Simple condensation of composite bosons in a number conserving approach to many fermion systems

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We recently derived the Hamiltonian of fermionic composites by an exact procedure of bosonization. In the present paper we expand this Hamiltonian in the inverse of the number of fermionic states in the composite wave function and give the necessary and sufficient conditions for the validity of such an expansion. We compare the results to the Random phase Approximation and the BCS theory and perform an illustrative application of the method.

The low energy physics of several many fermion systems is determined by the formation of composites, accompanied or not by their condensation. Examples of simple condensation (ground state built by a large number of composite bosons in one single-particle state while all other occupation numbers are of order 1) can be found in superconducting materials, ultracold fermionic atoms in magnetic traps [1], ultrasmall metallic grains [2] and atomic nuclei [3, 4]. Examples of multiple condensation (ground state built by a large number of bosons in 2 or more single-particle states) essentially occur in spatially separated systems as in the Josephson effect and superleak or in systems whose components differ by some internal quantum number of nongeometrical nature [5]. The theory of all such systems requires some bosonization procedure. For finite systems it is important to respect particle number conservation, and this becomes unavoidable in the study of effects related to the total number of fermions, its parity and supersymmetry [6]. But respecting this symmetry can be important also for infinite systems [5].

There is an infinite literature on this subject which we cannot review here, but to our knowledge there is no unified method which respects fermion number conservation and treats ground and excited states on the same footing. We recently proposed an exact bosonization procedure which, as such, implements these features. Starting from the operator form of the partition function, after discretization of the Euclidean time we perform an independent Bogoliubov transformation at each time slice. The time dependent parameters of the transformation are determined by the formation of composites, which is the number of fermionic states in their structure functions, assuming simple condensation with one-dimensional condensation sector. The condensation sector is the Fock subspace of composite bosons which contains the condensed boson and all other bosons whose mixing with the condensed one is allowed by symmetries. We call free space the complementary subspace. In the present work we generalize the results of Ref. [9] to a condensation sector of arbitrary dimension. In this framework we can study BCS-BEC transitions in ultracold systems in magnetic traps [10], effects related to the number of fermions and the parity of this number, shape transitions and shape coexistence [11] in atomic nuclei.

One of the motivations of our work is indeed to derive the phenomenological Interacting Boson Model [4] of atomic nuclei starting from an effective nuclear Hamiltonian in a model space. Fermion Hamiltonians in a model space can be written in the form

\[ H_F = \hat{c}^\dagger (e + \mathcal{M}) \hat{c} - \frac{1}{4} g_K \hat{c}^\dagger \hat{F}_K^\dagger \hat{e} \hat{F}_{K} \hat{c}. \]  

(1)

\( \hat{c} \) and \( \hat{c}^\dagger \) are fermion creation-annihilation operators and we adopt a summation convention over repeated indices and a matrix notation, for instance \( \hat{c} \hat{F}_K \hat{c} = \sum_{m_1 m_2} \hat{c}_{m_1} (F_K)_{m_1 m_2} \hat{c}_{m_2} \). \( e \) is the matrix of single-fermion energy, \( \mathcal{M} \) the matrix of any interaction with external fields and \( F_K \) are the potential form factors normalized according to \( \text{tr}(F_K^\dagger F_{K'}) = 2 \Omega \delta_{K,K'} \). The separable terms of the potential are assumed of particle-particle type: the particle-hole ones must be rearranged in this form. The Hamiltonian of composite bosons [9] is

\[ H_B =: \text{tr}(R B^\dagger e B) - \frac{1}{4} \sum_K g_K \text{tr}(R B^\dagger F_K^\dagger) \text{tr}(R F_K B) \]

\[ + \frac{1}{2} \sum_K g_K \text{tr} \left[ (R - 1) F_K^\dagger F_K - R B^\dagger F_K^\dagger R F_K B \right]. \]

(2)

where the colons mean normal ordering, \( B = \frac{1}{\sqrt{4 \pi}} \hat{b}_j B_j^\dagger \), \( R = (\mathbb{1} + B^\dagger B)^{-1} \) and we omitted the interaction with external fields \( H_I =: \text{tr}(R B^\dagger M B) : \). In the above equations the \( \hat{b}_j \) are destruction operators of composites with quantum numbers \( K \) and the matrices \( B_K \) are their structure functions. Unlike the composite operators \( \hat{B}_K = \frac{1}{\sqrt{4 \pi}} \hat{c} B_K \hat{c} \), they obey canonical commutation relations provided the conditions on the structure

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functions reported below are satisfied. In a sector of $n_F$ fermions $H_B$ must be used with the constraint
\[
\text{tr} \left( R B^\dagger B \right) = n_F. \tag{3}
\]
We denote the quantum numbers of the composite bosons in the condensation/free sector by $c_i / f_i$ respectively. We call "zero" the condensation mode and $\sigma$ the remaining states in the condensation sector. We will use the index $\vec{K}$ to represent both $\sigma$- and $f$-bosons.

The difficulty dealing with the bosonic Hamiltonian comes from the operator $R$ which is a nonpolynomial function of bosonic creation-destruction operators. If the number of composite bosons is much smaller than $\Omega$ we can overcome the difficulty by expanding $R$ with respect to $B^\dagger B$. Otherwise a subtraction of the condensate is necessary before an expansion can be done. Because only the "zero" mode will have a large occupation, we can make the number conserving approximation $\Omega^{-1} \langle \hat{b}_0 \hat{b}_0 \rangle \approx n / \Omega = \nu_0$, where $n = \frac{1}{2} n_F$ is the number of bosons. Now we can write the normalization conditions
\[
\frac{1}{2\Omega} \text{tr} \ C_{00} = 1, \quad \frac{1}{2\Omega} \text{tr} \left[ C_{\vec{K} \vec{K}_1} - \nu C_{\vec{K}_1 00 \vec{K}} \right] = \delta_{\vec{K}, \vec{K}_1} \tag{4}
\]
where $C_{\vec{K}_1 \vec{K}_2 \vec{K}_3 \vec{K}_4 \cdots} = \Gamma B_{\vec{K}_1} B_{\vec{K}_2} \Gamma B_{\vec{K}_3} B_{\vec{K}_4} \cdots$ and $\Gamma = \left( 1 + \nu B_0 B^\dagger_0 \right)^{-1}$. They are derived as in Ref.9 and coincide with those reported there if the condensation sector is one-dimensional. The subtraction parameter $\nu$ (a priori different from $\nu_0$) is determined by the constraint (3) which for simple condensation using Eqs. (4) becomes
\[
\nu (\nu_0 - \nu) = \text{terms of order $\Omega^0$.} \tag{5}
\]
This equation is satisfied by $\nu = \nu_0 + \text{terms of order $\Omega^{-1}$}$ which give contributions of order 1 which depend on the number of fermions but not on their state. Following Ref.9 $H_B$ can be expanded in powers of $\Omega^{-\frac{1}{2}}$. Neglecting terms of order $\Omega^{-\frac{1}{2}}$ it becomes
\[
H_B = \mathcal{E}_{00} n + \mathcal{E}_{0\sigma} \hat{b}_0 \hat{b}_0 + \mathcal{E}_{\sigma 0} \hat{b}_0 \hat{b}_0 + \mathcal{E}_{\vec{K}_1 \vec{K}_2} b_{\vec{K}_1}^\dagger b_{\vec{K}_2} + \mathcal{E}_0 \left( \frac{1}{2} \left( \mathcal{W}_{\vec{K}_1 \vec{K}_2} \mathcal{R}_0 \hat{b}_{\vec{K}_1} \hat{b}_{\vec{K}_2} \hat{b}_{\vec{K}_1} \hat{b}_{\vec{K}_2} + H.c. \right) \right)
\]
where
\[
\begin{align*}
\mathcal{E}_0 &= \nu_0 T_{0000} - \Omega \mathcal{G}_{0000} D_{0000}^\dagger + cc \\
\mathcal{E}_{0\sigma} &= 2 \pi + T_{0000} - \nu_0 T_{0000} \mathcal{G}_{0000} D_{0000}^\dagger \mathcal{G}_{0000} D_{0000}^\dagger \\
\mathcal{E}_{\sigma 0} &= \mathcal{E}_{\sigma 0} = 0 \\
\mathcal{E}_{\vec{K}_1 \vec{K}_2} &= \mathcal{E}_{\vec{K}_1 \vec{K}_2} = \nu_0 \left[ T_{0000} - \mathcal{G}_{0000} D_{0000}^\dagger + cc \right] \delta_{\vec{K}_1 \vec{K}_2} + T_{\vec{K}_1 \vec{K}_2} \mathcal{R}_0 \hat{b}_{\vec{K}_1} \hat{b}_{\vec{K}_2} \\
\mathcal{E}_{\vec{K}_1 \vec{K}_2} &= \mathcal{E}_{\vec{K}_1 \vec{K}_2} = \nu_0 \left[ T_{0000} - \mathcal{G}_{0000} D_{0000}^\dagger + cc \right] \delta_{\vec{K}_1 \vec{K}_2} + T_{\vec{K}_1 \vec{K}_2} \mathcal{R}_0 \hat{b}_{\vec{K}_1} \hat{b}_{\vec{K}_2} \\
\end{align*}
\]
where $l$ is any integer. The above equations are valid for an arbitrary choice of $\pi$ as a consequence of the constraint (3) on the number of fermions. All the constants appearing in $H_B$ are of order $\Omega^0$. Then assuming $n \sim \Omega$ the first term is of order $\Omega$, the second and third are of order $\Omega^{-\frac{1}{2}}$ (because the matrix elements of the operators $\hat{b}_0 \hat{b}_0$ are of order $\sqrt{n}$), and the other terms are of order $\Omega^0$. Estimating the order of the different terms we assume that the coupling constants scale according to $g_{K} \sim \Omega^{-\frac{1}{2}} b_{\vec{K}}$, where $b_{\vec{K}}$ is the single fermion energy spreading. This assumption is necessary to get finite energies in infinite systems. Two comments are in order: i) all the constants appearing in $H_B$ vanish unless both quantum numbers $\vec{K}_1 \vec{K}_2$ belong either to the condensed or to the free sector because of different symmetries in these sectors, ii) the zero-boson has a strong mixing with the $\sigma$-bosons due to the terms of order $\Omega^{-\frac{1}{2}}$. But if it is the true condensed boson such mixing must be absent
\[
\mathcal{E}_{\sigma 0} = \mathcal{E}_{\sigma 0} = 0. \tag{8}
\]
As we will see this decoupling prevents the occurrence of boson-particle-boson-hole states in the ground state, and it is therefore similar to an ordinary selfconsistency condition.

We can now derive a number of results without numerical calculations by introducing phonon operators. This can be done in two steps. First we introduce the phonon operators $\hat{A}_{\vec{K}} = \frac{1}{\sqrt{n}} \hat{b}_{\vec{K}} \hat{b}_0^\dagger$ and rewrite the Hamiltonian accordingly
\[
\hat{H}_B = \mathcal{E}_0 + \mathcal{E}_{00} n + \mathcal{E}_{\vec{K}_1 \vec{K}_2} \hat{A}^\dagger_{\vec{K}_1} \hat{A}_{\vec{K}_2}
\]
This is the Bogoliubov Hamiltonian for a superfluid bosonic system and can be diagonalized by a bosonic Bogoliubov transformation \( \hat{A} = \hat{A}^\dagger U^+ + \hat{V} \), \( \hat{A} = U \hat{A} + V \hat{A}^\dagger \). This transformation becomes simple when, due to symmetries, there is a one-to-one correspondence between the quantum numbers \( \vec{K} \) and \( \vec{K}: \vec{K} = \vec{K}/(\vec{K}) \). This is guaranteed only for the free sector, but we assume it to be true for all noncondensed modes in order to illustrate some general features. Then \( \hat{E}_{\vec{K}, \vec{K}} = \hat{E}_{\vec{K}, \vec{K}}^\dagger \), \( \hat{W}_{\vec{K}, \vec{K}} = \hat{W}_{\vec{K}, \vec{K}}^\dagger \). After transformation \( H_B \) takes its final form

\[
H_B = \hat{E}_0 + \sum_{\vec{K}} \hat{E}_{\vec{K}}^\dagger \hat{E}_{\vec{K}} + \hat{E}_\gamma \hat{\Phi} \hat{\Phi}^\dagger
\]

where \( E_{\vec{K}} = \sqrt{(\hat{E}_{\vec{K}}^2 - \nu_0^2)\hat{W}_{\vec{K}, \vec{K}}^2} \). The ground state is the vacuum of the phononic operators \( \hat{\Phi} \), which written in terms of the bosonic composites is

\[
|GS\rangle = |\exp\left(\frac{1}{2\hbar^2} \hat{b}_{\vec{K}}^\dagger (V(U^*)^{-1})_{\vec{K}, \vec{K}}^\dagger \hat{b}_{\vec{K}} \hat{b}_{\vec{K}}^\dagger \right)^n \rangle
\]

\( |GS\rangle \) is a coherent state of phonon pairs which are 2p-2h boson states and therefore 4p-4h fermion states built on the \( \nu_0 \) condensate, at variance \([12]\) with the RPA. The above results have been derived under the condition that the occupation of noncondensed bosons be of order 1

\[
<GS| \sum_{\vec{K}} \hat{b}_{\vec{K}}^\dagger \hat{b}_{\vec{K}} |GS> = \frac{1}{2} \sum_{\vec{K}} (\hat{E}_{\vec{K}} \hat{E}_{\vec{K}} - 1) \ll \Omega.
\]

This is the necessary and sufficient condition for the validity of the assumption of simple condensation and of the \( \Omega^{-1} \) expansion. So this is also the condition for condensation in a finite system.

The structure functions \( B_K \) must be determined by a variational calculation on ground state and phonon energies under the normalization and decoupling conditions. This can be done in the following way. We write \( B_0 = B_0^\dagger + \frac{1}{2} \delta B_0 \). We solve the variational equation for \( B_0 \) neglecting the first 2 terms of \([10]\) which are of order 1 and use the result to determine the correction \( \delta B_0 \). In the present approximation in which we neglect terms of order \( \Omega^{-1/2} \) this correction will alter only the contribution of the term \( \hat{E}_\gamma \hat{\Phi} \hat{\Phi}^\dagger \). A comparison with the BCS theory can clarify the meaning of this procedure. The parameter \( \hat{E}_\gamma \) is indeed the BCS energy per particle in the form of the quasichemical equilibrium theory \([13]\). To see this we must sketch an essential point in the derivation of \( H_B \). The time-dependent Bogoliubov transformation changes the fermion vacuum into the quasiparticle vacuum \( |B\rangle = \exp\left(\hat{b}_{\vec{K}}^\dagger \hat{B}_{\vec{K}} \right) |0\rangle \), where the \( \hat{B}_{\vec{K}} = \frac{1}{\sqrt{2B_{\vec{K}}}} + \hat{B}_{\vec{K}} \) are composite operators and the \( \hat{b}_{\vec{K}} \) time-dependent holomorphic variables. The partition function involves an integral over these variables which acquire the meaning of dynamical bosonic fields with fermion number 2, so that all the terms in the expansion of \( |B\rangle \) have fermion number zero. A further transformation of the partition function into a trace over a bosonic Fock space leads to the expression \([2]\). The coherent states \( |B\rangle \) can be identified with the BCS states setting

\[
v_m = \frac{b_0}{\sqrt{\Omega}} (B_0)_{m,-m}, \quad u_m = \left[1 + \frac{\nu_0^2}{\Omega} (B_0)_{m,-m} \right]^{-\frac{1}{2}}
\]

with standard BCS notation. But if one is ready to break fermion number conservation one can set \( b_0^\dagger \approx n \). Then the BCS normalization \( u_m^2 + v_m^2 = 1 \) is identically enforced and the first of the normalization conditions \([1]\) becomes the BCS condition on fermion number

\[
\sum_m v_m (1 + v_m^2)^{-1} = n_F.
\]

One can easily check that the variation of \( \hat{E}_\gamma \) with respect to \( B_0 \) yields the standard gap equation. But this equation must now be solved under the decoupling conditions \([2]\). These conditions are obviously absent when the condensation sector is one dimensional, in which case one can use results obtained in the BCS theory to evaluate the phonon energies and \( \delta B_0 \) which corresponds to the contribution arising from projection of the BCS wave function (but it includes the contribution of states in the free sector). We now show how our method can be applied in practice to the study of shape transitions in nuclei and the BEC-BCS transition at zero temperature, which can be regarded as the transition from molecular to Cooper structure of the condensed boson. In fact the convenience of the quasichemical equilibrium theory in this context has been advocated long ago \([14]\). In the principal frame of inertia of the nucleus the zero-mode will be a superposition of \( b_{LM} \)-bosons with \( M = 0 \), the \( \sigma \)-modes will be all the other independent superpositions of modes with \( M = 0 \) and the free modes will have \( M \neq 0 \). To determine the structure functions we must minimize the ground state and the phonon energies under the decoupling and normalization conditions \([8]\) \([4]\) \([5]\). The problem simplifies considerably if we assume the condensation sector to be 2-dimensional, including only the states \( L = 0, 2 \), the \( s \)- and \( d \)-bosons of the Interacting boson boson model. As a further simplification we assume the nucleons to live in a single \( j \)-shell and have constant single-particle energy and monopole and quadrupole paring interactions. The energy is therefore a function of the ratio of couplings \( \xi = g_2/g_0 \). In this model space \( \Omega = j + \frac{1}{2} \) and the potential form factors are proportional to Clebsch-Gordan coefficients \( (F_{LM})_{m_1,m_2} = \langle jm_1jm_2|LM > \sqrt{2j+1} \). Then the structure matrices in the condensation sector can be parametrized according to \( B_0 = \gamma_0 F_{00} + \gamma_2 F_{20}, \quad B_\sigma = N (\cos \beta F_{00} + \sin \beta F_{20}) \), and all the parameters are determined by the constraints, \( \beta \) and \( N \), are determined by Eqs. \([4]\) Eqs. \([5]\) and \([8]\) give rise respectively to a closed and open contour lines in the \( \gamma_0, \gamma_2 \) plane as shown in Fig.1 where only the upper part is shown (the lower one can be obtained by a parity inversion). The intersection for which \( \hat{E}_\gamma \) is minimum
FIG. 1: Contour plots of the first of normalization conditions (full circles) and of the decoupling condition (empty circles) for $\xi = 1.5$ and $\nu_0 = 0.5$. The minimum energy is for a spherical shape, at $\gamma_2 = 0, \gamma_0 = 1.4$.

FIG. 2: The critical line separating the deformed phase (upper part) from the spherical one (lower part).

determines the values of the $\gamma$-parameters and therefore the shape of the nucleus. In Fig. 2 we plot the critical line which separates the deformed from the spherical shape. When $\nu_0$ approaches 1 the shell is fully occupied, and because of the Pauli principle the bosonic approximation cannot be valid. However we have a tentative interpretation of the steep rise of the critical line in this region. For $\nu_0 = 1$ there is a unique nuclear state which is spherical. Therefore approaching 1, larger and larger values of the strength of the quadrupole pairing are necessary to get a deformed shape. Below the critical line the ground state is a condensate of bosons with zero angular momentum (seniority limit). The condensation sector is one-dimensional and

$$\hat{H}_B = 2n e + g_0 n^2 - \Omega g_0 n + E_L \hat{A}_{LM}^{\dagger} \hat{A}_{LM}$$ (12)

where

$$E_L = \Omega g_0 |1 - \xi| \sqrt{1 + \frac{1}{1 - \xi} \left[ 1 - 4 \left( \frac{1}{2} - \nu \right)^2 \right]}.$$ (13)

Note that the Hamiltonian is expressed in terms of the $\alpha$-phonons, because the coefficients $W$ vanish. The phonon energies are even functions of the deviation from half filling and vanish for $\xi = 1$, close to the critical line. For $\xi = 0$ we reproduce the spectrum of the pairing model [12]. Inclusion of a nonconstant single-particle energy does not require any modification of the procedure outlined. Instead if we increase the model space and/or the condensation sector, the structure functions will depend on more parameters and we will have to solve a constrained gap equation. The resulting Hamiltonian can be directly compared to that of the Interacting Boson model in the intrinsic frame.

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