCS and examines its extension to a higher order. To perform this procedure, keeping in mind that we want to describe 0^+ excited states, we introduce a set of zero angular-momentum boson operators b_j^\dagger in correspondence with the quasiparticle pair operators \mathcal{A}_j^\dagger . These boson operators obey the standard commutation relations

$$[b_i, b_j^\dagger] = \delta_{ij}, \quad [b_i, b_j] = [b_i^\dagger, b_j^\dagger] = 0. \quad (16)$$

We define the state $| \rangle$ as the vacuum of the operators b_j , i.e.,

$$b_j | \rangle = 0. \quad (17)$$

In correspondence with the fermion space

$$F \equiv \{ (\mathcal{A}_j^\dagger)^M (\mathcal{A}_{j'}^\dagger)^{M'} | \rangle \}, \quad 0 \leq M, M' \leq \Omega, \quad (18)$$

where the indices (j, M) and (j', M') refer to the lower and higher level, respectively, we therefore define the boson space

$$B \equiv \{ (b_j^\dagger)^M (b_{j'}^\dagger)^{M'} | \rangle \}, \quad 0 \leq M, M' \leq \Omega, \quad (19)$$

a one-to-one correspondence existing between the states of F and B . By resorting to a mapping procedure, we can construct the boson image in this space of any fermion operator. The procedure which has been employed in this work is the same which has been used in previous works [18] and is of Marumori-type. Namely, it is required that corresponding fermion and boson matrix elements are equal. Some details of the mapping procedure are given in the Appendix. Here we simply show the boson images of the Hamiltonian (9) and of the particle number operator (12). These are, respectively,

$$\begin{aligned} \hat{H}_B = & \alpha + \sum_i \beta_i (b_i^\dagger + b_i) + \sum_{ij} \gamma_{ij} b_i^\dagger b_j \\ & + \sum_{i \leq j} \phi_{ij} (b_i^\dagger b_j^\dagger + b_i b_j) + \sum_{i \leq j} \sum_k \epsilon_{ijk} (b_i^\dagger b_j^\dagger b_k + b_k^\dagger b_j b_i) \\ & + \sum_{i \leq j} \sum_{k \leq l} \delta_{ijkl} b_i^\dagger b_j^\dagger b_k b_l + \sum_{i \leq j \leq k} \sum_l \rho_{ijkl} \\ & \times (b_i^\dagger b_j^\dagger b_k^\dagger b_l + b_i^\dagger b_k b_j b_l), \end{aligned} \quad (20)$$

where the coefficients are given in the Appendix, and

$$\begin{aligned} \hat{N}_B = & \alpha_N + \sum_j (\beta_N)_j (b_j^\dagger + b_j) + \sum_j (\gamma_N)_j b_j^\dagger b_j \\ & + \sum_{i \leq j} \sum_k (\epsilon_N)_{ijk} (b_i^\dagger b_j^\dagger b_k + b_k^\dagger b_j b_i), \end{aligned} \quad (21)$$

with

$$\alpha_N = 2\Omega \sum_j v_j^2, \quad (22a)$$

$$(\beta_N)_j = 2\sqrt{\Omega} u_j v_j, \quad (22b)$$

$$(\gamma_N)_j = 2(u_j^2 - v_j^2), \quad (22c)$$

$$(\epsilon_N)_{ijk} = \frac{\sum_l (\beta_N)_l \left[\delta_{il} \delta_{jk} + \delta_{ik} \delta_{jl} \left(1 - \frac{2}{\Omega} \delta_{lk} \right) \right]}{\sqrt{1 + \delta_{ij}} \sqrt{1 + \delta_{ij} \left(1 - \frac{2}{\Omega} \right)}} - \frac{\delta_{ik}}{1 + \delta_{ij}} (\beta_N)_j - \frac{\delta_{jk}}{1 + \delta_{ij}} (\beta_N)_i. \quad (22d)$$

In both \hat{H}_B and \hat{N}_B the boson expansion has been truncated at four-boson terms but in the case of \hat{N}_B these last terms turn out to be zero. An analysis of the quality of the Hamiltonian (20) is provided in the Appendix.

We are now ready to implement a variational procedure of BCS type in the new boson space B . For this purpose we first perform the Bogoliubov transformation for bosons

$$q_v^\dagger = \sum_j (X_j^\nu b_j^\dagger - Y_j^\nu b_j), \quad (23)$$

where the X and Y coefficients are such to guarantee boson commutation relations to the q and q^\dagger operators, namely they satisfy the conditions

$$\sum_i (X_i^\nu X_i^{\nu'} - Y_i^\nu Y_i^{\nu'}) = \delta_{\nu\nu'}, \quad (24a)$$

$$\sum_i (X_i^\nu Y_i^{\nu'} - X_i^{\nu'} Y_i^\nu) = 0 \quad (24b)$$

(we suppose the X and Y coefficients to be real). We call $|0\rangle$ the vacuum of the operators q_ν , i.e.,

$$q_\nu |0\rangle = 0. \quad (25)$$

Inverting the expression (23) (and its Hermitian conjugate) and using Eq.(25) we can evaluate the expectation value of any boson operator in the vacuum $|0\rangle$ without explicitly knowing this state. These quantities are functions of the variables u, v, X , and Y . The variational procedure that we will explore in this work consists of minimizing the expectation value

$$\begin{aligned} \langle 0 | \hat{H}_B | 0 \rangle &= \Omega \sum_i v_i^2 (2\epsilon_i - Gv_i^2) - G\Omega^2 \left(\sum_i u_i v_i \right)^2 + \sum_{ij} \gamma_{ij} \sum_\nu Y_i^\nu Y_j^\nu + \sum_{i \leq j} \phi_{ij} \sum_\nu (Y_i^\nu X_j^\nu + X_i^\nu Y_j^\nu) \\ &+ \sum_{i \leq j} \sum_{k \leq l} \delta_{ijkl} \sum_{\nu\tau} (Y_i^\nu X_j^\nu X_k^\tau Y_l^\tau + Y_i^\nu Y_j^\tau Y_k^\tau Y_l^\nu + Y_i^\nu Y_j^\tau Y_k^\nu Y_l^\tau) \\ &+ \sum_{i \leq j \leq k} \sum_l \rho_{ijkl} \sum_{\nu\tau} (Y_i^\nu X_j^\nu Y_k^\tau Y_l^\tau + Y_i^\nu Y_j^\tau X_k^\tau Y_l^\nu + Y_i^\nu Y_j^\tau X_k^\nu Y_l^\tau + Y_i^\nu X_j^\tau Y_k^\tau Y_l^\nu + X_i^\nu Y_j^\tau Y_k^\tau Y_l^\nu + X_i^\nu Y_j^\tau Y_k^\nu Y_l^\tau) \end{aligned} \quad (26)$$

with respect to all these variables under the constraint that

$$\langle 0 | \hat{N}_B | 0 \rangle = 2\Omega \sum_j v_j^2 + 2 \sum_j (u_j^2 - v_j^2) \sum_\nu (Y_j^\nu)^2 = N, \quad (27)$$

and with the further constraints given by Eqs. (7), (24a), and (24b).

The formal similarity between this minimization and the one performed in BCS is evident. However, the new vacuum $|0\rangle$ exhibits a structure much richer than the BCS vacuum $|\rangle$. This can be seen in detail by noticing that, as a result of the condition (25), it is [22]

$$|0\rangle = N_0 \exp \left(\frac{1}{2} \sum_{ij} (YX^{-1})_{ij} b_i^\dagger b_j^\dagger \right) |\rangle \quad (28)$$

and remembering that $|\rangle$ is the image of the quasiparticle vacuum $|\rangle$. To the extent that \hat{H}_B and \hat{N}_B are good images of \hat{H} and \hat{N} , this minimization is expected to be more effective than the BCS one.

Following arguments similar to those employed in BCS and, in particular, by making use of the Thouless theorem for bosons [22], it is possible to show that such a minimization implies that

$$\langle 0 | \hat{H}'_B q_\nu^\dagger q_\nu^\dagger | 0 \rangle = 0 \quad (29)$$

(where $\hat{H}'_B \equiv \hat{H}_B - \lambda \hat{N}_B$ and λ is again a Lagrange multiplier), which closely recalls Eq. (15). However, differently from the BCS case where it is true by construction that

$$\langle |(\hat{H} - \lambda \hat{N}) \alpha_\nu^\dagger | \rangle = 0, \quad (30)$$

nothing can be said *a priori* concerning the matrix element $\langle 0 | \hat{H}'_B q_\nu^\dagger | 0 \rangle$. Whenever nonnegligible matrix elements of such a form were present, they would cause, of course, a ‘‘disturbance’’ in the definition of $|0\rangle$ and $q_\nu^\dagger |0\rangle$ as ground and excited states of the system, respectively. In such a case, one should resort to some extra operations like, for instance, a diagonalization in the space $\{|0\rangle, q_\nu^\dagger |0\rangle, \dots\}$. In general, the use of a more general Bogoliubov transformation (23) including a ‘‘shift’’ term [22] could also be taken into account. In all the cases examined in this work, however, this problem has never occurred since the matrix elements $\langle 0 | \hat{H}'_B q_\nu^\dagger | 0 \rangle$, although not exactly zero, have always remained much smaller than the matrix elements $\langle 0 | \hat{H}'_B | 0 \rangle$ or $\langle 0 | q_\nu \hat{H}'_B q_\nu^\dagger | 0 \rangle$. Therefore, we will not pay much attention to this problem in this work. We remark, in any case, that the

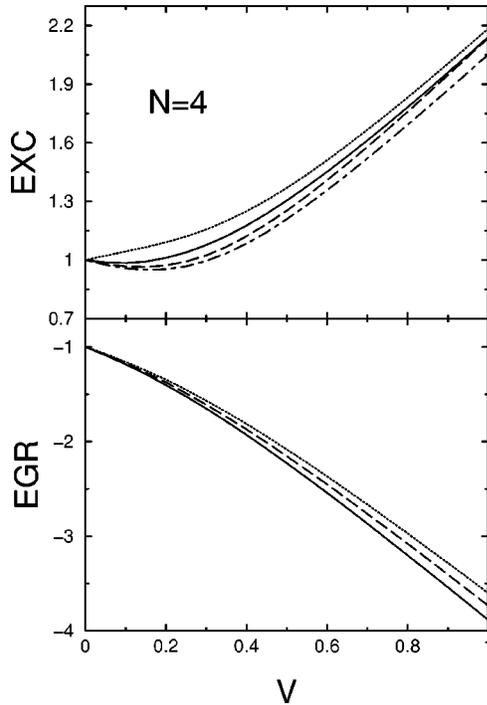


FIG. 1. Ground state energy (EGR) and excitation energy of the first 0^+ state (EXC) as a function of the variable V described in the text and for a number of particles $N=4$. Both energies are divided by 2ϵ , ϵ being the difference between the two single-particle energies. The angular momentum of the levels is $j=11/2$. The results refer to exact calculations (solid lines), BCS (dotted lines), QRPA (dot-dashed line), and the present approach (dashed lines).

Hamiltonian \hat{H}'_B is not diagonal in the one-phonon space $\{q_\nu^\dagger|0\rangle\}$ and so its diagonalization in this space is indispensable for a correct definition of the excited states.

III. CALCULATIONS AND DISCUSSION

The calculations that we will first discuss refer to the angular momentum $j=\frac{11}{2}$ and to single-particle energies $\epsilon_1=-1$ and $\epsilon_2=1$ (in arbitrary units). Results obtained are shown in Figs. 1–5. In each figure we plot, in the lower part, the ground state energy while, in the upper part, the excitation energy of the first 0^+ state [both energies are divided by $2\epsilon\equiv 2(\epsilon_2-\epsilon_1)$]. In Figs. 1–3, these energies are plotted as a function of the variable $V=G\Omega/2\epsilon$ and refer to systems with number of particles $N=4, 8$, and 12 , respectively. In Figs. 4 and 5, instead, we fix two values of this variable V ($V=0.5$ and 1.0 , respectively) and plot these energies for N ranging from 0 up to 4Ω . In each figure, results are shown for BCS (dotted line), present approach (dashed line), and exact calculations (solid line). In addition, in the case of the energy of the first excited state, we also show the results obtained within the QRPA [22] (dot-dashed line).

A. Ground state energies

Regarding the ground state energies, a glance at all figures shows that the results obtained within the present approach are systematically located between exact and BCS results. Particularly interesting is the case $N=2\Omega=12$ (half filling) shown in Fig. 3. In this case, in fact, BCS solutions exhibit a

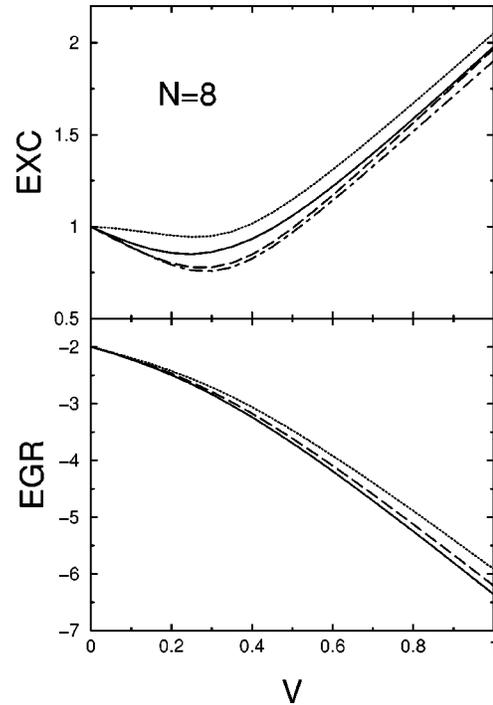


FIG. 2. As in Fig. 1 but for $N=8$.

transition from a normal to a superfluid phase at $V=0.28$. In the present approach, instead, this phase transition occurs at $V=0.37$. Both these transitions turn out to be hardly visible in the behavior of these energies. For a strength smaller than the critical value $V=0.37$, our results are almost identical to the exact ones whereas for larger values of V they start deviating although always remaining within 2% from the exact values. Similar calculations performed using other choices of the parameters of the Hamiltonian confirm qualitatively these results (see also another example in the following).

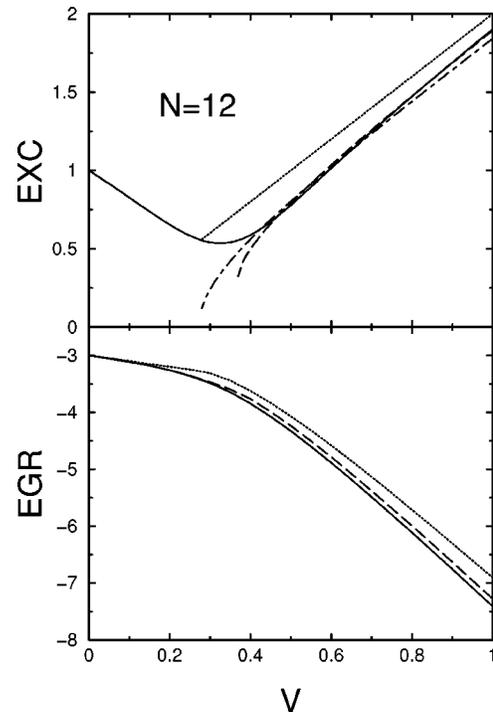


FIG. 3. As in Fig. 1 but for $N=12$.

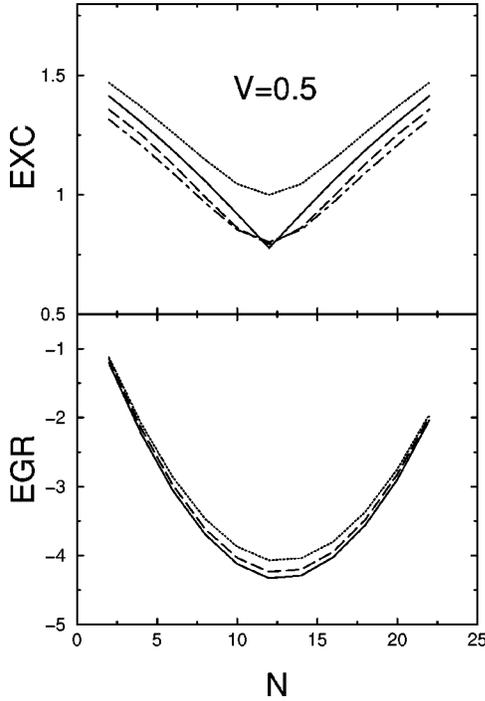


FIG. 4. Ground state energy (EGR) and excitation energy of the first 0^+ state (EXC) as a function of the particle number N and for a fixed value $V=0.5$. Further details are as in Fig. 1.

Before proceeding with the discussion of the results on the excited states, it is appropriate to insert a parenthesis on spurious states.

B. Spurious states

The case that we are going to treat in this paper, namely that of excited $J=0$ states, is a very delicate one in all the

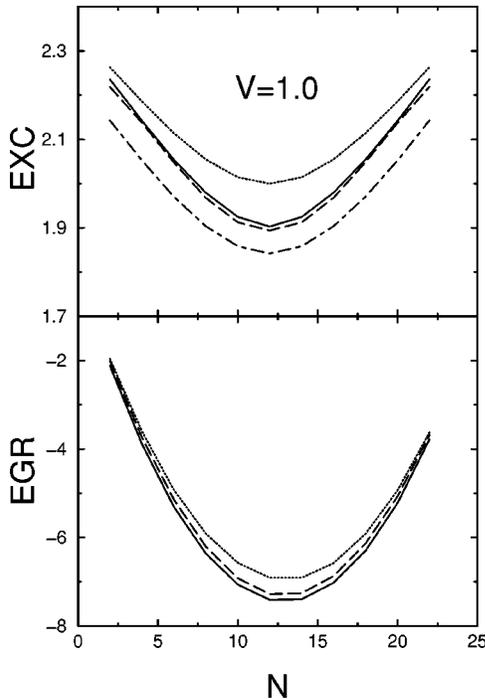


FIG. 5. As in Fig. 4 but for $V=1.0$.

three approaches that we are using. Let us begin with BCS, for instance. The problems concerning this case are well known in literature and are discussed in some detail in Ref. [23]. We will recall them here because they are of great help in examining our approach.

A low-lying excited state with $J=0$ can be written, in the quasiparticle formalism of this paper, as a linear combination of the type

$$|0, \nu\rangle = \sum_i c_i^\nu \mathcal{A}_i^\dagger | \rangle. \quad (31)$$

Such a state has components corresponding to various number of particles. However, in order to describe a system with N particles, it is reasonable to require that it should at least have an N -particle component. We can easily identify a state of the form (31) for which this is not the case. To see this we note that, remembering the quasiparticle version of the particle number operator \hat{N} (12), the constraint (14) and the definition (8) of the vacuum $| \rangle$, one has

$$(\hat{N} - N)| \rangle = 2\sqrt{\Omega} \sum_i u_i v_i \mathcal{A}_i^\dagger | \rangle. \quad (32)$$

If $|\psi_n\rangle$ is a normalized n -particle state and d_n^2 the probability that it is contained in $| \rangle$, we can write

$$(\hat{N} - N)| \rangle = \sum_n d_n^2 (\hat{N} - N) |\psi_n\rangle = \sum_n d_n^2 (n - N) |\psi_n\rangle. \quad (33)$$

This tells us that the state (32) has no component with $n = N$ and therefore should be excluded when calculating the properties of the excited two quasiparticle states with $J=0$.

In the special case of our two-level model, since we can form at most two linearly independent states of the form of Eq. (31), eliminating the state (32) means being left with only one state of this form. The coefficients c_i^ν of this state can be fixed by simply requiring its orthogonality to Eq. (32) and its normalization. One finds

$$c_1^\nu = -\frac{u_2 v_2}{\sqrt{u_1^2 v_1^2 + u_2^2 v_2^2}}, \quad c_2^\nu = \frac{u_1 v_1}{\sqrt{u_1^2 v_1^2 + u_2^2 v_2^2}}. \quad (34)$$

These coefficients define the structure of the excited BCS state with $J=0$ whose energy has been plotted in Figs. 1–5.

Spurious states are also observed in the approach under consideration in this paper and this fact can be understood on the basis of the same arguments already employed for BCS. Starting, in fact, from the expression (21) for the boson image of the number operator, expressing this in terms of the q^\dagger and q operators and making use of Eqs. (25) and (27), one can write

$$\begin{aligned}
(\hat{N}_B - N)|0\rangle &\approx \sum_\nu \left\{ \sum_j (\beta_N)_j (X_j^\nu + Y_j^\nu) + \sum_{i \leq j} \sum_k (\epsilon_N)_{ijk} \right. \\
&\quad \times \left[\left(\sum_\eta Y_k^\eta Y_i^\eta \right) (X_i^\nu + Y_i^\nu) + \left(\sum_\eta Y_k^\eta Y_i^\eta \right) \right. \\
&\quad \left. \left. \times (X_j^\nu + Y_j^\nu) + \left(\sum_\eta X_j^\eta Y_i^\eta \right) (X_k^\nu + Y_k^\nu) \right] \right\} q_{\nu}^\dagger |0\rangle \\
&\equiv q_{sp}^\dagger |0\rangle, \tag{35}
\end{aligned}$$

where we have truncated the expression at the one-phonon component. Following the same reasoning as for Eqs. (31)–(33), we see that this state has no component with $n=N$ particles and so has to be excluded from our calculations. We are, therefore, left with only one “physical” phonon q_{ph}^\dagger whose structure can be fixed by requiring its orthogonality to q_{sp}^\dagger and its normalization. The energies of the figures, for what concerns the procedure under study, refer to this “physical” phonon. It is worth noticing, in any case, that the phonons q_{sp}^\dagger and q_{ph}^\dagger are almost exactly those which result from the diagonalization of \hat{H}'_B in the one-phonon space $\{q_{\nu}^\dagger|0\rangle\}$. The energy of the state $q_{sp}^\dagger|0\rangle$, in particular, is always found quite low. So the same plots can also be obtained by performing this diagonalization and simply neglecting the lowest (or “spurious”) eigenvalue.

To complete these notes on spuriousity, we briefly comment also on the QRPA case. Here, one systematically observes a solution of the equations which is zero. The presence of such a spurious solution can be easily understood on the basis of Baranger’s remarks [24]. The starting point is the fact that the Hamiltonian of the system and the particle number operator commute:

$$[\hat{H}, \hat{N}] = 0. \tag{36}$$

If we use the expression (12) for \hat{N} and we approximate this commutator according to the method of the linearization [1] we find that

$$[\hat{H}, \hat{N}] \approx \left[H, 2\sqrt{\Omega} \sum_j u_j v_j (\mathcal{A}_j^\dagger + \mathcal{A}_j) \right] = 0. \tag{37}$$

In other words, the phonon

$$Q^\dagger = 2\sqrt{\Omega} \sum_j u_j v_j (\mathcal{A}_j^\dagger + \mathcal{A}_j) \tag{38}$$

is a solution of the equation

$$[\hat{H}, Q^\dagger] = \omega Q^\dagger, \tag{39}$$

with $\omega=0$. This ω is then a QRPA eigenvalue. Indeed, the X and Y coefficients of the QRPA spurious solution which are found numerically turn out to be exactly (within a normalization factor) those given by Eq. (38).

C. The first excited $J=0$ state

We can now proceed examining the energies of the first excited state with $J=0$. Also for these energies the present

approach provides a quite good agreement with the exact results for all three values of N examined. These values refer to the interval $(0, 2\Omega)$ but, as can also be seen in Figs. 4 and 5, excited energies are symmetrical with respect to the value $N=2\Omega$. We have already observed in Sec. III A that this last case (Fig. 3) is the one presenting a normal-superfluid phase transition and it can be noticed, especially in the case of QRPA and in the present approach, how the excited energies start deviating more and more from the exact ones while approaching the transition points. Still in this case we also see that our results are quite close to those obtained in QRPA while the difference with the BCS results is more marked. For the remaining N values and particularly for increasing values of the strength V (see Fig. 5, for instance) differences are more pronounced and the present approach is the one which provides the best agreement with the exact results.

D. Comparison with other recent calculations

In a quite recent publication by Dukelsky, Röpke, and Schuck [26], the same two-level model discussed in this paper has been used as a testing ground for three different many-body approaches for the treatment of correlations in Fermi systems: the self-consistent particle-particle RPA (SCppRPA), the variational RPA (VRPA) and the Brückner-Hartree-Fock (BHF) method. It is not our intention to make here a thorough discussion on these approaches and their interconnections for which we refer, of course, to Ref. [26]. We believe, however, that it is of some interest to see at least how these approaches compare with the one discussed in this paper within the same model.

For what concerns the SCppRPA method, we simply remind the reader that this is a generalization of the ppRPA [22] according to a fermion self-consistent scheme of the type outlined in the Introduction. In the special case of the model under discussion, two addition and removal phonons of the type used in the ppRPA are introduced and the SCppRPA ground state is defined as the vacuum of these phonons. RPA-like equations are then constructed which depend on the amplitudes defining these phonons as well as on one- and two-body density matrices (also depending on these amplitudes). The set of nonlinear equations so constructed is solved iteratively.

The VRPA, instead, is somehow closer in spirit to the one discussed in the present paper since it corresponds to a direct minimization of the expectation value of the Hamiltonian in the SCppRPA ground state. The main differences with respect to the present approach are the fact that the VRPA is fully developed in the fermion space and that it implies an explicit knowledge of the ground state wave function.

In Ref. [26] only ground state energies have been taken into account and only for $N=2\Omega$. However, differently from the cases of Figs. 1–5, also negative values of the pairing strength G have been considered to simulate repulsion among particles. Moreover, the calculations have been performed for $j=\frac{19}{2}$ while the single-particle energies are the same as in this work. In Table I, we have compared the results of the different approaches in the range $(-0.5-0.5)$ of the strength V explored in Ref. [26].

A glance at the table shows that our approach provides a very good agreement with the exact results in the whole

TABLE I. Results for the ground state energy (in arbitrary units) vs the variable V described in the text. The angular momentum of the levels is $j=19/2$ and the number of particles is $N=20$. For a description of the approaches involved see Sec. III D.

V	Exact	This work	VRPA	SCppRPA	BHF
-0.50	-18.55446	-18.55360	-18.55411	-18.55410	-18.68164
-0.45	-18.66849	-18.66784	-18.66821	-18.66821	-18.77071
-0.40	-18.78706	-18.78660	-18.78686	-18.78686	-18.86658
-0.35	-18.91072	-18.91040	-18.91058	-18.91058	-18.97002
-0.30	-19.04010	-19.03990	-19.04001	-19.04001	-19.08190
-0.25	-19.17600	-19.17588	-19.17594	-19.17594	-19.20324
-0.20	-19.31939	-19.31933	-19.31936	-19.31936	-19.33521
-0.15	-19.47153	-19.47150	-19.47151	-19.47151	-19.47916
-0.10	-19.63406	-19.63405	-19.63405	-19.63405	-19.63667
-0.05	-19.80919	-19.80919	-19.80919	-19.80919	-19.80957
0.00	-20.00000	-20.00000	-20.00000	-20.00000	-20.00000
0.05	-20.21101	-20.21101	-20.21101	-20.21101	-20.21047
0.10	-20.44921	-20.44917	-20.44918	-20.44918	-20.44390
0.15	-20.72625	-20.72593	-20.72600	-20.72599	-20.70373
0.20	-21.06339	-21.06100	-21.06132	-21.06130	-20.99397
0.25	-21.50260	-21.48640	-21.48772	-21.48733	-21.31929
0.30	-22.12491	-22.03620	-22.04037	-22.03638	-21.68509
0.35	-23.03321	-22.77899	-22.72688	-22.70769	-22.09757
0.40	-24.24608	-23.97001	-23.52903	-23.47803	-22.56372
0.45	-25.68929	-25.39821	-24.42583	-24.33106	-23.09128
0.50	-27.29077	-26.98390	-25.40086	-25.25808	-23.68858

range of V . The agreement remains quite good also outside this range: at $V=1.0$, for instance, our result deviates from the exact one still by less than 1%. As far as the comparison with the other approaches is concerned, in the interval (-0.5 – 0.3) our results are very close to the VRPA and SCppRPA ones. For larger values of V , instead, these approaches start to deviate more and more from the exact values.

To give a better insight into these results, we notice that, within our approach, a transition between normal and superfluid phases occurs at $V=0.32$. Therefore, beyond this point quasiparticles begin to play a crucial role in our calculations. The importance of a quasiparticle treatment is also stressed in Ref. [26] for $G>0.1$ (i.e., $V>0.25$). At this critical value, in fact, the RPA eigenvalue is seen to approach zero. However, although a SCRPA for superfluid systems can already be found in literature [13], none of the approaches discussed in Ref. [26] makes use of the quasiparticles formalism.

For completeness we also show in Table I the results which refer to BHF: this method appears to be the one with more difficulties in reproducing the exact results both for positive and negative values of the pairing strength. Further discussion on this point, however, goes beyond the purposes of the present work and we will skip it.

IV. SUMMARY AND CONCLUSIONS

In this article we have examined a variational approach to collective excitations within a boson formalism. Aiming at providing a simultaneous treatment of particle-hole and particle-particle (hole-hole) correlations, we have first introduced quasiparticles. Bosons have been defined in corre-

spondence with pairs of these quasiparticles. By means of a mapping procedure of Marumori-type we have constructed boson images of fermion operators truncating the expansion of the boson operators at four-boson terms. RPA-type phonons have been introduced as Bogoliubov transformations of the above bosons and we have also defined the ground state of the system as the vacuum of these phonons. The minimization of the expectation value of the boson Hamiltonian in this vacuum with respect to the variables defining the quasiparticles and the phonons operators has allowed to fix these variables.

Important features of this boson procedure are that (i) no RPA-type inconsistency occurs, (ii) no explicit knowledge of the ground state wave function is required and (iii) no ambiguities related to the noncommutativity of the phonon operators exist. Also the variational aspect of the procedure is an important feature always allowing to identify the exact ground state energy as a lower bound of the calculation.

As a test for our approach we have chosen an exactly solvable two-level model characterized by a pairing Hamiltonian. Ground state energies have been found in a quite good agreement with the exact results, always remaining located between these and the BCS ones. We have also calculated the energy of the first 0^+ excited state and compared it with the BCS and QRPA values. Also in this case our approach has offered a quite good agreement with the exact results providing globally the best results.

These calculations have all referred to a pairing Hamiltonian and, in some cases, differences between the various approaches have not been found relevant. It would certainly be quite interesting to perform a similar comparison in the

case of a more general Hamiltonian and some work is planned in this direction. Already on the basis of the present calculations, however, we can conclude that this approach shows itself as a valid alternative to the QRPA in all its different applications. Among these we mention, in particular, the proton-neutron QRPA which represents at the moment an essential tool of theoretical analysis in the field of double-beta decay and which has recently been the object of several studies [27].

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APPENDIX

The mapping technique used in this work follows the main lines of a procedure which has had several applications in the past both in the fermion-boson correspondence [28] and in the fermion-fermion one [29]. We refer to Ref. [30] for a general discussion of the method. Here, we simply outline its basic points.

The first step of the procedure consists in defining a fermion space F and a boson space B in a one-to-one correspondence. We have already seen that, in the present case, these spaces are those defined in Eqs. (18) and (19). In correspondence with a given fermion operator \hat{O}_F , the procedure searches for a boson operator \hat{O}_B such that all the eigenvalues of \hat{O}_F in F are also eigenvalues of \hat{O}_B in B . The operator \hat{O}_B defines the image of \hat{O}_F in B .

The boson operator is constructed via a step-by-step procedure. Each step involves the correspondence between increasingly larger fermion and boson subspaces. The larger these spaces are and, in general, the more complicated the n -body structure of the boson operator will be. In this work, wishing to construct boson images having at most four-boson terms, it is enough to consider up to the two subspaces

$$F' = \{ | \rangle, A_j^\dagger | \rangle, A_j^\dagger A_j^\dagger | \rangle, A_j^\dagger A_j^\dagger A_j^\dagger | \rangle, A_j^\dagger A_j^\dagger A_j^\dagger A_j^\dagger | \rangle \} \quad (\text{A1})$$

and

$$B' = \{ | \rangle, b_j^\dagger | \rangle, b_j^\dagger b_j^\dagger | \rangle, b_j^\dagger b_j^\dagger b_j^\dagger | \rangle, b_j^\dagger b_j^\dagger b_j^\dagger b_j^\dagger | \rangle \}. \quad (\text{A2})$$

Finding the boson image amounts to finding a boson operator such that corresponding matrix elements between these states (suitably normalized) are equal. The procedure is, therefore, of Marumori-type.

We have already discussed in Sec. II the case of the fermion number operator (12) which is mapped on the boson operator (21). In the case of the Hamiltonian (9), the boson image has the form (20) and the coefficients are

$$\alpha = c_0, \quad (\text{A3a})$$

$$\beta_i = (c_2)_i, \quad (\text{A3b})$$

$$\gamma_{ij} = 2\delta_{ij}(c_1)_j + (c_3)_{ij} + 4\delta_{ij}(c_6)_{ij}, \quad (\text{A3c})$$

$$\phi_{ij} = \sqrt{\frac{(\mathcal{N}_F)_{ij}^{(2)}}{(\mathcal{N}_B)_{ij}^{(2)}}} [(c_5)_{ij} + (c_5)_{ji}(1 - \delta_{ij})], \quad (\text{A3d})$$

$$\epsilon_{ijk} = \left\{ \sqrt{\frac{(\mathcal{N}_B)_{ij}^{(2)}}{(\mathcal{N}_F)_{ij}^{(2)}}} \left[\sum_{i'} ((c_2)_{i'} + 2(c_4)_{i'k}) \Delta_{ij,i'k}^{(2)} (\mathcal{N}_F)_{ij}^{(2)} \right] - \delta_{ik}\beta_j - \delta_{jk}\beta_i \right\} / (\mathcal{N}_B)_{ij}^{(2)}, \quad (\text{A3e})$$

$$\delta_{ijkl} = \left\{ \sqrt{\frac{(\mathcal{N}_F)_{ij}^{(2)}(\mathcal{N}_B)_{kl}^{(2)}}{(\mathcal{N}_F)_{kl}^{(2)}(\mathcal{N}_B)_{ij}^{(2)}}} \left[(c_0 + 2(c_1)_l + 2(c_1)_k + 4(c_6)_{ll} + 4(c_6)_{lk} + 4(c_6)_{kl} + 4(c_6)_{kk}) \Delta_{ij,kl}^{(2)} + \sum_{i'} \left((c_3)_{i'l} \Delta_{ij,i'l}^{(2)} + (c_3)_{i'k} \left(1 - \delta_{kl} \frac{2}{\Omega_k} \right) \Delta_{ij,i'l}^{(2)} \right) \right] - \alpha \Delta_{ij,kl}^{(2)} - \sum_{i'} (\gamma_{i'k} \Delta_{ij,i'l}^{(2)} + \gamma_{i'l} \Delta_{ij,i'k}^{(2)}) \right\} / (\mathcal{N}_B)_{kl}^{(2)}, \quad (\text{A3f})$$

$$\rho_{ijkl} = \sqrt{\frac{(\mathcal{N}_F)_{ijk}^{(3)}}{(\mathcal{N}_B)_{ijk}^{(3)}}} \sum_{i'j'} (c_5)_{i'j'} \Delta_{ijk,i'j'l}^{(3)} - \sum_{i' \leq j'} \phi_{i'j'} \Delta_{ijk,i'j'l}^{(3)}, \quad (\text{A3g})$$

where

$$(\mathcal{N}_F)_{ij}^{(2)} = \delta_{ij} \left(1 - \frac{1}{\Omega_i} \right) + 1, \quad (\text{A4a})$$

$$(\mathcal{N}_F)_{ijk}^{(3)} = \delta_{ij} \delta_{ik} \delta_{jk} 6 \left(1 - \frac{2}{\Omega_i} \right) \left(1 - \frac{1}{\Omega_i} \right) + (1 - \delta_{ij} \delta_{ik} \delta_{jk}) \times \left[(\delta_{ij} + \delta_{ik}) 2 \left(1 - \frac{1}{\Omega_i} \right) + \delta_{jk} 2 \left(1 - \frac{1}{\Omega_j} \right) \right], \quad (\text{A4b})$$

$$(\mathcal{N}_B)_{ij}^{(2)} = \delta_{ij} + 1, \quad (\text{A5a})$$

$$(\mathcal{N}_B)_{ijk}^{(3)} = \delta_{ij} \delta_{ik} \delta_{jk} 6 + (1 - \delta_{ij} \delta_{ik} \delta_{jk}) 2 (\delta_{ij} + \delta_{ik} + \delta_{jk}), \quad (\text{A5b})$$

$$\Delta_{ij,i'j'}^{(2)} = (\delta_{ii'} \delta_{jj'} + \delta_{ij'} \delta_{ji'}) / (\mathcal{N}_B)_{ij}^{(2)}, \quad (\text{A6a})$$

$$\Delta_{ijk,i'j'k'}^{(3)} = (\delta_{ii'} \delta_{jj'} \delta_{kk'} + \delta_{ii'} \delta_{jk'} \delta_{kj'} + \delta_{ij'} \delta_{jk'} \delta_{ki'} + \delta_{ij'} \delta_{ji'} \delta_{kk'} + \delta_{ik'} \delta_{ji'} \delta_{kj'} + \delta_{ik'} \delta_{jj'} \delta_{ki'}) / (\mathcal{N}_B)_{ijk}^{(3)}. \quad (\text{A6b})$$

TABLE II. Comparison between spectra of the Hamiltonians \hat{H}_F (9) and \hat{H}_B (20) for three values of the angular momentum j . Only the lowest 10 eigenvalues are shown. For further details see the Appendix.

	$j = 11/2$		$j = 15/2$		$j = 19/2$	
	E_F	E_B	E_F	E_B	E_F	E_B
1	-17.069	-17.072	-22.064	-22.065	-27.065	-27.065
2	-16.172	-16.194	-21.231	-21.239	-26.282	-26.286
3	-14.813	-14.912	-19.961	-20.002	-25.088	-25.109
4	-13.785	-13.812	-18.740	-18.751	-23.751	-23.816
5	-13.377	-13.717	-18.563	-18.692	-23.718	-23.725
6	-12.601	-12.700	-17.707	-17.755	-22.774	-22.807
7	-11.922	-12.623	-17.090	-17.391	-22.313	-22.462
8	-11.200	-12.369	-16.340	-16.484	-21.501	-21.591
9	-10.821	-11.440	-15.738	-16.275	-20.824	-21.118
10	-10.558	-10.920	-15.602	-15.759	-20.635	-20.646

As a test on the quality of the boson Hamiltonian (20) we have made a comparison between fermion and boson spectra. In Table II, columns E_F , we show the lowest 10 eigenvalues of the fermion Hamiltonian (9) diagonalized in the space (18) for three values of the angular momentum j : $\frac{11}{2}$, $\frac{15}{2}$, and $\frac{19}{2}$. The coefficients of this Hamiltonian are functions of the (u_i, v_i) Bogoliubov-Valatin variables and for these we have taken the values resulting from the procedure of Sec. II for a strength $V=0.5$ and a number of particles $N=2\Omega$.

In Table II, columns E_B , we show the corresponding spectra obtained by diagonalizing the boson Hamiltonian

(20) in the space (19). One observes a quite satisfactory agreement between fermion and boson spectra which testifies the good quality of this Hamiltonian. Of course, this agreement could be further improved by resorting to higher-order terms in the boson expansion of the Hamiltonian. However, with reference to possible realistic applications of the procedure, we have preferred to test an expansion containing up to four-boson terms. The use of the higher-order terms would very likely be avoided in such applications because of its complexity.

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