

Bogoliubov transformation for distinguishable particles

M. Holzmann and F. Laloë
Laboratoire de Physique de l'ENS,
LKB et LPS, 24 rue Lhomond, F-75005 Paris, France

July 13, 2006

Abstract

The Bogoliubov transformation is generally derived in the context of identical bosons with the use of “second quantized” a and a^\dagger operators (or, equivalently, in field theory). Here, we show that the transformation, together with its characteristic energy spectrum, can also be derived within the Hilbert space of distinguishable particles, obeying Boltzmann statistics; in this derivation, ordinary dyadic operators play the role usually played by the a and a^\dagger operators; therefore, breaking the symmetry of particle conservation is not necessary.

The Bogoliubov transformation [1][2] is an essential tool in the theory of Bose-Einstein condensation of identical bosons¹. It modifies the quadratic energy spectrum of free particles into a quasiparticle spectrum which includes a linear variation for small momenta; this feature is generally associated with the existence of phonons and, since it introduces a non zero minimum value for the ratio between the energy and momentum, it allows a natural derivation of the notion of critical velocity (a maximum velocity for the system to remain superfluid). Usually, the mathematics of the Bogoliubov transformation is performed within the formalism of creation and annihilation operators (often called “second quantization” for historical reasons); assuming that the system is entirely made of identical particles, one then uses a formalism which automatically ensures a full symmetrization of the state vector. Nevertheless, the notion of phonons has a much broader scope in physics than just identical quantum particles; it is even often discussed in the context of classical systems, solids or even fluids. One can therefore wonder whether it is possible to re-derive the Bogoliubov spectrum in a context where the particles are considered as distinguishable and where, as a consequence, the effect of exchange operators remains completely

¹Historically, the first introduction of the mathematical transformation seems to be the work of Holstein and Primakoff in 1940 [3], in the context of magnetic systems.

explicit. The purpose of the present article is to show how this is indeed possible. Another motivation for a mathematical derivation of the Bogoliubov transformation within the Hilbert space of distinguishable particles arises for the use of Ursell operators in statistical mechanics [4], a formalism in which the symmetrization of the states is not introduced implicitly from the beginning of the calculations, but explicitly and at a later stage with the help of exchange cycles.

1 Hamiltonian

The hamiltonian of the problem is:

$$H = \sum_{i=1}^N \frac{(\mathbf{P}_i)^2}{2m} + \frac{1}{2} \sum_{i \neq j} V(i, j) \quad (1)$$

where N is the number of particles, m their mass, \mathbf{P}_i the momentum of particle numbered i , and $V(i, j)$ the interaction energy of particles numbered i and j . The simplest assumption is to take the matrix elements of this interaction potential as constant, provided they satisfy momentum conservation (otherwise they of course vanish):

$$\langle i : \mathbf{k}, j : \mathbf{k}' | V(i, j) | i : \mathbf{k} + \mathbf{q}, j : \mathbf{k}' - \mathbf{q} \rangle = g \quad (2)$$

where g is the coupling constant, inversely proportional to the volume of the system². The hamiltonian can then be written:

$$H = \sum_{i=1}^N \frac{(\mathbf{P}_i)^2}{2m} + \frac{g}{2} \sum_{i \neq j} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} | i : \mathbf{k}, j : \mathbf{k}' \rangle \langle i : \mathbf{k} + \mathbf{q}, j : \mathbf{k}' - \mathbf{q} | \quad (3)$$

In this expression the interaction term contains, first, the forward scattering terms $\mathbf{q} = 0$ which can be written:

$$\begin{aligned} & \frac{g}{2} \sum_{i \neq j} \sum_{\mathbf{k}, \mathbf{k}'} | i : \mathbf{k} \rangle \langle i : \mathbf{k} | \otimes | j : \mathbf{k}' \rangle \langle j : \mathbf{k}' | \\ &= \frac{g}{2} \sum_{i, j} \sum_{\mathbf{k}, \mathbf{k}'} | i : \mathbf{k} \rangle \langle i : \mathbf{k} | \otimes | j : \mathbf{k}' \rangle \langle j : \mathbf{k}' | - \frac{g}{2} N \end{aligned} \quad (4)$$

or simply:

$$\frac{g}{2} N(N - 1) \quad (5)$$

²In the thermodynamic limit, g itself tends to zero, but products such as gN keep a finite value.

As for the $\mathbf{q} \neq 0$ terms, they never contain 4, or even 3, vanishing momenta; the terms containing 2 vanishing momenta can include them, either in the same side of the operator, or in opposite sides:

$$\begin{aligned} & \frac{g}{2} \sum_{i \neq j} \sum_{\mathbf{k} \neq 0} \left[|i : \mathbf{0}, j : \mathbf{0}\rangle \langle i : \mathbf{k}, j : -\mathbf{k}| + h.c. \right] \\ & + \frac{g}{2} \sum_{i \neq j} \sum_{\mathbf{k} \neq 0} \left[|i : \mathbf{0}, j : \mathbf{k}\rangle \langle i : \mathbf{k}, j : \mathbf{0}| + h.c. \right] \end{aligned} \quad (6)$$

where $h.c.$ is for Hermitian conjugate. It is convenient to express the second line³ of this expression as a function of simpler (diagonal) operators by re-writing it in the form:

$$g \sum_{i \neq j} \sum_{\mathbf{k} \neq 0} \left[|i : \mathbf{k}, j : \mathbf{0}\rangle \langle i : \mathbf{k}, j : \mathbf{0}| \right] + W_{as.} \quad (7)$$

where $W_{as.}$ is the (antisymmetrical) interaction operator:

$$W_{as.} = -g \sum_{i \neq j} \sum_{\mathbf{k}} \left[1 - P_{exch.}(i, j) \right] |i : \mathbf{k}, j : \mathbf{0}\rangle \langle i : \mathbf{k}, j : \mathbf{0}| \quad (8)$$

Here, $P_{exch.}(i, j)$ is the exchange operator of particles i and j (the condition $\mathbf{k} \neq \mathbf{0}$ in the summation can be released since the corresponding term vanishes); another equivalent expression of $W_{as.}$ can be obtained by applying the exchange operator to the right⁴:

$$W_{as.} = -g \sum_{i \neq j} \sum_{\mathbf{k}} |i : \mathbf{0}, j : \mathbf{k}\rangle \langle i : \mathbf{0}, j : \mathbf{k}| \left[1 - P_{exch.}(i, j) \right] \quad (9)$$

(in passing, we see that $W_{as.}$ is Hermitian). Now, the first operator in (7) can be simplified into:

$$g \sum_{i, j} \sum_{\mathbf{k} \neq 0} \left[|i : \mathbf{k}\rangle \langle i : \mathbf{k}| \otimes |j : \mathbf{0}\rangle \langle j : \mathbf{0}| \right] \quad (10)$$

(the constraint $i \neq j$ can be released since every term $i = j$ in the summation is zero, due to the orthogonality of single particle states), or again:

$$g N_0 \sum_{\mathbf{k} \neq 0} n_{\mathbf{k}} = g N_0 N_e \quad (11)$$

³For this operator in the second line, interchanging the dummy indices i and j is equivalent to an hermitian conjugate operation; for this term, we can therefore ignore the $h.c.$ and just replace $g/2$ by g .

⁴In (7), (8) or (9), interchanging the dummy indices i and j is equivalent to interchanging the states labelled by $\mathbf{0}$ and \mathbf{k} .

where $n_{\mathbf{k}}$ is the population of the excited state labelled by momentum \mathbf{k} :

$$n_{\mathbf{k}} = \sum_i |i : \mathbf{k} \rangle \langle i : \mathbf{k}| \quad (12)$$

N_0 the population of the ground state (for the ground state, we use a capital letter to emphasize that it has an extensive population, but N_0 is in fact the same operator as n_0):

$$N_0 = \sum_i |i : \mathbf{0} \rangle \langle i : \mathbf{0}| \quad (13)$$

N_e as the operator associated with the total number of excited particles:

$$N_e = \sum_{\mathbf{k} \neq \mathbf{0}} n_{\mathbf{k}} = N - N_0 \quad (14)$$

Finally, the interaction terms with 2 vanishing momenta can be written:

$$\frac{g}{2} \sum_{i \neq j} \sum_{\mathbf{k} \neq \mathbf{0}} \left[|i : \mathbf{0}, j : \mathbf{0} \rangle \langle i : \mathbf{k}, j : -\mathbf{k}| + h.c. \right] + g N_0 N_e + W_{as}. \quad (15)$$

Last, the only interaction term that we have not yet included corresponds to the interaction between particles in excited states; we call this operator V_{ee} :

$$V_{ee} = \frac{g}{2} \sum_{i \neq j} \sum_{\mathbf{k}, \mathbf{k}' \neq \mathbf{0}} \sum_{\mathbf{q} \neq \mathbf{0}, -\mathbf{k}, +\mathbf{k}'} \left[|i : \mathbf{k}, j : \mathbf{k}' \rangle \langle i : \mathbf{k} + \mathbf{q}, j : \mathbf{k}' - \mathbf{q}| + h.c. \right] \quad (16)$$

but, in what follows, we will merely neglect its effect; this is because the system will be supposed to be at sufficiently low temperature and to be sufficiently dilute so that most of the particles remain in the ground state; interaction effects proportional to the square of the excited state populations are then negligible.

To summarize, we have obtained the following expression for the Hamiltonian:

$$\begin{aligned} H &= \sum_{\mathbf{k} \neq \mathbf{0}} (e_k + g N_0) n_{\mathbf{k}} + \frac{g}{2} N (N - 1) \\ &+ \frac{g}{2} \sum_{i \neq j} \sum_{\mathbf{k} \neq \mathbf{0}} [|i : \mathbf{0}, j : \mathbf{0} \rangle \langle i : \mathbf{k}, j : -\mathbf{k}| + h.c.] \\ &+ V_{ee} + W_{as}. \end{aligned} \quad (17)$$

where the free particle energy e_k is defined, as usual, by:

$$e_k = \frac{\hbar^2 k^2}{2m} \quad (18)$$

2 Another expression of the hamiltonian

We introduce in this section a new hamiltonian H' which in a second step, we will identify with H term by term.

2.1 Introducing new creation and annihilation operators

We now define the operator $A_{\mathbf{k}}$ by:

$$A_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_i \{ \alpha_{\mathbf{k}} | i : \mathbf{0} \rangle \langle i : \mathbf{k} | + \beta_{\mathbf{k}} | i : -\mathbf{k} \rangle \langle i : \mathbf{0} | \} \quad (19)$$

where we assume that $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ are real numbers, which are for the moment not fixed, but which are supposed to be even functions of the vector \mathbf{k} :

$$\alpha_{\mathbf{k}} = \alpha_{-\mathbf{k}} \quad ; \quad \beta_{\mathbf{k}} = \beta_{-\mathbf{k}} \quad (20)$$

$A_{\mathbf{k}}$ is defined as an operator which removes a momentum $\hbar \mathbf{k}$ from the system by, either transferring one particle from momentum \mathbf{k} to zero, or from zero to $-\mathbf{k}$; it is a single particle operator which, if restricted within the totally symmetric part \mathcal{E}_S of the Hilbert space, could be expressed (through the well known expression of single particle operators) as:

$$A_{\mathbf{k}}^S = \frac{1}{\sqrt{N}} \left\{ \alpha_{\mathbf{k}} a_0^\dagger a_{\mathbf{k}} + \beta_{\mathbf{k}} a_0 a_{-\mathbf{k}}^\dagger \right\} \quad (21)$$

with the usual notation for the creation and annihilation operators $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^\dagger$.

The Hermitian conjugate of $A_{\mathbf{k}}$ is equal to:

$$A_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{N}} \sum_j \{ \alpha_{\mathbf{k}} | j : \mathbf{k} \rangle \langle j : \mathbf{0} | + \beta_{\mathbf{k}} | j : \mathbf{0} \rangle \langle j : -\mathbf{k} | \} \quad (22)$$

We can now calculate the commutator of $A_{\mathbf{k}}$ and $A_{\mathbf{k}}^\dagger$ term by term. For instance, the commutator of $| i : \mathbf{0} \rangle \langle i : \mathbf{k} |$ with $| j : \mathbf{k} \rangle \langle j : \mathbf{0} |$ is zero except if $i = j$; assuming that this is the case, the commutator is given by:

$$| i : \mathbf{0} \rangle \langle i : \mathbf{k} | | i : \mathbf{k} \rangle \langle i : \mathbf{0} | - | i : \mathbf{k} \rangle \langle i : \mathbf{0} | | i : \mathbf{0} \rangle \langle i : \mathbf{k} | \quad (23)$$

which is merely the difference $| i : \mathbf{0} \rangle \langle i : \mathbf{0} | - | i : \mathbf{k} \rangle \langle i : \mathbf{k} |$. Taking the sum of all four terms in a similar way gives (the crossed term in $\alpha_{\mathbf{k}} \times \beta_{\mathbf{k}}$ vanish):

$$\begin{aligned} [A_{\mathbf{k}}, A_{\mathbf{k}}^\dagger] &= N^{-1} \sum_i \left\{ \alpha_{\mathbf{k}}^2 \left[| i : \mathbf{0} \rangle \langle i : \mathbf{0} | - | i : \mathbf{k} \rangle \langle i : \mathbf{k} | \right] \right. \\ &\quad \left. + \beta_{\mathbf{k}}^2 \left[| i : -\mathbf{k} \rangle \langle i : -\mathbf{k} | - | i : \mathbf{0} \rangle \langle i : \mathbf{0} | \right] \right\} \end{aligned} \quad (24)$$

or:

$$\left[A_{\mathbf{k}} , A_{\mathbf{k}}^{\dagger} \right] = (\alpha_{\mathbf{k}}^2 - \beta_{\mathbf{k}}^2) \frac{N_0}{N} + \beta_{\mathbf{k}}^2 \frac{n_{-\mathbf{k}}}{N} - \alpha_{\mathbf{k}}^2 \frac{n_{\mathbf{k}}}{N} \quad (25)$$

or again:

$$\left[A_{\mathbf{k}} , A_{\mathbf{k}}^{\dagger} \right] = (\alpha_{\mathbf{k}}^2 - \beta_{\mathbf{k}}^2) + \beta_{\mathbf{k}}^2 \frac{n_{-\mathbf{k}} + N_e}{N} - \alpha_{\mathbf{k}}^2 \frac{n_{\mathbf{k}} + N_e}{N} \quad (26)$$

We now calculate the product $A_{\mathbf{k}}^{\dagger} A_{\mathbf{k}}$ for any $\mathbf{k} \neq \mathbf{0}$; the terms $i = j$ provide:

$$\begin{aligned} & N^{-1} \sum \left[\alpha_{\mathbf{k}}^2 | i : \mathbf{k} \rangle \langle i : \mathbf{k} | + \beta_{\mathbf{k}}^2 | i : \mathbf{0} \rangle \langle i : \mathbf{0} | \right] \\ &= N^{-1} \left[\alpha_{\mathbf{k}}^2 n_{\mathbf{k}} + \beta_{\mathbf{k}}^2 N_0 \right] \end{aligned} \quad (27)$$

while the terms $i \neq j$ contain a summation of the expression:

$$\begin{aligned} & N^{-1} \left\{ \alpha_{\mathbf{k}}^2 | i : \mathbf{0}, j : \mathbf{k} \rangle \langle i : \mathbf{k}, j : \mathbf{0} | + \beta_{\mathbf{k}}^2 | i : -\mathbf{k}, j : \mathbf{0} \rangle \langle i : \mathbf{0}, j : -\mathbf{k} | \right. \\ & \left. + \alpha_{\mathbf{k}} \times \beta_{\mathbf{k}} \left[| i : \mathbf{0}, j : \mathbf{0} \rangle \langle i : \mathbf{k}, j : -i\mathbf{k} | + h.c. \right] \right\} \end{aligned} \quad (28)$$

where, as above, *h.c.* is for Hermitian conjugate⁵. We can now use the same method as in § 1 to distinguish, within the first line of (28), a “diagonal” part and an antisymmetrical part $B_{as.}(\mathbf{k})$:

$$\frac{1}{N} \left[\alpha_{\mathbf{k}}^2 N_0 n_{\mathbf{k}} + \beta_{\mathbf{k}}^2 N_0 n_{-\mathbf{k}} \right] + B_{as.}(\mathbf{k}) \quad (29)$$

with the definition:

$$\begin{aligned} B_{as.}(\mathbf{k}) = -\frac{1}{N} \sum_{i \neq j} [1 - P_{exch.}(i, j)] \left\{ \left[\alpha_{\mathbf{k}}^2 | i : \mathbf{k}, j : \mathbf{0} \rangle \langle i : \mathbf{k}, j : \mathbf{0} | \right. \right. \\ \left. \left. + \beta_{\mathbf{k}}^2 | i : \mathbf{0}, j : -\mathbf{k} \rangle \langle i : \mathbf{0}, j : -\mathbf{k} | \right] \right\} \end{aligned} \quad (30)$$

or, equivalently, by applying the exchange operator on the other side:

$$\begin{aligned} B_{as.}(\mathbf{k}) = -\frac{1}{N} \sum_{i \neq j} \left\{ \left[\alpha_{\mathbf{k}}^2 | i : \mathbf{0}, j : \mathbf{k} \rangle \langle i : \mathbf{0}, j : \mathbf{k} | \right. \right. \\ \left. \left. + \beta_{\mathbf{k}}^2 | i : -\mathbf{k}, j : \mathbf{0} \rangle \langle i : -\mathbf{k}, j : \mathbf{0} | \right] \right\} [1 - P_{exch.}(i, j)] \end{aligned} \quad (31)$$

Finally, we obtain:

$$\begin{aligned} A_{\mathbf{k}}^{\dagger} A_{\mathbf{k}} &= \alpha_{\mathbf{k}}^2 n_{\mathbf{k}} \left(\frac{1 + N_0}{N} \right) + \beta_{\mathbf{k}}^2 \frac{N_0}{N} (1 + n_{-\mathbf{k}}) \\ &+ N^{-1} \alpha_{\mathbf{k}} \beta_{\mathbf{k}} \left\{ \sum_{i \neq j} | i : \mathbf{0}, j : \mathbf{0} \rangle \langle i : \mathbf{k}, j : -\mathbf{k} | + h.c. \right\} + B_{as.}(\mathbf{k}) \end{aligned} \quad (32)$$

⁵For this hermitian conjugate term, we have interchanged the dummy indices i and j .

2.2 Identification of two expressions

Let us introduce a new hamiltonian H' by:

$$H' = \sum_{\mathbf{k} \neq \mathbf{0}} \widetilde{e}_k A_{\mathbf{k}}^\dagger A_{\mathbf{k}} + \lambda_N N + \lambda_e N_e \quad (33)$$

where $\alpha_{\mathbf{k}}$, $\beta_{\mathbf{k}}$, \widetilde{e}_k , λ_N and λ_e are for the moment free parameters - in a second step they will be chosen in order to make the new hamiltonian equal to the initial Hamiltonian:

$$\begin{aligned} H &= \sum_{\mathbf{k} \neq \mathbf{0}} (e_k + gN_0) n_{\mathbf{k}} + \frac{g}{2} N(N-1) \\ &+ \frac{g}{2} \sum_{i \neq j} \sum_{\mathbf{k} \neq \mathbf{0}} [|i : \mathbf{0}, j : \mathbf{0} \rangle \langle i : \mathbf{k}, j : -\mathbf{k}| + h.c.] \end{aligned} \quad (34)$$

In addition, $A_{\mathbf{k}}$ and $A_{\mathbf{k}}^\dagger$ will have commutation relation that are similar to those of ordinary creation and annihilation operators.

(i) first condition (commutation relation); if:

$$\alpha_{\mathbf{k}}^2 - \beta_{\mathbf{k}}^2 = 1 \quad (35)$$

(for any value of \mathbf{k}), relation (26) shows that the commutator of $A_{\mathbf{k}}$ and $A_{\mathbf{k}}^\dagger$ is equal to one in the limit of very low temperatures and very dilute systems (when almost all the particles are in the ground state, $N_e \ll N$). Relation (35) is automatically fulfilled with the following choice of the two parameters $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ as a function of a single parameter $\xi_{\mathbf{k}}$:

$$\begin{aligned} \alpha_{\mathbf{k}} &= \cosh \xi_{\mathbf{k}} \\ \beta_{\mathbf{k}} &= \sinh \xi_{\mathbf{k}} \end{aligned} \quad (36)$$

(ii) second condition (identification of the main interaction terms); from (17), (32) and (33) we get that the terms in $|i : \mathbf{0}, j : \mathbf{0} \rangle \langle i : \mathbf{k}, j : -\mathbf{k}|$ can be made identical if we set:

$$\widetilde{e}_k \alpha_{\mathbf{k}} \beta_{\mathbf{k}} = \frac{gN}{2} \quad (37)$$

which, through (36), is equivalent to:

$$\widetilde{e}_k \sinh 2\xi_{\mathbf{k}} = gN \quad (38)$$

(iii) third condition (kinetic terms in $n_{\mathbf{k}}$); the identification of the terms which, in (32), are linear in the excited population operators $n_{\mathbf{k}}$ (or $n_{-\mathbf{k}}$) provides the condition:

$$\widetilde{e}_k \left\{ \alpha_{\mathbf{k}}^2 \frac{1 + N_0}{N} + (\beta_{-\mathbf{k}})^2 \frac{N_0}{N} \right\} = e_k + gN_0 \quad (39)$$

or, through the relation $N = N_0 + N_e$:

$$\widetilde{e_k} \left\{ \alpha_{\mathbf{k}}^2 \frac{1 + N - N_e}{N} + (\beta_{-\mathbf{k}})^2 \frac{N - N_e}{N} \right\} = e_k + gN - gN_e \quad (40)$$

In this equation, N is a number while N_e is an operator; term by term identification then provides the two conditions:

$$\begin{aligned} \widetilde{e_k} \left[\alpha_{\mathbf{k}}^2 (1 + N^{-1}) + (\beta_{-\mathbf{k}})^2 \right] &= e_k + gN \\ \widetilde{e_k} \left[\alpha_{\mathbf{k}}^2 - (\beta_{-\mathbf{k}})^2 \right] \frac{N_e}{N} &= gN_e \end{aligned} \quad (41)$$

Assuming that $N \gg 1$, and taking into account the parity relation (20) as well as definition (36), we can write the former in the form :

$$\widetilde{e_k} (\alpha_{\mathbf{k}}^2 + \beta_{\mathbf{k}}^2) = \widetilde{e_k} \cosh 2\xi_{\mathbf{k}} = e_k + gN \quad (42)$$

an equality which, together with (38), will provide the Bogoliubov quasiparticle spectrum. In the second line of (41), we have intentionally left in both sides the operator N_e ; in this way we emphasize that, in the expression of H' , this term appears as a product of N_e by the population operator $n_{\mathbf{k}}$ of the excited state \mathbf{k} , in other words as a second order correction in N_e/N which can be neglected in the limit of low temperatures and very dilute systems. Therefore, the major constraint of the identification is contained in (42) and, from now on, we will leave aside the second condition of (41).

(iv) terms in N and N_e ; in (32), we have not yet included the effect of the term $(\beta_{\mathbf{k}})^2 N_0/N$ which, when N_0 is replaced by $N - N_e$, provides:

$$\frac{g}{2} N(N-1) = \sum_{\mathbf{k}} \widetilde{e_k} (\beta_{\mathbf{k}})^2 \left(1 - \frac{N_e}{N} \right) + \lambda_N N + \lambda_e N_e \quad (43)$$

Term by term identification then provides⁶:

$$\lambda_N = \frac{g}{2} (N-1) - \frac{1}{N} \sum_{\mathbf{k}} \widetilde{e_k} (\beta_{\mathbf{k}})^2 \quad (44)$$

and:

$$\lambda_e = \frac{1}{N} \sum_{\mathbf{k}} \widetilde{e_k} (\beta_{\mathbf{k}})^2 \quad (45)$$

We will neglect λ_e in what follows.

⁶Since, according to (47), $\beta_{\mathbf{k}}$ will be proportional to $1/e_k$ when k is large, the sums in equation (43) and following are linearly divergent at infinity. We discuss in § 3.1.2 how this divergence can be eliminated.

(v) antisymmetric terms $B_{as.}$ and $W_{as.}$; the initial hamiltonian contains the operator $W_{as.}$ while H' contains the operator:

$$W'_{as.} = \sum_{\mathbf{k}} \widetilde{e_k} B_{as}(\mathbf{k}) \quad (46)$$

where $B_{as.}(\mathbf{k})$ is defined in (30) or (31). We note that both these terms contain two particle antisymmetrizers $[1 - P_{exch. i, j}]$ and will therefore always vanish when multiplied (on any side) by the N particle symmetrization operator S_N ; their contribution is therefore exactly zero if the particles in the system are identical bosons. By the same token, the same remains true if the particles are distinguishable but in their ground state, which is also completely symmetrical (it is actually exactly the same as for bosons). The property obviously extends to any excited state having the same permutation symmetry, but not necessarily for energy states which correspond to other representations of the permutation group; in general, there is no reason why the difference $W_{as.} - W'_{as.}$ should play no role for distinguishable particles⁷.

2.3 Bogoliubov spectrum

From (38) and (42) we get by taking the ratio:

$$\tanh 2\xi_{\mathbf{k}} = \frac{gN}{e_k + gN} \quad (47)$$

which fixes the value of $\xi_{\mathbf{k}}$; to determine $\widetilde{e_k}$ we express $\cosh 2\xi_{\mathbf{k}}$ as a function of this result:

$$\frac{1}{\cosh^2 2\xi_{\mathbf{k}}} = 1 - \tanh^2 2\xi_{\mathbf{k}} = \frac{e_k (e_k + 2gN)}{(e_k + gN)^2} \quad (48)$$

which, combined with (42), gives:

$$\widetilde{e_k} = \sqrt{e_k (e_k + 2gN)} \quad (49)$$

This is the well known Bogoliubov result for the energy of the quasi-particles; actually relations (47) and (49) are exactly the basic relations obtained in the usual calculation in terms of annihilation and creation operators.

⁷Using the parity of $\beta_{\mathbf{k}}$ and interchanging the dummy indices i and j in (30) allows to show that $W'_{as.}$ is equal to the sum over \mathbf{k} of the product $\widetilde{e_k} (\alpha_{\mathbf{k}}^2 + \beta_{\mathbf{k}}^2)$ by the same sum over $i \neq j$ which appears in (8); the strict equality of $W'_{as.}$ and $W_{as.}$ would require the condition $\sum_{\mathbf{k}} \widetilde{e_k} (\alpha_{\mathbf{k}}^2 + \beta_{\mathbf{k}}^2) = gN$, which is reminiscent of the second condition (41), but introduces convergence problems. Requesting a strict equality of the operators H and H' in the whole Hilbert state of Boltzmann particles would then lead to difficulties.

With the above relations, the two Hamiltonians H and H' can be identified, with three approximations:

* (A1) we assume that the difference $W_{as.} - W'_{as.}$ can be ignored, which is exact for totally symmetric states.

* (A2) we ignore the effect of V_{ee} , corresponding to the interactions between excited particles.

* (A3) we ignore the condition expressed in the second line of (41).

The third approximation is consistent with the second and remains valid at low density and temperature, exactly as in the usual derivation for bosons. The first is of different nature since it is necessary only for Boltzmann particles; we have already mentioned that the operator $W_{as.} - W'_{as.}$ plays no role for the ground state of the system, as well as for all states which are fully symmetric - for instance for all states that are obtained from the ground state by action of any product of creation operators $A_{\mathbf{k}}^\dagger$'s, since these operators do not change the permutation symmetry of the states.

3 Discussion

We now discuss more precisely how the operators $A_{\mathbf{k}}$ and $A_{\mathbf{k}}^\dagger$ can be used to construct eigenstates of the hamiltonian.

3.1 Commutation relations

One of the commutation relations between the new creation and annihilation operators has already been studied above, and led us to an approximation which is consistent with approximation (A2):

* (A4) we ignore, in (26), the terms in N_e/N (as well as those in $n_{\mathbf{k}}/N$, but the latter tend to zero in the thermodynamic limit and therefore raise no question).

But we also have to study the situation for different values of \mathbf{k} as well as other commutations relations. We see in the definition (19) of $A_{\mathbf{k}}$ that its commutator with $A_{\mathbf{k}'}$ will, first, contain the commutator:

$$\left[|i : \mathbf{0} \rangle \langle i : \mathbf{k} |, |i : \mathbf{0} \rangle \langle i : \mathbf{k}' | \right] \quad (50)$$

which vanishes since both products of the operators do so (orthogonality of single particle states if \mathbf{k} and \mathbf{k}' are both different from zero). Similarly:

$$\left[|i : -\mathbf{k} \rangle \langle i : \mathbf{0} |, |i : -\mathbf{k}' \rangle \langle i : \mathbf{0} | \right] = 0 \quad (51)$$

Two other commutators do not vanish, for instance:

$$\begin{aligned} & \left[|i : -\mathbf{k} \rangle \langle i : \mathbf{0} |, |i : -\mathbf{k}' \rangle \langle i : \mathbf{0} | \right] \\ &= |i : -\mathbf{k} \rangle \langle i : \mathbf{k}' | - \delta_{\mathbf{k}, -\mathbf{k}'} |i : \mathbf{0} \rangle \langle i : \mathbf{0} | \end{aligned} \quad (52)$$

so that we obtain the result:

$$\begin{aligned} [A_{\mathbf{k}}, A_{\mathbf{k}'}] &= \delta_{\mathbf{k}, -\mathbf{k}'} (\alpha_{\mathbf{k}} \beta_{-\mathbf{k}} - \alpha_{-\mathbf{k}} \beta_{\mathbf{k}}) \frac{N_0}{N} \\ &- \frac{\alpha_{\mathbf{k}} \beta_{\mathbf{k}'}}{N} \sum_i |i : -\mathbf{k}' \rangle \langle i : \mathbf{k}| + \frac{\alpha_{\mathbf{k}'} \beta_{\mathbf{k}}}{N} \sum_i |i : -\mathbf{k} \rangle \langle i : \mathbf{k}'| \end{aligned} \quad (53)$$

The parity relation (20) ensures that the main term in the right hand side, proportional to N_0/N , vanishes exactly. The remaining terms, on the second line, are as V_{ee} “excited-excited terms” which act only on excited particles, and leave them excited; it is therefore natural to introduce one more assumption:

* (A5) the operators in the second line of (53) can be neglected in our calculation, so that the $A_{\mathbf{k}}$ ’s get the usual commutation relations of annihilation operators for orthogonal states.

We do not have to study the commutation relations of $A_{\mathbf{k}}^\dagger$ and $A_{\mathbf{k}'}^\dagger$, since they can be obtained from (53) by Hermitian conjugation, but we have to study the commutator of $A_{\mathbf{k}}$ and $A_{\mathbf{k}'}^\dagger$. The calculation from (19) and (22) is actually very similar to that which leads to (53) and provides:

$$\begin{aligned} [A_{\mathbf{k}}, A_{\mathbf{k}'}^\dagger] &= \delta_{\mathbf{k}, \mathbf{k}'} (\alpha_{\mathbf{k}}^2 - \beta_{\mathbf{k}}^2) \frac{N_0}{N} \\ &- \frac{\alpha_{\mathbf{k}} \alpha_{\mathbf{k}'}}{N} \sum_i |i : \mathbf{k}' \rangle \langle i : \mathbf{k}| + \frac{\beta_{\mathbf{k}} \beta_{\mathbf{k}'}}{N} \sum_i |i : -\mathbf{k} \rangle \langle i : -\mathbf{k}'| \end{aligned} \quad (54)$$

When $\mathbf{k} = \mathbf{k}'$, this relation has already been studied; when $\mathbf{k} \neq \mathbf{k}'$, we introduce the additional assumption, similar to (A5):

* (A6) the operators in the second line of (54) can be neglected in our calculation since they also correspond to “excited-excited terms”.

3.1.1 effect of the operators $A_{\mathbf{k}}$ and $A_{\mathbf{k}}^\dagger$

For completeness, we recall here a last approximation, which has already been discussed above and which is consistent with all preceding approximations (valid if the gas is very dilute and at a very low temperature):

* (A7) we ignore, in the expression (33), the effect of the term in N_e (the term in N creates no problem since this number is unchanged under the action of all operators introduced; this term is studied below).

Assume then that $|\Phi_E\rangle$ is an eigenstate of the Hamiltonian H , with eigenvalue E ; we introduce the new ket $|\Phi_E^-(\mathbf{k})\rangle$ as:

$$|\Phi_E^-(\mathbf{k})\rangle = A_{\mathbf{k}} |\Phi_E\rangle \quad (55)$$

Now, since all usual commutation relations are satisfied by the operators $A_{\mathbf{k}}$, we can easily show that $|\Phi_E^-(\mathbf{k})\rangle$ is another eigenstate of the

Hamiltonian H , with eigenvalue $E - \widetilde{e}_k$; $A_{\mathbf{k}}$ then plays the role of a “ladder” operator which changes the energy step by step, by decreasing values; similarly, $A_{\mathbf{k}}^\dagger$ will increase the energy eigenvalues.

Let $|\Phi_0\rangle$ be ground state of the hamiltonian H . By action of $A_{\mathbf{k}}$ onto this ket we obtain, either a ket which is zero, or a ket in which the average of H has decreased by \widetilde{e}_k , plus possibly some corrections related to the terms in the commutators that have been neglected. As noted above, $|\Phi_0\rangle$ is a common ground state to bosons and Boltzmann particles, since it is fully symmetric; so is $A_{\mathbf{k}}|\Phi_0\rangle$, which shows that the effect of $W_{as.} - W'_{as.}$ on this ket is strictly zero. We then just have to deal with approximations (A2) to (A7), which amount to assuming that the ratio N_e/N has a small average value in the ground state. If the gas is sufficiently dilute, all the corrections in N_e/N will not be able to make up for the decrease in energy \widetilde{e}_k and change it into an increase of energy. But no state has an average energy below that of the ground state, so that one necessarily has:

$$A_{\mathbf{k}}|\Phi_0\rangle = 0 \quad (56)$$

This equation is valid for any value of \mathbf{k} , except very small values for which the density corrections in N_e/N may be comparable to the decrease in energy \widetilde{e}_k , so that the cancellation of the ket is no longer a necessity. We have obtained in this way a set of equations that the ground state of the system has to obey.

Now, applying any power of the operator $A_{\mathbf{k}}^\dagger$ to this ground state will not change the permutation symmetry of the state and therefore allow us to still ignore the effect of $W_{as.} - W'_{as.}$; we will therefore obtain good approximations to energy eigenstates, as long as not too many particles are excited in the operation. The Bogoliubov energies therefore play the role of quasiparticle energies, as in the usual derivation for bosons, which is not surprising since the completely symmetric subspace \mathcal{E}_S of the Hilbert space of Boltzmann particles remains invariant under all the operators considered.

3.1.2 ground state energy

Finally, it is interesting to come back to the term in λ_N that we have obtained in (44). We have:

$$\sum_{\mathbf{k}} \widetilde{e}_k (\beta_{\mathbf{k}})^2 = \sum_{\mathbf{k}} \widetilde{e}_k \sinh^2(\xi_{\mathbf{k}}) \quad (57)$$

where, if we use (48), we can insert:

$$\sinh^2(\xi_{\mathbf{k}}) = \frac{1}{2}(\cosh 2\xi_{\mathbf{k}} - 1) = \frac{1}{2} \left\{ \frac{1}{\sqrt{e_k(e_k + 2gN)}} - 1 \right\} \quad (58)$$

which gives:

$$\lambda_N = \frac{g}{2}(N-1) + \left\{ \sum_{\mathbf{k}} \sqrt{e_k(e_k + 2gN)} - e_k - gN \right\} \quad (59)$$

When k tends to infinity, the expression under the sum is equivalent to:

$$-\frac{(gN)^2}{e_k} \quad (60)$$

A cancellation of first order terms occurs, but not of second order terms, so that the sum over all values of \mathbf{k} remain (linearly) divergent.

This divergence is well known and takes place in all derivations of the Bogoliubov transformation. A classical way to solve the problem [2] is to replace the coupling constant g (which is directly the matrix element of the potential) by its second order expansion as a function of the scattering length a :

$$g = \frac{4\pi a \hbar^2}{mV} \left\{ 1 + \frac{4\pi a \hbar^2}{V} \sum_{\mathbf{k}} \frac{1}{\hbar^2 k^2} + \dots \right\} \quad (61)$$

where V is the volume. Expressing the mean interaction term $gN(N-1)/2$ as a function of a instead of g then introduced a counterterm in (59) which merely amounts to adding inside the sum $(gN)^2/e_k$, which pushes the cancellation of orders up to second order, makes the sum convergent, and proportional to the integral:

$$\int_0^\infty x^2 dx \left\{ \sqrt{x^2(x^2 + 2)} - x^2 - 1 + \frac{1}{2x^2} \right\} \quad (62)$$

The value of this integral turns out to be $\sqrt{128}/15$ and, finally, one gets for the following well-known result for the energy of the ground state:

$$\lambda_N N = \frac{g}{2} N(N-1) \left\{ 1 + \frac{128}{15} \sqrt{\frac{Na^3}{\pi V}} \right\} \quad (63)$$

Another method to eliminate the divergence is to use a pseudopotential⁸ which directly contains the scattering length a in its matrix elements, so that any renormalization of the coupling constant such as (61) becomes unnecessary. In our calculations, we have replaced all matrix elements of the potential by the same constant g , but it would be possible to make a

⁸Not to be confused with an ordinary delta function potential; a real pseudopotential contains, in addition, a r derivation operator[5][6] and leads to a scattering length which is indeed proportional to its matrix elements, while it turns out the cross section associated with an ordinary delta function potential vanishes.

more careful calculation with a correct expression of the matrix elements of a pseudopotential; as shown by Castin [7], the method also allows one to recover (63). Beliaev [8] has studied systematically how the Bogoliubov energy spectrum with the scattering length a as an interaction parameter is recovered from a resummation of diagrams, as well as corrections to the Bogoliubov theory.

CONCLUSION

The mathematics of the Bogoliubov transformation can be performed within the space of states \mathcal{E}_B of distinguishable particles, and leads exactly to the same formulas than in its fully symmetrical subspace \mathcal{E}_S ; in other words, the proof can be generalized to include quantum states which are not necessarily completely symmetric by exchange and, as one would naturally expect, renders explicit additional conditions of validity. Even within the completely symmetric space \mathcal{E}_S , the proof is not only a mathematical curiosity since it does necessitate a symmetry breaking of the number of particles; it therefore reveals more precisely what is behind the usual approximations that is made by replacing the operators a_0 and a_0^\dagger by c-numbers, a brutal approximation whose effects are not necessarily easy to control quantitatively. Here one gets a precise view of the exact list of operators which have been neglected (approximations A2 to A7) - see for instance the terms in N_e/N in (26) or those appearing in the second lines of (53) and (54), which arise precisely from the fact that a_0 and a_0^\dagger have not been treated as numbers; if one wished to push the approximation beyond the usual derivation of the Bogoliubov transformation, the consideration of the exact expression of these terms would be useful. Needless to say, during the derivation, we have also obtained trivial terms such as the interaction term between excited particles, $V_{ee.}$, which is ignored exactly in the same way as in the traditional derivation: it should be no surprise that, for bosons as well as for Boltzmann particles, the ratio N_e/N should remain small for the Bogoliubov spectrum to be established.

In a sense, the most interesting correction term is the operator $W_{as.} - W'_{as.}$, even if it has no effect on the whole class of states that are common to bosons and Boltzmann particles (those which can be obtained by the action of $A_{\mathbf{k}}^\dagger$ operators onto the ground state). Indeed, we know the low energy spectrum of a system of distinguishable particles is richer than that of a system of bosons, and here this fact is reflected in our calculation by the presence of these antisymmetric operators⁹. It is well known that the major difference between a Boltzmann system and a boson system is not to be

⁹In all calculations based on the Ursell operator formalism for bosons, where a complete symmetrization is applied in a second step, the two operators $W_{as.}$ and $W'_{as.}$ give contributions which exactly vanish, so that the presence of these antisymmetric operators will create no problem.

found in the condensate, which is basically described by exactly the same many-body wave function in both statistics; it is in fact contained in the excitations, which are much more numerous for Boltzmann particles since the numbering of the particles which are excited becomes relevant. For non-interacting particles, this just associates much more entropy to excitation processes than for identical particles - this is actually the reason behind the instability of the condensate for Boltzmann particles at any non-zero temperature, as opposed to a Bose system where it remains stable until the Bose Einstein temperature is reached.. As soon as interactions are included, energetic effects also occur and, in our approach, they are reflected by the presence of the operators W_{as} . and W'_{as} .

LKB and LPS are Unités associées au CNRS et à l'Université Pierre et Marie Curie, UMR 8552 and 8551.

References

- [1] N.N. Bogoliubov, J. Phys. USSR **11**, 23 (1947).
- [2] see for instance R.K. Pathria, "Statistical mechanics", Pergamon Press (1972), §11.2 or A.L. Fetter and J.D. Walecka, "Quantum theory of many-particle systems", Mc Graw Hill (1971), §35.
- [3] T. Holstein and H. Primakoff, Phys. Rev. **58**, 1098 (1940).
- [4] P. Grüter and F. Laloë, J. Physique **5**, 181 and 1255 (1995); M. Holzmann, P. Grüter and F. Laloë, Eur. Phys. J. B **10**, 739 (1999).
- [5] K. Huang and C.N. Yang, Phys. Rev. **105**, 767 (1956)
- [6] K. Huang, "Statistical mechanics", Wiley (1963), chap. 13.
- [7] Y. Castin, seminar given in 1995 at ENS and unpublished notes.
- [8] S.T. Beliaev, Zh. Eksp. Teor. Fiz. **34**, 417 and 433 (1958); JETP **7**, 289 and 299 (1958).