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Collective excitations in an interacting boson gas beyond Bogoliubov theory

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ABSTRACT

In a gas of N interacting bosons, the Hamiltonian H_c, obtained by dropping all the interaction terms between free bosons with moment $\hbar\mathbf{k} \neq \mathbf{0}$, is diagonalized exactly. The resulting eigenstates $|S, \mathbf{k}, \eta\rangle$ depend on two discrete indices S, $\eta = 0, 1, \ldots$, where η numerates the *quasiphonons* carrying a moment $\hbar\mathbf{k}$, responsible for transport or dissipation processes. S, in turn, numerates a ladder of 'vacua' $|S, \mathbf{k}, 0\rangle$, with increasing equispaced energies, formed by boson pairs with opposite moment. Passing from one vacuum to another ($S \to S \pm 1$), results from creation/annihilation of new momentless collective excitations, that we call *pseudobosons*. Exact quasiphonons originate from one of the vacua by 'creating' an asymmetry in the number of opposite moment bosons. The well known Bogoliubov collective excitations (CEs) are shown to coincide with the exact eigenstates $|0, \mathbf{k}, \eta\rangle$, i.e. with the quasiphonons (QPs) created from the lowest-level vacuum (S=0). All this is discussed, in view of existing or future experimental observations of the pseudobosons (PBs), a sort of bosonic Cooper pairs, which are the main factor of novelty beyond Bogoliubov theory.

1. Introduction

In his approach to the weakly interacting bosons gas [1,2], Bogoliubov's first step was eliminating from the N-bosons Hamiltonian:

$$H_{bos} = \sum_{\mathbf{k}} \overbrace{(\hbar^2 k^2/2M)}^{\mathcal{T}(k)} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \frac{1}{2}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} \hat{u}(q) b_{\mathbf{k}_2-\mathbf{q}}^\dagger b_{\mathbf{k}_1+\mathbf{q}}^\dagger b_{\mathbf{k}_1} b_{\mathbf{k}_2} \tag{1}$$

all the interaction terms that couple bosons in the excited states. This is a first-order approximation in the ratio N_{out}/N_{in}, between the number of particles outside and inside the free particle ground state, which yields the truncated canonic Hamiltonian:

$$H_c = \overbrace{\frac{\hat{u}(0)N^2}{2}}^{E_{in}} + \sum_{\mathbf{k}\neq 0} \overbrace{[\mathcal{T}(k) + \widetilde{N}_{in}\hat{u}(k)]}^{\tilde{\epsilon}_1(k)} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \frac{1}{2}\sum_{\mathbf{k}\neq 0} \hat{u}(k)[b_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger (b_{\mathbf{0}})^2 + b_{\mathbf{k}} b_{-\mathbf{k}} (b_{\mathbf{0}}^\dagger)^2], \tag{2}$$

in the thermodynamic limit (TL). The operators $b_{\mathbf{k}}^\dagger$ and $b_{\mathbf{k}}$ create/destroy a spinless boson in the free-particle state $\langle \mathbf{r}|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V}$ and

$$\hat{u}(q) = \frac{1}{V}\int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} u(r),$$

is the Fourier transform of the *repulsive* interaction energy $u(r)$ (> 0). The number operator $\widetilde{N}_{in} = b_{\mathbf{0}}^\dagger b_{\mathbf{0}}$ refers to the bosons in the free particle ground state. Overtilded symbols indicate operators to avoid confusion with their (non-overtilded) eigenvalues.

Bogoliubov's next step is reducing H_c to a bi-linear form, which is realized in the TL, by assuming $|N_{in} \pm 2, N_{out}\rangle \approx |N_{in}, N_{out}\rangle$ for the bosonic Fock states [3], which yields the approximated Hamiltonian:

$$H_{BCA} = E_{in} + \sum_{\mathbf{k}\neq 0} \overbrace{[\mathcal{T}(k) + N\hat{u}(k)]}^{\epsilon_1(k)} \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} + \frac{N}{2}\sum_{\mathbf{k}\neq 0} \hat{u}(k)[\beta_{\mathbf{k}}^\dagger \beta_{-\mathbf{k}}^\dagger + \beta_{\mathbf{k}}\beta_{-\mathbf{k}}], \tag{3a}$$

where new creation/annihilation operators are introduced:

$$\beta_{\mathbf{k}} = b_{\mathbf{0}}^\dagger (\widetilde{N}_{in} + 1)^{-1/2} b_{\mathbf{k}}, \quad \beta_{\mathbf{k}}^\dagger = b_{\mathbf{k}}^\dagger (\widetilde{N}_{in} + 1)^{-1/2} b_{\mathbf{0}}, \tag{3b}$$

ensuring the conservation of the number N of real bosons. Note that $\beta_{\mathbf{k}}$ and $\beta_{\mathbf{k}}^\dagger$ satisfy the bosonic commutation rules *exactly* [4,5]. This is what we call the Bogoliubov Canonic Approximation (BCA). Since H_{BCA} is a bi-linear form in bosonic creation/annihilation operators, it is possible to eliminate the interactions by a suitable Bogoliubov transformation:

$$B_{\mathbf{k}}^\dagger = w_+^* \beta_{\mathbf{k}}^\dagger - w_-^* \beta_{-\mathbf{k}}; \quad B_{\mathbf{k}} = w_+ \beta_{\mathbf{k}} - w_- \beta_{-\mathbf{k}}^\dagger, \tag{4}$$

which leads to a *free* gas of new 'particles', which is customary to call *collective excitations* (CEs), or 'quasiparticles'. In the present work, the terms 'quasiphonon' (QP) and 'pseudoboson' (PB) will be used to distinguish, respectively, between a CE displaying a genuine particle nature, from one that does not, as will be seen in what follows.

In Ref. [3], since now on referred to as (I), the present author has diagonalized the Hamiltonian (2) exactly, in the special subspace

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spanned by the states $|j,\ \mathbf{k}\rangle_0$ with the same number j of bosons in $|\mathbf{k}\rangle$ and $|-\mathbf{k}\rangle$ and $N-2j$ bosons in $|\mathbf{0}\rangle$:

$$|j,\ \mathbf{k}\rangle_0=\frac{(b_{\mathbf{0}}^{\dagger})^{N-2j}}{\sqrt{(N-2j)!}}\frac{(b_{\mathbf{k}}^{\dagger})^{j}(b_{-\mathbf{k}}^{\dagger})^{j}}{j!}|\varnothing\rangle \tag{5}$$

($|\varnothing\rangle$ being the real bosons' vacuum). The resulting eigenvalues $E_S(k,0)$ (see, in particular, [6]) turn out to be *twice as large as* the BCA energies $\mathcal{E}_S(k,0)$ reported in the current literature [7]:

$$E_S(k,0)=2\underbrace{\left[\epsilon(k)\left(S+\frac{1}{2}\right)-\frac{\epsilon_1(k)}{2}\right]}_{\mathcal{E}_S(k,0)}\quad(S=0,\ 1,\ \ldots), \tag{6a}$$

where:

$$\epsilon(k)=\sqrt{\epsilon_1^2(k)-N^2\hat{u}^2(k)}, \tag{6b}$$

$\epsilon_1(k)$ being defined in Eq. (3a). The exact eigenstates of H_c calculated in (I) are, in turn, quite different from the BCA eigenstates: the latter have total moment $S\hbar\mathbf{k}$, corresponding to a number S of QPs, while the formers have *zero* total moment, for any S. In this case, the eigenstate is formed by a 'sea' of opposite moment pairs, and S numerates what we call the 'pseudobosons' (PBs) carried by the eigenstate. Hence a PB corresponds to the creation of a momentless quantum $2\epsilon(k)$ of energy, which cannot be considered a particle in its full sense, but, rather, a sort of bosonic Cooper pair. The next question is, thereby, which *exact* QPs do follow from the diagonalization of H_c. This question was left to future investigations in (I), where the diagonalization of H_c was limited to the subspace spanned by the momentless states equation (5). In the present work the diagonalization of H_c is extended to the subspaces containing a different number of bosons with opposite moment:

$$|j,\ \mathbf{k}\rangle_\eta=\frac{(b_{\mathbf{0}}^{\dagger})^{N-2j-\eta}}{\sqrt{(N-2j-\eta)!}}\frac{(b_{\mathbf{k}}^{\dagger})^{j+\eta}(b_{-\mathbf{k}}^{\dagger})^{j}}{\sqrt{j!(j+\eta)!}}|\varnothing\rangle, \tag{7}$$

with $j+\eta$ bosons in $|\mathbf{k}\rangle$, j bosons in $|-\mathbf{k}\rangle$ and $N-2j-\eta$ bosons in $|\mathbf{0}\rangle$, so that the total moment is, manifestly, $\eta\hbar\mathbf{k}$. From a formal viewpoint, this is the main factor of novelty, with respect to (I) (Section 2). However, the results obtained open the way to other new items and perspectives. In particular, in Section 3 it is shown that the creation/annihilation of a QP ($\eta\to\eta\pm1$) corresponds to enhance/reduce the asymmetry between opposite moment populations. Creating/annihilating a PB ($S\to S\pm1$), instead, corresponds to the passage between different 'vacua' of QPs, which are the states with symmetric populations studied in (I). Furthermore, Bogoliubov theory turns out to be a special case of the general exact solution developed in Section 2, in which the symmetry breaking occurs on the zero-PBs state (S=0). Finally, possible effects revealing the existence of the PBs are outlined in Section 4, with some insight about their experimental observation.

2. Complete diagonalization of H_c

Before entering the main subject, it should be recalled that in the present work the results are 'exact' with respect to Bogoliubov's approximations BCA, not with respect to the truncation of Hamiltonian (1), leading to H_c (Eq. (2)).

Hamiltonian H_c can be written as a sum of independent one-moment Hamiltonians

$$H_c=E_{in}+\sum_{\mathbf{k}\neq0}h_c(\mathbf{k}), \tag{8a}$$

where:

$$h_c(\mathbf{k})=\frac{1}{2}\tilde{\epsilon}_1(k)[b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}+b_{-\mathbf{k}}^{\dagger}b_{-\mathbf{k}}]+\frac{1}{2}\hat{u}(k)[b_{\mathbf{k}}^{\dagger}b_{-\mathbf{k}}^{\dagger}(b_{\mathbf{0}})^2+b_{\mathbf{k}}b_{-\mathbf{k}}(b_{\mathbf{0}}^{\dagger})^2]. \tag{8b}$$

Hence the whole problem can be reduced to the study of the exact eigenstates of $h_c(\mathbf{k})$,[1] by solving the eigenvalue equation

$$h_c|S,\ \mathbf{k},\ \eta\rangle=\mathcal{E}_S(k,\eta)|S,\ \mathbf{k},\ \eta\rangle, \tag{9}$$

with exact QPs expressed as linear combinations of the states equation (7). Thanks to a suitable transformation [8], Eq. (9) can be reduced to the same problem already solved *analytically* in (I). This makes it possible to write the eigenstates of h_c (Eq. (8b)) as:

$$|S,\ \mathbf{k},\ \eta\rangle=\sum_{j=0}^{\infty}\overbrace{x^j(k)\sqrt{\binom{j+\eta}{j}}\sum_{m=0}^{S}C_{S,\eta}(m,k)j^m}^{\phi_{S,\eta}(j,\,k)}|j,\ \mathbf{k}\rangle_\eta, \tag{10}$$

with boundary conditions $\lim_{j\to\infty}\phi_{S,\eta}(j,k)=0$ (necessary for normalizability) and $\phi_{S,\eta}(-1,k)=0$ (exclusion of negative populations). It should be noticed that $\left|\phi_{S,\eta}(j,k)\right|^2\propto j^{2S+\eta}x^{2j}(k)$ for $j\gg1$, i.e. the pre-exponential factor in the probability amplitude on the Fock states $|j,\ \mathbf{k}\rangle_\eta$ (Eq. (7)) tends to a polynomial of degree $2S+\eta$ in $j\gg1$. The quantity $x(k)$, the coefficients $C_{S,\eta}(m,k)$ and the eigenvalue $\mathcal{E}_S(k,\eta)$ are determined by a system of $S+2$ equations (see Ref. [8]), and by normalization. The resulting expressions for $x(k)$ (fixing the exponential decay in j) and the eigenvalue $\mathcal{E}_S(k,\eta)$ read:

$$x(k)=\frac{\epsilon(k)-\epsilon_1(k)}{N\hat{u}(k)} \tag{11a}$$

$$\mathcal{E}_S(k,\ \eta)=\frac{\epsilon(k)}{2}(\eta+2S)-\frac{\epsilon_1(k)-\epsilon(k)}{2}\quad(S,\ \eta=0,\ 1,\ \ldots). \tag{11b}$$

Notice that $x(k)$ is negative and smaller than 1 in modulus, which ensures normalizability. Since $h_c(\mathbf{k})=h_c(-\mathbf{k})$ (Eq. (8b)), $\mathcal{E}_S(k,\ \eta)$ must be counted twice in the sum equation (8a).[2] Hence the energy eigenvalues of H_c-E_{in} are:

$$E_S(k,\ \eta)=2\mathcal{E}_S(k,\ \eta)=\epsilon(k)(\eta+2S)-[\epsilon_1(k)-\epsilon(k)] \tag{12a}$$

$$E_S(k,\eta)=\epsilon(k)\left(\eta+\frac{1}{2}\right)+2\epsilon(k)\left(S+\frac{1}{2}\right)-\underbrace{\left[\epsilon_1(k)+\frac{\epsilon(k)}{2}\right]}_{\mathcal{E}_0(k)}. \tag{12b}$$

For the calculations in what follows, it is useful to recall that the coefficients $w_\pm(\mathbf{k})$ in the Bogoliubov transformation equation (4) can be expressed in terms of $x(\mathbf{k})$ (Eq. (11a)) as follows:

$$w_+=\frac{1}{\sqrt{1-x^2}};\quad w_-=\frac{x}{\sqrt{1-x^2}}. \tag{13}$$

The limit of large $k\gg\xi^{-1}\equiv\sqrt{2M\hat{u}(0)N}/\hbar$ that marks the passage from collective to single-particle dynamics, yields $\epsilon_1(k)\to\mathcal{T}(k)$ and $\epsilon(k)-\epsilon_1(k)\to0$. Hence, from Eq. (12), one has:

$$E_S(k,\ \eta)\to(2S+\eta)\mathcal{T}(k)\quad(k\gg\xi^{-1}). \tag{14}$$

Since the CEs (QPs and PBs) become non-interacting *real* bosons when their kinetic energy $\mathcal{T}(k)=\hbar^2k^2/(2M)$ largely exceeds the interaction energy, the number $2S+\eta$ corresponds to the total number of real bosons excited in the limit $k\gg\xi^{-1}$. This agrees with physical intuition: each PB corresponds to the creation of a sort of bosonic Cooper pair, i.e. *two* bosons in $|\pm\mathbf{k}\rangle$, with opposite momenta and identical kinetic energy; each QP corresponds to the additional activation of a *single* boson in $|\mathbf{k}\rangle$.

3. Discussion and comparison with Bogoliubov theory

Unlike some thermodynamic results [9], the differences between Bogoliubov's *dynamics* and exact dynamics do not vanish in the TL. In

[1] In (I) those exact QPs have been improperly denoted as 'η-pseudobosons'.

[2] Ignoring the double counting was the error in the original version of Ref. [3], emended in [6].