Mean field description of the ground state of many boson systems relevant to nuclei

F. Aldabe* and G. G. Dussel†
Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Pabellón 1, Ciudad Universitaria, (1428) Buenos Aires, Argentina

H. M. Sofia‡
Departamento de Física, Comisión Nacional de Energía Atómica, Avenida del Libertador 8250, (1429) Buenos Aires, Argentina
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In the present paper we give the explicit expressions for the ground state of a many boson system in different mean field approximations, such as Hartree-Bose, Bogoliubov, the particle-hole random phase approximation (RPA), and its coupling with the particle-particle RPA. The ground states obtained satisfy the requirement that the annihilation operators of the "elementary excitations" annihilates them. In all cases the ground state wave functions can be understood as a condensate of pairs of bosons.

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I. INTRODUCTION

The mean field description of fermion systems was studied in detail at the beginning of the 1960s. At that time it was shown that a mean field description can be obtained using the Hartree-Fock (HF) or Hartree-Fock-Bolgoliuvov (HFB) approximations, depending on the relevance of the two-particle (two-hole) degrees of freedom. Moreover, the importance of the particle-hole and particle-particle excitations and their relation to the stability of the HF or HFB vacuum was also studied [1,2]. It was found that the stability of the HF solution was guaranteed once the roots of the random phase approximation (RPA) are real [2,3]. The RPA was thought of as a "fluctuation" on the Fermi surface defined by the HF approximation. It was also shown that when the correlations introduced by the RPA were taken into account the structure of the ground state was not changed in a qualitative way. It is also well known that there are two different types of instabilities: one related to the particle-hole RPA (PHRPA), which in nuclei is related to shape fluctuations, and the other one corresponding to fluctuations in the number of particles or, similarly, to the two-particle (and two-hole) RPA (TPRPA). This second instability is related to the existence or not of Cooper pairs or to the existence of a nonvanishing solution for the HFB equations.

The initial tool used to obtain the stability theorem for particle-hole excitations was developed by Thouless [2]. He proved that the variations of the HF vacuum, nonorthogonal to it, can be written in terms of one-body operators. The relevant variations are given by states of the form

$$|0'\rangle = \exp\left(\sum_{ki} C_{ki} a_k^\dagger a_i\right)|0\rangle \, , \tag{1.1}$$

where $a_k^\dagger$ (a_i) creates (annihilates) a particle above (below) the Fermi sea, while $|0\rangle$ corresponds to the HF vacuum. The coefficients C_{ki} must be determined by some physical prescription. In the minimization of the ground state energy, using the HF method, they are arbitrary numbers, while in the calculation of the instability of the RPA, they are related to the RPA eigenstates.

For bosons, the state of the art was in a sense rather poor and the problem is quite different. The more noticeable difference is the existence of Bose condensation [4]. This phenomenon complicates the application of field theoretical methods to Bose systems, a problem that was solved for dilute systems in Refs. [5,6]. The studies done at that time were mainly interested in the thermodynamic limit. In that limit bosons are prone to collapse for an attractive interaction. This fact makes necessary the existence of short range repulsion for physical systems.

Due to the existence of Bose condensation it was assumed that the ground state at zero temperature can be described as a condensate of the lower-energy boson (Γ_0). The bosonic excitations of the systems were obtained via a Dyson-like equation that contained not only the usual self-energy but also the anomalous one [5]. It was implicitly assumed, as it is valid for fermionic systems, that the structure of the ground state does not change "drastically" when the correlations introduced by the different types of RPA's are taken into account. The study of this aspect will be the main point that we will develop in the present paper.

*Present address: Departamento de Física-CNEA.
†On leave of absence from the Comisión Nacional de Energía Atómica.
‡Member of the Consejo Nacional de Investigaciones Científicas y Técnicas.

A similar problem, but in nuclear physics, was studied more recently; see for instance [7,8]. In this case the characteristics of the Hartree-Bose (HB) method for a finite (and not so large) number of bosons were considered in some detail. All the steps used in fermion systems can be reproduced for boson systems, but the presence of Bose condensation changes some of the relevant characteristics of the problem, the more noticeable being the similarity between the Bogoliubov transformation for bosons and the excitations described by the PHRPA [8,9]. At the time of the appearance of the BCS treatment for fermion systems there was much interest in the application of similar methods to bosons [10–12]. The results obtained for boson systems have some different "signs" if they are compared with the fermion ones: normalization conditions, the relation between the energy of the excitations and the gap, etc.

For boson systems the comparison between the characteristics of a condensate of bosons and a condensate of pairs of boson was studied variationally [13]. We will show in our conclusions why this comparison was not completely meaningful. Also in nuclear physics a model was considered that has essentially the same competition: on one side a condensate of bosons, considering as a "quasiboson" the pair of fermions that originates the superconductive description, and on the other hand a condensate of α-like structures that can be considered as a pair of bosons [14–16] (or a pair of "deuteronlike structures" coupled to the quantum numbers of an α particle).

In the present paper we will give explicit expressions for the ground state wave function of the system of structureless bosons, in different mean field approximations. We will initially make a review of the usual Hartree-Bose approximation and we will study its stability conditions that will yield the particle-hole random phase approximation (PHRPA). We will write down explicitly the ground state of the PHRPA using an operator $\mathcal{R}^\dagger$ [see Eq. (2.31)] that commutes with all the annihilation operators of the excitations of the PHRPA. The operator $\mathcal{R}^\dagger$ can be thought of as the creator of a "bosonic" Cooper pair, and that comparison clarifies why it is possible to write down the RPA ground state as a condensate of pairs of bosons.

We then will show that the assumption that the ground state of the type obtained in the PHRPA yields, naturally, excitations that have a structure identical to the one proposed by Bogoliubov [4,9]. The complex excitations of this system can be obtained studying the coupling of the "elementary excitations."

There exists a profound difference between the behavior of boson and fermion systems already at the level of the mean field. In the fermionic case one may have or not the anomalous self-energy [17], and if it vanishes (or not), the HF (or HFB) approximation provides an appropriate starting point for the description of the system. In the bosonic case both types of terms must be necessarily taken into account [4,5]. This difference is also related to the fact that for fermions the appearance of Cooper pairs marks a phase transition that cannot be obtained in a perturbative way, but only after a deep change in the structure of the ground state. This phase transition can be understood in terms of the Bose condensation of the Cooper pairs. For bosons, once the HB approximation is used, its ground state is a Bose condensate and the fluctuations around this condensate will result in a ground state wave function that can be written either as a condensate of pairs or as a coherent state formed by these pairs (this is the main conclusion of the present paper). In any case the depletion factor will inform us about how much of the ground state is composed of bosons in the lowest energy state and will be an appropriate order parameter [16].

In Sec. II we will review the HB approximation, its stability conditions, and the fluctuations induced by the PHRPA. In Sec. III we will present in a unified language different mean field approximations: again the PHRPA, a BCS-like treatment (Bogoliubov approximation), and the particle-particle RPA (PPRPA) coupled to the PH RPA. In the nuclear case the coupling between the PHRPA and the PPRPA is relevant only in open shell nuclei, i.e., when the system is superconductive (see for instance Ref. [18]). If the arguments used for fermions are valid in the bosonic case, we will show that this coupling must always be considered; i.e., the bosons are always on a superfluid ground state.

In all the cases we write explicitly the ground state wave function in such a way as to guarantee that the annihilation operators for the excitations of the system, acting on the ground state, give zero, showing that it can be always expressed in terms of a coherent mixture of pairs of bosons. In Sec. IV we will discuss the obtained results.

II. FLUCTUATIONS AROUND THE HARTREE-BOSE VACUUM

A. Hartree-Bose approximation

In this subsection we will follow closely the derivation of the HB approximation used in [8]. One starts by considering a system formed by N interacting bosons. In the lowest order, which is just the HB approximation, this system can be described as arising from independent (dressed) bosons moving in an average self-consistent field. Due to the boson structure of the degrees of freedom the ground state will be a condensate of bosons corresponding to the lowest single-particle energy. The vacuum wave function is

$$|\Psi_N\rangle = \sqrt{\frac{1}{N!}}\Gamma_0^{\dagger N}|0\rangle \; , \tag{2.1}$$

where $\Gamma_0^\dagger$ is the creation operator of the dressed boson in the lowest-energy single-particle state and $|0\rangle$ is the bare vacuum. The main purpose of the HB approximation is to express the operator $\Gamma_0^\dagger$ in terms of the initial undressed-boson operators.

To fix the ideas we will consider a two-body boson Hamiltonian that is written as

$$H=\sum_{ij}t_{ij}\gamma_i^\dagger\gamma_j+\frac{1}{4}\sum_{ijkm}V^{\rm sym}_{ij,km}\gamma_i^\dagger\gamma_j^\dagger\gamma_k\gamma_m\ , \qquad (2.2)$$

where $V^{\rm sym}_{ij,km}$ is related to the symmetrized matrix element of the two-body interaction [8], and $\gamma_k^\dagger$ creates a boson with quantum numbers k.

One can use a theorem similar to the Thouless theorem for bosons. The variations not orthogonal to the ground state can be written as [2,3,7]

$$|\Psi_N'\rangle=A\left(\Gamma_0^\dagger+\sum_p c_p\Gamma_p^\dagger\right)^N|0\rangle\ , \qquad (2.3)$$

where

$$A=\left(1+\sum_p|c_p|^2\right)^{-\frac{N}{2}}\ . \qquad (2.4)$$

Here the coefficients c_p are arbitrary. The p's label the remaining dressed bosons states that together with the 0 state form the complete HB basis.

This variational wave function can be written in an alternative way as

$$|\Psi_N'\rangle=Ae^{\Theta}|\Psi_N\rangle\ , \qquad (2.5)$$

where

$$\Theta=\sum_p c_p\Gamma_p^\dagger\Gamma_0\ . \qquad (2.6)$$

In order to find the solution for the HB problem we will study the expectation value of the Hamiltonian with the variational wave function $|\Psi_N'\rangle$, i.e.,

$$\langle\Psi_N'|H|\Psi_N'\rangle=A^2[\langle\Psi_N|H|\Psi_N\rangle+\langle\Psi_N|\Theta^\dagger H+H\Theta|\Psi_N\rangle+\langle\Psi_N|\Theta^\dagger H\Theta+\tfrac{1}{2}\left(\Theta^{+2}H+H\Theta^2\right)|\Psi_N\rangle+\cdots]\ . \qquad (2.7)$$

If $|\Psi_N\rangle$ corresponds to a solution of the HB problem, any variation not orthogonal to it can only increase the expectation value of the ground state energy. Therefore, the HB approximation is obtained by requiring the cancellation of the linear terms in Θ in Eq. (2.7), and as usual, the stability conditions will come out from the requirement that the second order terms must be positive definite.

To do explicitly the HB approximation we will define the $\Gamma^\dagger$ operators in terms of the $\gamma^\dagger$ by performing a unitary transformation

$$\Gamma_0^\dagger=\sum_i\eta_{0i}^*\gamma_i^\dagger\ , \qquad (2.8)$$

$$\Gamma_p^\dagger=\sum_i\eta_{pi}^*\gamma_i^\dagger\ , \qquad (2.9)$$

$$\delta_{\mu\nu}=\sum_i\eta_{\mu i}^*\eta_{\nu i}\ , \qquad (2.10)$$

$$\delta_{ij}=\sum_\mu\eta_{\mu j}^*\eta_{\mu i}\ . \qquad (2.11)$$

We can write the Hamiltonian of Eq. (2.2) in the $\{0,p\}$ basis

$$H=H_{00}+H_{10}+H_{01}+H_{11}+H_{20}+H_{02}+H_{21}+H_{12}+H_{22}\ , \qquad (2.12)$$

where

$$H_{00}=\sum_{ik}t_{ik}\eta_{0i}\eta_{0k}^*\Gamma_0^\dagger\Gamma_0+\frac{1}{4}\sum_{ijkl}V^{\rm sym}_{ij,kl}\eta_{0i}\eta_{0j}\eta_{0k}^*\eta_{0l}^*\Gamma_0^\dagger\Gamma_0^\dagger\Gamma_0\Gamma_0\ , \qquad (2.13)$$

$$H_{01}=H_{10}^\dagger=\sum_p\left(\sum_{ik}t_{ik}\eta_{pi}\eta_{0k}^*\Gamma_p^\dagger\Gamma_0+\frac{1}{2}\sum_{ijkl}V^{\rm sym}_{ij,kl}\eta_{pi}\eta_{0j}\eta_{0k}^*\eta_{0l}^*\Gamma_p^\dagger\Gamma_0^\dagger\Gamma_0\Gamma_0\right)\ , \qquad (2.14)$$

$$H_{11}=\sum_{pq}\left(\sum_{ik}t_{ik}\eta_{pi}\eta_{qk}^*\Gamma_p^\dagger\Gamma_q+\sum_{ijkl}V^{\rm sym}_{ij,kl}\eta_{0i}\eta_{pj}\eta_{qk}^*\eta_{0l}^*\Gamma_0^\dagger\Gamma_p^\dagger\Gamma_q\Gamma_0\right)\ , \qquad (2.15)$$

$$H_{02} = H_{20}^{\dagger} = \frac{1}{4}\sum_{pq}\sum_{ijkl} V^{\rm sym}_{ij,kl}\eta_{pi}\eta_{qj}\eta^{*}_{0k}\eta^{*}_{0l}\Gamma^{\dagger}_{p}\Gamma^{\dagger}_{q}\Gamma_{0}\Gamma_{0}\ , \tag{2.16}$$

$$H_{12} = H_{21}^{\dagger} = \frac{1}{2}\sum_{pqr}\sum_{ijkl} V^{\rm sym}_{ij,kl}\eta_{pi}\eta_{qj}\eta^{*}_{rk}\eta^{*}_{0l}\Gamma^{\dagger}_{p}\Gamma^{\dagger}_{q}\Gamma_{r}\Gamma_{0}\ , \tag{2.17}$$

$$H_{22} = \frac{1}{4}\sum_{pqrs}\sum_{ijkl} V^{\rm sym}_{ij,kl}\eta_{pi}\eta_{qj}\eta^{*}_{rk}\eta^{*}_{rl}\Gamma^{\dagger}_{p}\Gamma^{\dagger}_{q}\Gamma_{r}\Gamma_{s}\ . \tag{2.18}$$

The indices p, q, r, and s refer to states different from 0. It can be seen that the only parts of the Hamiltonian involved in the stationary condition [when the linear term of Eq. (2.7) vanishes] are H_{10} and H_{01}. We notice that, the coefficients c_p being arbitrary numbers, the stationary condition is fulfilled if

$$\sum_{j}\eta^{*}_{0j}h_{ij} = E_0\eta^{*}_{0i}\ , \tag{2.19}$$

where

$$h_{ij} = t_{ij} + \frac{1}{2}\langle\Psi_N|\Gamma^{\dagger}_{0}\Gamma_{0} - 1|\Psi_N\rangle\sum_{kl}V^{\rm sym}_{ik,lj}\eta_{0k}\eta^{*}_{0l} \tag{2.20}$$

and

$$E_0 = \sum_{ij}\left(t_{ij}\eta_{0i}\eta^{*}_{0j} + \frac{1}{2}\langle\Psi_N|\Gamma^{\dagger}_{0}\Gamma_{0} - 1|\Psi_N\rangle\sum_{kl}V^{\rm sym}_{ij,kl}\eta_{0i}\eta_{0j}\eta^{*}_{0k}\eta^{*}_{0l}\right)\ . \tag{2.21}$$

The one-body Hamiltonian h_{ij} corresponds to an average distorted field generated self-consistently by the N bosons of the system. We call Eq. (2.20) the Hartree-Bose Hamiltonian because of the similarity to the fermionic case. It must be noticed that, in the bosonic case, there is only one state that is occupied and can be considered as belonging to Fermi sea. The procedure to obtain the HB state involves only the coefficients η_{0i}, leaving the $\eta_{pi}(p \neq 0)$ undetermined. We can go further and construct a complete orthogonal basis of bosons from the equation

$$\sum_{j}\eta^{*}_{xj}h_{ij} = E_x\eta^{*}_{xi}, \qquad x = 0, p\ , \tag{2.22}$$

where the eigenvalue solutions of Eq. (2.21), E_x, are the energies required to add one more dressed boson of the "type x" to the $(N-1)$ particle condensate. In general [8] the expectation value $\langle\Psi_N|\Gamma^{\dagger}_{0}\Gamma_{0} - 1|\Psi_N\rangle$ is replaced by $N-1$. The energy E_0 should not be confused with the ground state energy which is the expectation value of H_{00} (note the difference of a factor $\frac{1}{2}$ in the two-body part, as well as an overall factor N):

$$\mathcal{E}_{HB}(N) = \langle\Psi_N|H_{00}|\Psi_N\rangle = N\sum_{ij}t_{ij}\eta_{0i}\eta^{*}_{0j} + \frac{1}{4}\langle\Psi_N|\Gamma^{\dagger}_{0}\Gamma^{\dagger}_{0}\Gamma_{0}\Gamma_{0}|\Psi_N\rangle\sum_{ijkl}V^{\rm sym}_{ij,kl}\eta_{0i}\eta_{0j}\eta^{*}_{0k}\eta^{*}_{0l}\ . \tag{2.23}$$

If one makes an expansion of the energy in terms of N, it is well known that the HB approximation corresponds to consider the leading order terms in N. Therefore, one has the freedom to change the matrix by N instead of $N-1$, but we do not see any special reason to make this replacement. We will preserve the dependence that appears more naturally, i.e., to replace $\langle\Psi_N|\Gamma^{\dagger}_{0}\Gamma^{\dagger}_{0}\Gamma_{0}\Gamma_{0}|\Psi_N\rangle$ by $N(N-1)$. This completes the definition of the HB procedure and, if one is interested in considering all the $O(N)$ terms, the RPA must be performed.

B. Particle-hole random phase approximation

We will consider single-boson excitations that correspond to the eigenvalues of the one-body Hamiltonian h_{ij}. In this way these excitations will be orthogonal to $\Gamma^{\dagger}_{0}$. Their energies E_p will be the energy required to add one more boson to the ground state of $(N-1)$ bosons. This prescription has the disadvantage that H_{11} will not be diagonal in this basis.

These energies will be wrong in order $O(1/N)$ (compared to the leading order, which is of order N^2) as terms of that order in the Hamiltonian have not been considered. In order to take into account all such terms we must perform the RPA, which is equivalent to linearizing the equation of motion of the excitation operators

$$B^{\dagger}_{\alpha} = \frac{1}{\sqrt{N}}\sum_{p}(X^{\alpha}_{p}\Gamma^{\dagger}_{p}\Gamma_{0} - Y^{\alpha}_{p}\Gamma^{\dagger}_{0}\Gamma_{\bar{p}})\ , \tag{2.24}$$

$$\sum_{p}[(X^{\alpha}_{p})^2 - (Y^{\alpha}_{p})^2] = 1\ , \tag{2.25}$$

which act on the correlated ground state of the system with N bosons. This procedure was discussed in detail in Ref. [8] and will only be sketched here.

We assume that the Hamiltonian of Eq. (2.2) has been diagonalized in the HB approximation. Since we only study excitation energies of one-boson states, it is convenient to define the zero of the energy scale at the lowest-energy state E_0. Therefore, we will take as single-boson energies $\mathcal{E}_p = E_p - E_0$. The linearization of the equations of motion, given by the commutators

$$[H, B_\alpha^\dagger] = \Omega_\alpha B_\alpha^\dagger \ , \tag{2.26}$$

leads to the RPA equations

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^\alpha \\ Y^\alpha \end{pmatrix} = \Omega_\alpha \begin{pmatrix} X^\alpha \\ Y^\alpha \end{pmatrix} \ , \tag{2.27}$$

where

$$\begin{aligned} A_{p,q} &= \frac{1}{N}\langle \Psi_N | [\Gamma_0^\dagger \Gamma_p, [H, \Gamma_q^\dagger \Gamma_0]] | \Psi_N \rangle \\ &= \mathcal{E}_p \delta_{pq} + (N-1) \sum_{ij,kl} V_{ij,kl}^{\text{sym}} \eta_{pi} \eta_{0j} \eta_{qk}^* \eta_{0l}^* \ , \end{aligned} \tag{2.28}$$

$$\begin{aligned} B_{p,q} &= -\frac{1}{N}\langle \Psi_N | [\Gamma_0^\dagger \Gamma_p, [H, \Gamma_0^\dagger \Gamma_q]] | \Psi_N \rangle \\ &= \frac{1}{2}(N-1) \sum_{ij,kl} V_{ij,kl}^{\text{sym}} \eta_{pi} \eta_{qj} \eta_{0k}^* \eta_{0l}^* \ . \end{aligned}$$

In calculating the commutators neither H_{21} nor H_{22} contribute.

As was already noted in Ref. [8] the structure of the creation operators of the RPA bosons is equivalent, to order $O(1/N)$, to a Bogoliubov transformation defining quasiparticles. We will later show that this similarity is by no means fortuitous.

C. Stability conditions and the particle-hole RPA vacuum

We will now study the stability condition for Bose systems in the HB approximation. The proof is essentially the same as for fermion systems. We will start by considering the requirement that the second order term in the coefficients c_p in Eq. (2.7) be positive definite. That implies, as in the fermionic case, that in the Hermitian eigenvalue problem

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} C \\ C^* \end{pmatrix} = \lambda \begin{pmatrix} C \\ C^* \end{pmatrix} \tag{2.29}$$

the eigenvalues λ should all be non-negative. If we multiply the RPA equation on the left by the row vector (X, Y), we find

$$\begin{aligned} & (X_\alpha^\dagger \quad Y_\alpha^\dagger) \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X_\alpha^\dagger \\ Y_\alpha^\dagger \end{pmatrix} \\ &\qquad = \Omega_\alpha \left(X_\alpha^\dagger X_\alpha - Y_\alpha^\dagger Y_\alpha \right) \ , \end{aligned} \tag{2.30}$$

which is the sufficient condition to which Thouless arrived. We can therefore conclude that if all the eigenvalues of the RPA are real, then the HB solution will be stable. It is important to remark that we have only considered the particle-hole RPA. We will now give an explicit expression for the PHRPA ground state. We want to define it by imposing the conditions

$$B_\alpha |\text{RPA}\rangle = 0 \ , \tag{2.31}$$

for all α. It is convenient to define the operators

$$\eta_p^\dagger = \Gamma_p^\dagger \Gamma_0 - \sum_q \mathcal{Z}_{pq} \Gamma_0^\dagger \Gamma_{\bar{q}} \ , \tag{2.32}$$

$$\mathcal{R}^\dagger = \Gamma_0^\dagger \Gamma_0^\dagger + \sum_{pq} \mathcal{Z}_{pq} \Gamma_p^\dagger \Gamma_q^\dagger \ , \tag{2.33}$$

where

$$\mathcal{Z}_{pq} = \sum_\alpha Y_p^\alpha \left(\frac{1}{X} \right)_{\alpha,q} \ . \tag{2.34}$$

Due to their construction, η_p and $\mathcal{R}^\dagger$ commute. Moreover, the operators $\eta_p^\dagger$ are a linear combination of the operators that create the PHRPA excitations. With these auxiliary operators it is simple to arrive to an explicit expression for the RPA vacuum. It can be written as[1]

$$|\text{RPA}\rangle = \mathcal{A} \mathcal{R}^{\dagger \frac{N}{2}} |0\rangle \ . \tag{2.36}$$

The structure of this state is rather amusing; it corresponds to a condensate of pairs of bosons, and therefore its structure is similar to the one corresponding to a number-conserving HBB wave function. We will now study the possibility that this state is variational; i.e., we will consider the energy of the RPA ground state and will make variations with regard to the parameters $\mathcal{Z}$.

The contribution coming from the RPA to the ground state energy, in leading order in N (i.e., if one considers that the commutator between B_α and $B_\alpha^\dagger$ is equal to 1, neglecting the higher order terms), can be written as [7]

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[1] In the case of a system with odd number of bosons

$$|\text{RPA}\rangle = \mathcal{A} D_p^\dagger \mathcal{R}^{\dagger \frac{N}{2}} |0\rangle \ , \tag{2.35}$$

where

$$\begin{aligned} D_p^\dagger &= (N+2) Y_p^\alpha \Gamma^\dagger - X_p^\alpha \Gamma_{\bar{p}} \mathcal{R}^\dagger , \qquad p \neq 0, \\ D_0^\dagger &= (N+2) \Gamma_0^\dagger - \Gamma_0 \mathcal{R}^\dagger \end{aligned}$$

fulfilled the condition that $B_\alpha |\text{RPA}\rangle = 0$.

$$\mathcal{E}_{0,\mathrm{RPA}} = \mathcal{E}_{\mathrm{HB}} - \sum_{\alpha} \Omega_\alpha \sum_p (Y_p^\alpha)^2 = \mathcal{E}_{\mathrm{HB}} - \frac{1}{2}\mathrm{Tr}[A] + \frac{1}{2}\sum_\alpha \Omega_\alpha,$$

$$\mathcal{E}_{0,\mathrm{RPA}} = \mathcal{E}_{\mathrm{HB}} - \frac{1}{2}\mathrm{Tr}[A] + \frac{1}{2}\mathrm{Tr}_\alpha \left[\begin{pmatrix} X_\alpha^\dagger & Y_\alpha^\dagger \end{pmatrix} \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X_\alpha^\dagger \\ Y_\alpha^\dagger \end{pmatrix} \right] . \tag{2.37}$$

The variation with respect to $\mathcal{Z}$ is equivalent to a variation with respect to Y_p^α, taking into account the normalization condition Eq. (2.25). This normalization condition relates the variation with respect to Y_p^α to variations with respect to X_q^α yielding

$$\frac{\delta X_q^\beta}{\delta Y_q^\alpha} = \left(\frac{X_q^{\beta\dagger}}{Y_q^{\alpha\dagger}} \right)^{-1} . \tag{2.38}$$

With this constraint, Eq. (2.37) is satisfied automatically once the RPA is satisfied. This implies that the wave function that we have obtained for the ground state of the PHRPA of a bosonic system is the same that will be obtained if one performs a number-conserving HBB calculation (to higher order in N).

III. STRUCTURE OF THE ELEMENTARY EXCITATIONS

To simplify the treatment we will rewrite the Hamiltonian of Eqs. (2.12)–(2.18) in terms of the number operators $n_p = \Gamma_p^\dagger \Gamma_p$ and the two-particle creation operators $P_p^\dagger = \Gamma_p^\dagger \Gamma_{\overline{p}}^\dagger$, where $|\overline{p}\rangle$ is the time-reversal state of $|p\rangle$. The Hamiltonian can then be written as

$$H = \sum_p (E_p - \mu) n_p + \sum_{p,q} T_{pq} n_p n_q + \sum_{q \neq p} S_{pq} P_p^\dagger P_q + W , \tag{3.1}$$

where in the summation the subindices p, q can also have the value 0. The energies E_p are the HB energies, solutions of Eq. (2.22), and we have also introduced the chemical potential μ. T_{pq} and S_{pq} are parts of the residual Hamiltonian H_{11} [Eq. (2.15)], H_{20}, H_{02} [Eq. (2.16)], and H_{22} [Eq. (2.18)]. In W are included all the terms which are not explicitly included (for example, H_{31}). In particular, W is not relevant for the ground state calculation and can be treated perturbatively if necessary.

In order to study the excitations of the system, it is convenient to introduce the concept that the creators of the elementary modes of excitation $C_\alpha^\dagger$ are defined through the linearization conditions

$$[H, C_\alpha^\dagger] = \omega_\alpha C_\alpha^\dagger , \tag{3.2}$$

where the structure of the operators $C_\alpha^\dagger$ must be specified. When performing this linearization, one has in the commutator written on the left hand side, in general, a different structure than the one that was assumed on the right hand side of the linearization condition. It is customary to replace the supernumerary operators that are on the left in the left member of Eq. (3.2) by their corresponding mean values in the ground state such as to reduce it to the proper structure. The assumptions with respect to this point make the difference between the different mean field approximations.

A. Elementary excitations of the Bogoliubov approximation

If one chooses for $C_p^\dagger$ the Bogoliubov prescription

$$C_p^\dagger = U_p \Gamma_p^\dagger - V_p \Gamma_{\overline{p}} , \tag{3.3}$$

Eq. (3.2) corresponds to the Bogoliubov description of the system.

To evaluate the commutator between the Hamiltonian and the operator that creates the elementary excitation, one needs the commutators

$$[n_q, \Gamma_p^\dagger] = \delta_{q,p} \Gamma_p^\dagger \tag{3.4}$$

and

$$[P_q, \Gamma_p^\dagger] = \delta_{q,p} \Gamma_{\overline{p}} . \tag{3.5}$$

Therefore,

$$[H, \Gamma_p^\dagger] = \left(E_p - \mu + \sum_q T_{qp}(2n_q - 1) \right) \Gamma_p^\dagger + \sum_{q \neq p} \left(S_{qp} P_q^\dagger \right) \Gamma_{\overline{p}} . \tag{3.6}$$

In the Bogoliubov approximation one replaces the operators n_q and $P_q^\dagger$ by their corresponding mean values in the ground state, i.e., by $\langle n_q \rangle$ and $\langle P_q^\dagger \rangle = \Delta_q$, respectively. Therefore one has for the commutator between the elementary excitation and the Hamiltonian

$$[H, C_p^\dagger] = [U_p \eta_{11}(p) + V_p \eta_{20}(p)] \Gamma_p^\dagger + [U_p \eta_{20}(p) + V_p \eta_{11}(p)] \Gamma_{\overline{p}} = E_p \left(U_p \Gamma_p^\dagger - V_p \Gamma_{\overline{p}} \right) , \tag{3.7}$$

where

$$\eta_{11}(p) = E_p - \mu + \sum_q T_{qp}\langle 2n_q - 1\rangle \quad (3.8)$$

and

$$\eta_{20}(p) = \sum_{q\neq p} S_{qp}\Delta_q \, . \quad (3.9)$$

Equation (3.7) allows us to write down explicitly U_p, V_p, and the "quasiparticle" energy E_p. The energies of the excitations satisfy the condition

$$E_p^2 = \eta_{11}(p)^2 - \eta_{20}(p)^2 \, . \quad (3.10)$$

The amplitudes U_p and V_p must satisfy also the normalization condition

$$U_p^2 - V_p^2 = 1 \, , \quad (3.11)$$

and therefore their values are given by

$$U_p^2 = \frac{1}{2}\left(1 + \frac{\eta_{11}(p)}{E_p}\right) \quad (3.12)$$

and

$$V_p^2 = \frac{1}{2}\left(-1 + \frac{\eta_{11}(p)}{E_p}\right) \, . \quad (3.13)$$

This completes the description of the excitations in the Bogoliubov approximation.

To construct the vacuum explicitly one must remember that it must satisfy

$$C_p|\mathrm{Bog}\rangle = 0 \, . \quad (3.14)$$

If one chooses for $|\mathrm{Bog}\rangle$ a state of the form

$$|\mathrm{Bog}\rangle = \mathcal{N}_{\mathrm{Bog}} \exp\left(\mathcal{T}^\dagger\right)|0\rangle \, , \quad (3.15)$$

where

$$\mathcal{T}^\dagger = \sum_p \rho_p \Gamma_p^\dagger \Gamma_{\bar{p}}^\dagger \, , \quad (3.16)$$

one obtains

$$C_p|\mathrm{Bog}\rangle = \mathcal{N}_{\mathrm{Bog}} \sum_m \frac{\mathcal{T}^{\dagger m}}{m!}\left(-V_p + U_p\rho_p\right)\Gamma_p^\dagger|0\rangle \, , \quad (3.17)$$

and therefore, with $\rho_p = \frac{V_p}{U_p}$, Eq. (3.15) corresponds to the vacuum of the system in the Bogoliubov approximation.

B. Elementary excitations of the PHRPA

If one assumes that

$$C_p^\dagger = \frac{1}{\sqrt{\mathcal{N}_p}}\left(X_p\Gamma_p^\dagger\Gamma_0 - Y_p\Gamma_0^\dagger\Gamma_{\bar{p}}\right) \, , \quad (3.18)$$

then Eq. (3.2) corresponds to the particle-hole RPA. The constant $\mathcal{N}_p$ is determined from the normalization condition $[C_\alpha, C_\beta^\dagger] = \delta_{\alpha,\beta}$, which reads

$$\mathcal{N}_p{}^2 = (X_p^2 - Y_p^2)(\langle n_0\rangle - \langle n_p\rangle) \, , \quad (3.19)$$

where $\langle n_0\rangle$ and $\langle n_p\rangle$ are the expectation values in the ground state of the number of bosons in the levels 0 and p respectively. As we have one degree of freedom in the determination of the constant we will use

$$\mathcal{N}_p{}^2 = \langle n_0\rangle - \langle n_p\rangle \quad (3.20)$$

and

$$X_p^2 - Y_p^2 = 1 \, . \quad (3.21)$$

We will start by evaluating the commutator of the Hamiltonian given by Eq. (3.1) with the operator defined in Eq. (3.18).

If we call $t_p = \Gamma_0^\dagger\Gamma_p$ (we assume $p \neq 0$), then we can write for the commutators

$$[n_q, t_p^\dagger] = (-\delta_{q,0} + \delta_{q,p})t_p^\dagger \, , \quad (3.22)$$

$$[t_q, t_p^\dagger] = \delta_{q,p}(n_0 - n_p) \, , \quad (3.23)$$

$$[t_q, P_p^\dagger] = \delta_{q,p}\Gamma_{\bar{p}}^\dagger\Gamma_0^\dagger \, , \quad (3.24)$$

$$[t_q, P_0] = -2\Gamma_q\Gamma_0 \, . \quad (3.25)$$

As $p \neq 0$ we can write

$$[H, t_p^\dagger] = \left(E_p - E_0 + \sum_q T_{pq}(2n_q - \delta_{q,p})\right) t_p^\dagger + \sum_{q\neq p} S_{pq} P_q^\dagger u_{\bar{p}} - \sum_{q\neq 0} 2S_{0q} u_p^\dagger P_q \, , \quad (3.26)$$

where we have defined

$$u_p^\dagger = \Gamma_p^\dagger\Gamma_0^\dagger \, . \quad (3.27)$$

In the linearization procedure, it is usual to replace operators by their expectation values on the vacuum. In this case we will need to make the replacement

$$u_p^\dagger P_q = \delta_{p,q} t_{\bar{p}}\langle n_p\rangle, \qquad q \neq 0 \, , \quad (3.28)$$

and

$$P_q^\dagger u_{\bar{p}} = 2\delta_{q,0} t_{\bar{p}}\langle n_0\rangle, \qquad q \neq p \, . \quad (3.29)$$

Therefore, we have

$$[H, t_p^\dagger] = \Lambda_{11}(p) t_p^\dagger + \Lambda_{20}(p) t_{\bar{p}} \, , \quad (3.30)$$

where

$$\Lambda_{11}(p) = \left(E_p - E_0 + \sum_q T_{pq}(2n_q - \delta_{q,p})\right) \quad (3.31)$$

and

$$\Lambda_{20}(p) = 2S_{0p}(\langle n_0\rangle - \langle n_p\rangle) . \quad (3.32)$$

These expressions allow us to write explicitly Eq. (3.2) as

$$\begin{aligned}[H, C_p^\dagger] &= [X_p\Lambda_{11}(p) + Y_p\Lambda_{20}(p)]\, t_p^\dagger \\ &\quad + [X_p\Lambda_{20}(p) + Y_p\Lambda_{11}(p)]\, t_{\overline{p}} \\ &= \Omega^p_{\rm RPA}\left(X_p t_p^\dagger - Y_p t_{\overline{p}}\right) , \end{aligned} \quad (3.33)$$

and therefore one obtains for the RPA amplitudes the conditions

$$X_p[\Lambda_{11}(p) - \Omega^p_{\rm RPA}] = -Y_p\Lambda_{20}(p) \quad (3.34)$$

and

$$Y_p[\Lambda_{11}(p) + \Omega^p_{\rm RPA}] = -X_p\Lambda_{20}(p). \quad (3.35)$$

These equations can be satisfied simultaneously if the energy of the RPA excitation satisfies the condition

$$(\Omega^p_{\rm RPA})^2 = \Lambda_{11}(p)^2 - \Lambda_{20}(p)^2 . \quad (3.36)$$

The amplitudes X_P and Y_p must satisfy also the normalization condition Eq. (3.21), and therefore their values are given by

$$X_p^2 = \frac{1}{2}\left(1 + \frac{\Lambda_{11}(p)}{\Omega^p_{\rm RPA}}\right) \quad (3.37)$$

and

$$Y_p^2 = \frac{1}{2}\left(-1 + \frac{\Lambda_{11}(p)}{\Omega^p_{\rm RPA}}\right) . \quad (3.38)$$

Once X_p and Y_p are known, the vacuum can be written down explicitly as it was done in Sec. II.

C. Elementary excitations of the coupled PPRPA and PHRPA

If one assumes that

$$C_p^\dagger = \frac{1}{\sqrt{\mathcal{N}_p}}\left(X_p\Gamma_p^\dagger\Gamma_0 - Y_p\Gamma_0^\dagger\Gamma_{\overline{p}} + Z_\alpha\Gamma_0^\dagger\Gamma_p^\dagger - W_\alpha\Gamma_0\Gamma_{\overline{p}}\right) , \quad (3.39)$$

then Eq. (3.2) corresponds to a RPA that couples the particle-hole and the particle-particle modes. The constant $\mathcal{N}_p$ is determined from the normalization condition $[C_\alpha, C_\beta^\dagger] = \delta_{\alpha,\beta}$.

We will now study the structure of the ground state of the excitations defined in Eq. (3.39). It follows from inspection that a state having the structure

$$|{\rm CRPA}\rangle = \exp\left(\rho\mathcal{R}^\dagger\right)|0\rangle , \quad (3.40)$$

where we have defined

$$\mathcal{R}^\dagger = \Gamma_0^\dagger\Gamma_0^\dagger + \sum_p \eta_p\Gamma_p^\dagger\Gamma_{\overline{p}}^\dagger , \quad (3.41)$$

satisfies the condition that all the annihilation operators related to Eq. (3.39) acting over the state $|{\rm CRPA}\rangle$ give zero once the commutations of those operators and $\mathcal{R}^\dagger$ are properly adjusted. These commutators can be written as

$$\begin{aligned}[C_p, \mathcal{R}^\dagger] &= X_p[t_p, \mathcal{R}^\dagger] - Y_p[t_{\overline{p}}^\dagger, \mathcal{R}^\dagger] + Z_p[u_p, \mathcal{R}^\dagger] \\ &= X_p\eta_p u_{\overline{p}}^\dagger - Y_p 2u_{\overline{p}}^\dagger + Z_p(2t_p + \eta_p t_{\overline{p}}^\dagger) \end{aligned} \quad (3.42)$$

and

$$[[C_p, \mathcal{R}^\dagger], \mathcal{R}^\dagger] = 4Z_p\eta_p u_{\overline{p}}^\dagger, \quad (3.43)$$

and therefore we have that

$$C_p \exp\left(\rho\mathcal{R}^\dagger\right)|0\rangle = \left[\sum_n \frac{\rho^n}{n!}\mathcal{R}^{\dagger n} u_{\overline{p}}^\dagger\right]\left[-W_p + \rho(X_p\eta_p - 2Y_p) + 4\rho^2 Z_p\eta_p\right]|0\rangle . \quad (3.44)$$

The determination of the number of particles fixes completely the coefficient ρ. For each value of p one must determine η_p in such a way that the parentheses in Eq. (3.44) cancel. It must be noted that when the particle-particle part of the RPA operators are irrelevant (i.e., when Z_p and W_p are equal to zero) we obtain the PHRPA wave function.

IV. CONCLUSIONS

In this paper we have studied several mean field approximations based on the Hartree-Bose description of many boson systems. We have studied the explicit structure that the corresponding ground states have in these different approximations. We have imposed in all the cases that it must be destroyed by the annihilation operators related with its excitations.

We have obtained a rather simple and general result: In all the approximations the ground state can be written in terms of operators that create pairs of bosons. We only discussed the even N case because if N is odd we saw in Sec. II that one must introduce an operator that takes into account the nonpaired boson and does not generate any collective phenomena. In number-conserving descriptions one obtains for the ground state a condensate of pairs of bosons, but when the approximation does not conserve the number of particles we obtained a coherent state where the basic operator creates a pair of bosons. The result that we have obtained seems to contradict the results of Ref. [13], where the competition between the single-boson condensation versus the condensation of pairs of bosons was studied. There the bosons have momentum (p) as a good quantum number and the wave function for the ground state of the single-boson condensate was assumed to be of the type

$$|1\rangle = \exp\left(\mathcal{S}^\dagger\right)|0\rangle \,, \tag{4.1}$$

where

$$\mathcal{S}^\dagger = \phi\Gamma_0^\dagger + \sum_p \lambda_p \Gamma_p^\dagger \Gamma_{-p}^\dagger \,. \tag{4.2}$$

It is useful to compare the part of the wave function $|1\rangle$ that has N particles ($|1,N\rangle$) with a condensate of $N/2$ pairs of bosons. One can write

$$|1,N\rangle = \sum_m \frac{\phi^{N-2m}}{(N-2m)!m!} {\Gamma_0^\dagger}^{N-2m} * (\mathcal{P}^\dagger)^m = \sum_m b_m {\Gamma_0^\dagger}^{N-2m} * (\mathcal{P}^\dagger)^m \tag{4.3}$$

where $\mathcal{P}^\dagger = \sum_p \lambda_p \Gamma_p^\dagger \Gamma_{-p}^\dagger$ On the other hand, the wave function of the condensate of a pair of bosons (CPB) is

$$|\text{CPB}\rangle = \mathcal{N}_{\text{CPB}} {\mathcal{R}^\dagger}^{N/2} |0\rangle \,, \tag{4.4}$$

where we can write for $\mathcal{R}^\dagger = \gamma\Gamma_0^\dagger\Gamma_0^\dagger + \mathcal{P}^\dagger$, or writing it explicitly

$$|\text{CPB}\rangle = \mathcal{N}_{\text{CPB}} \sum_m \frac{(N/2)!}{m!(N/2-m)!} \left(\gamma\Gamma_0^\dagger\right)^{N-2m} * \beta{\mathcal{P}^\dagger}^m = \sum_m a_m \left(\gamma\Gamma_0^\dagger\right)^{N-2m} * \beta{\mathcal{P}^\dagger}^m \,. \tag{4.5}$$

As both wave functions must be normalized we can assume that the ratio of the coefficients a_m/b_m for $m = 0$ has to be equal to 1. Taking into account this factor, the coefficients of the same terms in both wave functions have the ratio

$$\left(\frac{a_m}{a_0}\right)\left(\frac{b_0}{b_m}\right) = \frac{(N/2)!(N-2m)!}{(N/2-m)!N!}\left(\frac{\phi}{\gamma}\right)^{2m} . \tag{4.6}$$

For large N ($\gg m$) we can replace $\frac{N!}{(N-m)!}$ by $N^m[1 + O(\frac{m}{N}) + \cdots]$. If one neglects the terms of order $O(\frac{m}{N})$ and takes into account that $\phi = \sqrt{n_0} = \alpha\sqrt{N}$, the ratio has the value

$$\left(\frac{a_m}{a_0}\right)\left(\frac{b_0}{b_m}\right) = \left(\frac{\alpha}{\sqrt{2}\gamma}\right)^{2m} , \tag{4.7}$$

and therefore for $\sqrt{2}\gamma = \alpha$ both wave functions will be equal to leading order (in $\frac{m}{N}$).

We thus conclude that the wave function $|1,N\rangle$ can also be interpreted as describing a condensate of pairs of bosons, and therefore the assumption of Ref. [13] that the wave function $|1\rangle$ has to be considered as an alternative to a condensate of pairs of bosons is not justified. The system will be essentially a single-boson condensate if ϕ is of order $\sqrt{N}$ or equivalently if α is a number of order 1. When α is much smaller than 1, then the system will be described in terms of the operator $\mathcal{P}^\dagger$. But in both cases one cannot ignore the presence of pairs of bosons in the ground state. The type of phase transition that can happen is illustrated for example in Fig. 2 of Ref. [16], where a pairinglike Hamiltonian between the bosons was diagonalized exactly and the order parameter that is related to the occupation of the 0 level was calculated for different strengths of the interaction. The features of the phase transition will be of course dependent on the characteristics of the Hamiltonian.

In the nuclear case there may be a competition between a condensate of pairs of like bosons (superfluid description both for protons and neutrons) and a condensate of alphalike clusters (that can take into account the phase transition that appears when one moves from spherical to deformed nuclei). For spherical nuclei it is necessary to introduce two types of bosons Γ_0 and $\Gamma_{\bar{0}}$ as the minimum-energy bosons for protons and neutrons, respectively [16]. In these cases n_0 plus $n_{\bar{0}}$ is almost equal to the total number of bosons N and the bosons are simulating, both for protons and neutrons, superconductive systems.

The α-like particle can be understood as pairs of bosons with isoespin $T = 0$ (dueteronlike bosons), where the pairs of bosons may have the same quantum numbers as alpha particles. The α-cluster condensates (n_0 is almost zero) may be related to deformed nuclei, as has been discussed, for instance, in Refs. [16,19].

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