

Thermodynamics of a dilute Bose-Einstein gas with repulsive interactions

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2000 J. Phys. A: Math. Gen. 33 691

(<http://iopscience.iop.org/0305-4470/33/4/303>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.123

The article was downloaded on 02/06/2010 at 08:32

Please note that [terms and conditions apply](#).

Thermodynamics of a dilute Bose–Einstein gas with repulsive interactions

Yves Pomeau and Sergio Rica

Laboratoire de Physique Statistique de l'École Normale Supérieure, Associé au CNRS, 24 Rue Lhomond, 75231 Paris Cedex 05, France

Received 2 September 1999, in final form 16 November 1999

Abstract. The thermodynamics of a system with N identical Bose particles is studied in the diluted gas limit. Not too close to the Bose–Einstein transition we find results differing from the ones in the literature. A relevant consequence of this work is that at low momenta the momentum distribution of quasiparticles is not in the usual form of the Bose factor.

1. Introduction

We explore the properties of a dilute Bose gas by taking into account the effect of the interactions and the possible existence of a condensate. This is indeed not a new topic, it has been studied before by Bogoliubov [1] and by Huang *et al* in a series of papers [2–5]. A rather detailed calculation can be found in Huang's book on statistical mechanics [6] which, however, leaves open the question of the order of the phase transition, once the interaction is turned on.

There are two possibilities for representing a dilute Bose gas. One may resort to a regular perturbation method, as done by Huang, by considering the interaction as a small perturbation and computing the first-order corrections, the unperturbed state being given by the usual Bose–Einstein (BE) theory, without interactions. Another approach was used later by Lee and Yang [5]. It amounts to making a Bogoliubov transformation [1] to diagonalize the Hamiltonian by taking into account at the dominant order (i.e. not as a perturbative effect) the interaction between particles at finite momentum and the condensate. Lee and Yang [5] have also studied the model with a Bogoliubov spectrum, but their results differ from ours for a reason which will be given in section 3. One interesting thing to notice is that, generally, the effect of the Bogoliubov renormalization is to make the transition to condensation first order, that could be perhaps compared with the experimental findings of the BE transition in atomic vapours [7]. The neighbourhood of the transition has been studied recently in a number of publications [8, 9], but this paper is concerned with corrections far from the transition. One of our results is to show that the momentum distribution is not given by a simple Bose factor, for reasons explained in section 3.

That the transition is first order in those theories can be understood by the following argument. If the density of the condensate is finite, the excitation spectrum becomes a Bogoliubov spectrum, with a linear dependence of energy on momentum at low energies, although energy is a quadratic function of this momentum for free particles (that is noninteracting with the condensate). Therefore, for a given momentum, the quasiparticle energy is larger than the free-particle energy and it is more difficult at a given temperature

to excite thermally low-momenta quasiparticles than free particles with the same momentum. This depletes the density of the thermal particles to the benefit of the condensate, and yields a feedback making the transition first order.

We reconsider this question, and show that the Bogoliubov transformation is necessary to get the correct dominant correction to the thermodynamics of a dilute BE perfect gas. In the calculation of the thermodynamical quantities, a chemical potential must be introduced in the spectrum of the quasiparticles, in a way differing from most previous works on this topic (in [10] formulae rather similar to ours are presented, although with a different starting point—see the comments after equation (9)). This calculation gives a correct first-order correction to the thermodynamics only when the density of the condensate and of the thermal particles are of the same order of magnitude. It fails when the density of the condensate becomes so small that the interaction of quasiparticles with the condensate becomes smaller than their self-interaction. In this paper we do not address the question of the order of the transition in the presence of higher-order interactions, which turns out to be rather complex. One of the reasons for that is that the order of the transition in the noninteracting case is, in some sense, undefined. Actually, as soon as the pressure at the BE transition (now in the noninteracting case) is reached at constant temperature, for any density larger than the critical density, the pressure and the chemical potential keep their value at the transition. Therefore, according to the general principles of phase equilibria, any phase with a density larger than the critical one can coexist with any other one also at a density larger than the critical density. This degeneracy explains that profound changes may be brought about by a small perturbation, as the one due to the interaction in a dilute gas.

2. Thermodynamics of the dilute Bose gas with an energy perturbed to first order

We shall discuss first the calculation exposed by Huang [6], assuming (something that we shall discuss later on) that the interaction is a perturbation to the energy of the noninteracting particles. Accordingly, the first correction to the energy coming from the interaction is assumed to be given by terms that are diagonal in states with a fixed number of particles at each momentum: the unperturbed energy operator itself is diagonal with respect to those states. As shown in [6], this operator with the first-order perturbation is given by

$$H[n_p] = \sum_p \frac{p^2}{2m} n_p + \frac{4\pi f \hbar^2}{m\Omega} \left(N^2 - \frac{n_0^2}{2} \right) \quad (1)$$

where f is the positive scattering length that characterizes the potential (we assume the temperature low enough to yield only s -wave scattering in the long wave limit), n_p is the number of particles of momentum p , all particles being identical and of mass m . Furthermore Ω is the total volume, N the total number of particles and n_0 the number of particles in the ground state. In section 3, we recover (1) by analysing the full energy operator. The thermodynamic sum can be carried explicitly with this energy. This model, as well as some variants without the off-diagonal terms but with a more general interaction, have been studied extensively since the early work of Huang *et al* [4], leading in particular to some rigorous results [11–13].

The canonical partition function associated to the energy written in (1) reads

$$Q_N = \sum_{n_p} \exp \left[- \frac{1}{k_B T} \left(\sum_p \frac{p^2}{2m} n_p + \frac{4\pi f \hbar^2}{m\Omega} \left(N^2 - \frac{n_0^2}{2} \right) \right) \right]$$

with k_B the Boltzmann constant and T the absolute temperature. This partition function is computed by performing first the partial sum \sum_{n_p} over states with p different from zero,

at $\sum_p' n_p = N - n_0$ fixed and equal to N' (hereafter $\sum_p' \equiv \sum_{p \neq 0}$). This sum is as in a noninteracting BE gas and the result is borrowed from the standard Bose calculation:

$$\begin{aligned} Q_{N'} &= \sum_{n_p, p \neq 0} \exp \left[-\frac{1}{k_B T} \sum_p' \frac{p^2}{2m} n_p \right] \\ &= \exp \left[-\frac{\mu(N - n_0)}{k_B T} - \frac{\Omega}{(2\pi\hbar)^3} \int d^3 p \ln(1 - e^{-\frac{\epsilon(p)-\mu}{k_B T}}) \right] \end{aligned}$$

where $\epsilon(p) = \frac{p^2}{2m}$. The chemical potential μ is the Lagrange multiplier associated to N' , and is related to it by the condition $\frac{\partial Q_{N'}}{\partial \mu} = 0$, which gives

$$\rho'(\mu) = \frac{1}{(2\pi\hbar)^3} \int d^3 p \frac{1}{e^{\frac{\epsilon(p)-\mu}{k_B T}} - 1} \equiv \left(\frac{mk_B T}{2\pi\hbar^2} \right)^{3/2} \sum_{k=1}^{\infty} \frac{e^{\mu k/k_B T}}{k^{3/2}} \quad (2)$$

where $\rho'(\mu) = \frac{N'}{\Omega}$ is the number density of the particles outside of the condensate (the ‘thermal particles’ later on). The next step consists in tracing over the momentumless particle, that is to sum over all values of n_0 keeping N fixed:

$$\begin{aligned} Q_N &= \sum_{n_0} \exp \left\{ -\frac{1}{k_B T} \left[\frac{4\pi f \hbar^2}{m\Omega} \left(N^2 - \frac{n_0^2}{2} \right) \right. \right. \\ &\quad \left. \left. + \mu(N - n_0) + \frac{\Omega k_B T}{(2\pi\hbar)^3} \int d^3 p \ln(1 - e^{-\frac{\epsilon(p)-\mu}{k_B T}}) \right] \right\}. \end{aligned} \quad (3)$$

This sum is centred around a saddle at \bar{n}_0 , found by looking for the root of $\frac{\partial \ln Q_N}{\partial \bar{n}_0} = 0$, giving the condition $\frac{4\pi f \hbar^2}{m\omega} \bar{n}_0 + \mu = 0$. Note that the chemical potential μ depends on n_0 through equation (2), although the contribution to $\frac{\partial \ln Q_N}{\partial \bar{n}_0}$ proportional to $\frac{\partial \mu}{\partial n_0}$ vanishes identically because of (2). The partition function (3) can be approximated in the thermodynamic limit by the value of Q_N at its maximum, that is for \bar{n}_0 . The total free energy is, in the thermodynamic limit,

$$-k_B T \ln(Q_N) = \mu(N - \bar{n}_0) + \frac{4\pi f \hbar^2}{m\Omega} \left(N^2 - \frac{\bar{n}_0^2}{2} \right) + \frac{\Omega k_B T}{(2\pi\hbar)^3} \int d^3 p \ln(1 - e^{-\frac{\epsilon(p)-\mu}{k_B T}}). \quad (4)$$

This quantity is stationary under variations around \bar{n}_0 at N fixed; physically, this means that at equilibrium there is no exchange of mass between the condensate and the thermal particles, as was shown by Landau [14]. The relation between the chemical potential (Lagrange multiplier) imposing the number of particles outside the condensate (and inside as well, because N is fixed), and the particle density of the condensate is, as before,

$$\mu + \frac{4\pi f \hbar^2}{m} \rho_s = 0 \quad (5)$$

where $\rho_s = \bar{n}_0/\Omega = \rho - \rho'(\mu)$ and $\rho = \frac{N}{\Omega}$ is the total number density, an imposed quantity.

Equation (5) together with the above relation (2) for $\rho'(\mu)$ solves the problem, although one has ρ as a function of ρ_s . One writes the latter as

$$\tilde{\rho} - \tilde{\rho}_s = \frac{4}{\sqrt{\pi} \zeta(3/2)} \int_0^{\infty} x^2 dx \frac{1}{e^{x^2 + \alpha \tilde{\rho}_s} - 1} \equiv \frac{1}{\zeta(3/2)} \sum_{k=1}^{\infty} \frac{e^{-\alpha \tilde{\rho}_s k}}{k^{3/2}} \quad (6)$$

where $\zeta(s)$ is the Riemann ζ function, equal to $\sum_{k=1}^{\infty} \frac{1}{k^s}$ when the series converges and where $\tilde{\rho} = \frac{\rho}{\rho_c}$, $\tilde{\rho}_s$ standing for $\frac{\rho_s}{\rho_c}$ where ρ_c is the number density at the transition in the noninteracting BE case:

$$\rho_c = \left(\frac{mk_B T}{2\pi\hbar^2} \right)^{3/2} \zeta \left(\frac{3}{2} \right).$$

Finally,

$$\alpha = 2\left(\zeta\left(\frac{3}{2}\right)\right)^{2/3} f \rho_c^{1/3}$$

is the only dimensionless parameter. It is, actually, the small parameter of the problem. Because it is proportional to the scattering length f , we shall consider later on f as the small parameter, so that for instance any term of order f^2 will be considered as small compared with another one of order f . This is because their dimensionless ratio should be actually proportional to α times a constant of order 1. Equation (6) yields $\frac{\rho}{\rho_c}$ as a function of $\frac{\rho_s}{\rho_c}$ as represented in the figure 2.

An explicit representation of $\frac{\rho}{\rho_c}$ follows from the expansion for a noninteger s [15]:

$$\sum_{k=1}^{\infty} \frac{e^{-zk}}{k^s} = \Gamma(1-s)z^{s-1} + \sum_{r=0}^{\infty} \frac{(-z)^r}{\Gamma(r+1)} \zeta(s-r). \quad (7)$$

Putting this into (6), one gets the following expansion for $\alpha \tilde{\rho}_s$ a small quantity:

$$\tilde{\rho} - \tilde{\rho}_s = 1 - \frac{2\sqrt{\pi}}{\zeta(3/2)} (\alpha \tilde{\rho}_s)^{1/2} - \frac{\zeta(1/2)}{\zeta(3/2)} (\alpha \tilde{\rho}_s) + \dots$$

Writing now $\delta \tilde{\rho} = \tilde{\rho} - 1$, one obtains up to the dominant term

$$(\delta \tilde{\rho} - \tilde{\rho}_s)^2 = \frac{4\pi}{\zeta(3/2)^2} \alpha \tilde{\rho}_s.$$

Huang replaces this relation by $\delta \tilde{\rho} = \tilde{\rho}_s$, which represents well the dominant term far from the transition, where $\tilde{\rho}_s$ may become small and of the same order as $\delta \tilde{\rho}$. Near threshold, one sees that $\delta \tilde{\rho}$ and $\tilde{\rho}_s$ scale as α .

Finally, we shall derive the equation of state (that is a relation between ρ and the pressure P). This is obtained from the general expression for the pressure, i.e. minus the derivative of the free energy (4) with respect to the volume Ω at T and N constant:

$$\begin{aligned} P &= \frac{4\pi f \hbar^2}{m} \left(\rho^2 - \frac{\rho_s^2}{2} \right) - \frac{k_B T}{(2\pi \hbar)^3} \int d^3 p \ln(1 - e^{-\frac{\epsilon(p) - \mu}{k_B T}}) \\ &= \frac{4\pi f \hbar^2}{m} \left(\rho^2 - \frac{\rho_s^2}{2} \right) + \frac{P_c}{\zeta(5/2)} \sum_{k=1}^{\infty} \frac{e^{-\alpha \tilde{\rho}_s k}}{k^{5/2}} \end{aligned}$$

where P_c is the pressure at the BE transition in a perfect gas:

$$P_c = k_B T \left(\frac{mk_B T}{2\pi \hbar^2} \right)^{3/2} \zeta\left(\frac{5}{2}\right).$$

The pressure depends explicitly on ρ and ρ_s , however, it can be written as a function of the total density ρ only. The dimensionless ratio P/P_c reads, in general,

$$P/P_c = \alpha \frac{\zeta(3/2)}{\zeta(5/2)} \left(\tilde{\rho}^2 - \frac{\tilde{\rho}_s^2}{2} \right) + \frac{1}{\zeta(5/2)} \sum_{k=1}^{\infty} \frac{e^{-\alpha \tilde{\rho}_s k}}{k^{5/2}}. \quad (8)$$

which gives at first order in α :

$$\tilde{P} = 1 - \frac{\zeta(3/2)}{\zeta(5/2)} \alpha \tilde{\rho}_s + \frac{\zeta(3/2)}{\zeta(5/2)} \alpha \left(\tilde{\rho}^2 - \frac{\tilde{\rho}_s^2}{2} \right).$$

Combining this with the relation between $\tilde{\rho}_s$ and ρ one gets that the transition is first order because P is a multivalued function of ρ near the transition, as can be seen in figure 1. An equal-area Maxwell construction (see figure 2 in [4]) near the transition point in the $P/P_c, 1/\tilde{\rho}$ coordinates shows that the jump in ρ from one stable phase to the other is of order $\alpha \rho_c$ near ρ_c , the pressure variation being of order αP_c .

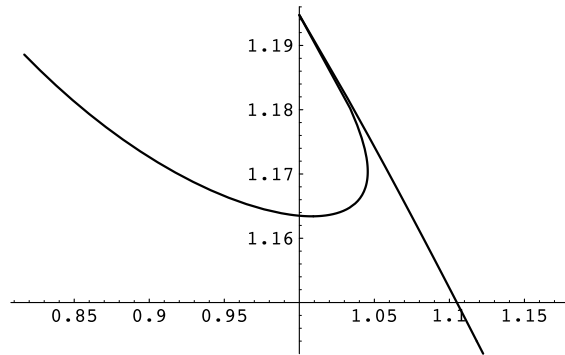


Figure 1. The equilibrium pressure P/P_c as a function of the specific volume $v = \frac{\rho_c}{\rho}$. Here $\alpha = 0.1$.

3. Thermodynamics of the dilute Bose gas at the Bogoliubov order

The results exposed in the previous section are qualitatively correct, in the sense that the order of magnitude of the first-order corrections to macroscopic quantities like P and ρ_s are correct, at least not too close to the transition point. But the calculations of section 2 do not capture quantitatively the thermodynamical properties at first order in f . This is because they miss the effect of the Bogoliubov renormalization on the energy spectrum at low momenta. It turns out that, at finite temperature, this Bogoliubov renormalization is quite different from the original zero-temperature renormalization. One essential ingredient of the derivation above was the assumption that the interaction appears as a first-order perturbation. This is indeed so, for the bulk of the energy spectrum. However, this is not quite true for that part of the spectrum responsible for the expansion of $\rho'(\mu)$ near $\mu = 0$. The first nontrivial and relevant term (beyond ρ_c) is of order $(-\mu)^{1/2}$ and comes from the contribution to the integral over the momenta such that $p^2/2m$ is of order μ , in other words such that p is of order $(-\mu)^{1/2}$. Those momenta are small enough to make the interaction and kinetic energy of the same order. This raises the question of the magnitude of the kinetic versus the interaction energy for this range of momenta. For those particles, as for any particle, the order of magnitude of the interaction energy with the condensate (we shall come to the question of the interaction energy with the other thermal particles later) follows at once from Bogoliubov theory. According to Bogoliubov [1], the energy of the quasiparticles of momentum p is given by

$$\epsilon_B(p) = \sqrt{\frac{p^4}{4m^2} + \frac{4\pi\hbar^2 f}{m^2} \rho_s p^2}.$$

From this formula together with the above expression (5) for μ and for momenta such that $\frac{p^2}{2m} \approx -\mu$, the kinetic part of the Bogoliubov energy ($\frac{p^2}{2m}$) and the energy of interaction with the condensate ($\frac{4\pi\hbar^2 f \rho_s}{m}$) are of the same order of magnitude. Therefore, the interaction cannot be considered as a perturbation in this range of momenta, and practically, all the calculations of section 2 must be reconsidered there, because the interaction was assumed to be a uniformly small perturbation to the kinetic energy. The starting point of a theory following the principles outlined by Bogoliubov at zero temperature is the splitting of the interaction part of the energy into pieces involving the condensate and pieces not involving this condensate. Let $a_\alpha^\dagger (a_\alpha)$ be the creation(destruction) operator in the state of momentum p_α . The operators a with different subscripts commute, although the commutation rule for the same subscript is $aa^\dagger - a^\dagger a = 1$.

The interaction part of the energy operator reads

$$V_{\text{int}} = \frac{4\pi f\hbar^2}{2m\Omega} \sum_{\alpha, \beta, \nu, \omega} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\nu} a_{\omega} \delta(p_{\alpha} + p_{\beta} - p_{\nu} - p_{\omega})$$

where the δ -function is the Kronecker discrete function, equal to zero if its argument is not zero and to 1 otherwise. The sum $\sum_{\alpha, \dots, \omega}$ may be decomposed in various terms, depending on the way in which the condensate wavefunction enters into those terms. As shown by Bogoliubov, if there is condensation in the state of zero momentum, the operators of index zero become c-numbers: $a_0 = \Psi_0 \Omega^{1/2}$, $a_0^{\dagger} = \bar{\Psi}_0 \Omega^{1/2}$, where Ψ_0 is the ground state wavefunction, practically a complex constant here, $\bar{\Psi}_0$ being its complex conjugate.

Let us derive first the expression (1) for the interaction energy from the above formula for V_{int} . At first order, this interaction energy is the average value of V_{int} computed with the unperturbed equilibrium ensemble. In this ensemble the occupation numbers at different momenta p are uncorrelated. The terms with nonzero momentum are finite quantities in the thermodynamic limit. Therefore, the terms such that all four momenta α, \dots, ω are equal and not zero yield a finite contribution to V_{int} , negligible because we expect a contribution of order Ω (or N') in the thermodynamic limit. In the absence of condensate, the average value of V_{int} is therefore equal to

$$\frac{2\pi f\hbar^2}{m\Omega} 2 \sum_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} \sum_{\beta} a_{\beta}^{\dagger} a_{\beta}$$

where the factor 2 in front of the sum is for the two possibilities of choosing either ν or ω equal to α (and so ω or ν equal to β) to satisfy the Kronecker condition. But if the state of momentum zero is macroscopically occupied, this factor 2 should not be there, because it amounts to counting twice the contribution

$$\frac{2\pi f\hbar^2}{m\Omega} a_0^{\dagger} a_0^{\dagger} a_0 a_0.$$

Therefore to avoid this double counting, one subtracts once this last contribution, which yields the sought value of the average value of V_{int} :

$$\langle V_{\text{int}} \rangle = \frac{4\pi f\hbar^2}{2m\Omega} (2N^2 - n_0^2)$$

the result used previously in (1). By singling out the ground state contribution to the sum over the momenta that gives V_{int} , one gets four types of terms:

- (1) The terms such that all four wavenumbers $p_{\alpha, \dots, \omega}$ differ from zero. The corresponding contribution to V_{int} , denoted as $V_{\text{int},1}$, can be computed as follows. This contribution is a small perturbation, and it is estimated by assuming that it is equal to its average value on the unperturbed state (a direct consequence of the general formula for estimating the first-order perturbation, as presented in the previous section), that is for the pure BE system. This amounts to neglecting the quantum correlations between states of different wavenumbers. If one does this the only surviving terms in the sum are such that indices are paired in such a way that the same index appears once in a creation and in a destruction operator:

$$\begin{aligned} V_{\text{int},1} &= \frac{2\pi f\hbar^2}{m\Omega} \sum_{\alpha, \dots, \omega, \text{all} \neq 0} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\nu} a_{\omega} \delta(p_{\alpha} + p_{\beta} - p_{\nu} - p_{\omega}) \\ &\approx \frac{4\pi f\hbar^2}{m\Omega} \left(\sum_{\alpha \neq 0} a_{\alpha}^{\dagger} a_{\alpha} \right) \left(\sum_{\beta \neq 0} a_{\beta}^{\dagger} a_{\beta} \right) = \frac{4\pi f\hbar^2}{m\Omega} (N - n_0)^2. \end{aligned}$$

The Bogoliubov renormalization does not change this result at the dominant order, because does change the contribution to energy of particles with a small momentum only, which is a small proportion of the total number of particles. Therefore, as we are considering the dominant corrections, we can safely use the above formula for $V_{\text{int},1}$ when estimating the perturbation brought by $V_{\text{int},1}$ to the thermodynamical properties.

- (2) The terms such that one wavenumber is zero: $\frac{4\pi f \hbar^2}{m\Omega} \sum'_{\alpha, \nu, \omega} (a_0^\dagger a_\alpha^\dagger a_\nu a_\omega + a_0 a_\nu^\dagger a_\omega^\dagger a_\alpha) \delta(p_\alpha - p_\nu - p_\omega)$.
- (3) The terms such that two wavenumbers are zero: $\frac{2\pi \hbar^2 f}{m\Omega} \sum'_p (a_0^2 a_p^\dagger a_{-p}^\dagger + a_0^{\dagger 2} a_p a_{-p} + 4|a_0|^2 a_p^\dagger a_p)$. These are precisely the ones kept by Bogoliubov and considered below.
- (4) The terms with three zero wavenumbers do not exist because of the Kronecker delta.
- (5) Finally, the ones with four zero wavenumbers: $\frac{2\pi \hbar^2 f}{m\Omega} |a_0|^4$.

We are going to study now the thermodynamics of a system at the ‘Bogoliubov’ order, that is with the interaction just listed in (1)–(5). It turns out that interaction (2) is always negligible compared with the other interaction terms except near the transition. This is because it has the lowest order in a_0 , with respect to any other term involving a_0 , and so becomes the most important term involving a_0 as the superfluid density tends to zero. However, outside this neighbourhood of the transition, this term may be neglected. In a regular perturbation scheme, the effect of (2) would require one to go to the second order in α (because any combination cubic in creation–annihilation operators brings no first-order contribution), although we shall deal with terms of at most first order in α .

Therefore, the energy operator that we are going to use can be written as

$$H = \sum_p \epsilon(p) a_p^\dagger a_p + \frac{2\pi \hbar^2 f}{m\Omega} [2(N - n_0)^2 + n_0^2] + \frac{2\pi \hbar^2 f}{m} \sum'_p (\Psi_0^2 a_p^\dagger a_{-p}^\dagger + \bar{\Psi}_0^2 a_p a_{-p} + 4|\Psi_0|^2 a_p^\dagger a_p). \quad (9)$$

Notice that when neglecting the off-diagonal terms one recovers formula (1) of section 2 because $|\Psi_0|^2 \equiv \rho_s$. Several studies have been devoted to situations where the energy operator is quite similar to the one given in (9), see [10, 13]. They are restricted, however, to cases where the energy is exactly quadratic in the operators a_p and a_p^\dagger , with $p \neq 0$, not the case of our energy operator, because of the contribution $\frac{2\pi \hbar^2 f}{m\Omega} 2(N - n_0)^2$. This last contribution is necessary to get consistently all the interaction effects at first order in the smallness parameter α . Therefore, there are important differences between the formulae deduced from our consistent approach and the results of [10]. In particular, the explicit relation between the chemical potential and the number densities (of the condensate and of the excited particles) are quite different. Following now the same general method as outlined in section 2, we are going to compute the partition function $Q_N^B = \text{Tr}(e^{-\frac{H}{k_B T}})$, for a given total number of particles N in a box of volume Ω . This does not lead to any difficulty, in principle, because the energy operator is a function of n_0 and N and a quadratic functional of the operators a_p^\dagger and a_p . However, the calculation is not that straightforward, and we shall decompose the main steps. The first step consists in computing the contribution to the partition function that depends explicitly on the operators a_p^\dagger and a_p , with a fixed total number of particles in the condensate. To obtain $Q_{N'}^B$, we compute the corresponding grandcanonical partition function $Q^B(\mu) = \sum_{N'} e^{-\frac{\mu N'}{k_B T}} Q_{N'}^B$, and then write $Q_{N'}^B$ as $\exp(+\frac{\mu N'}{k_B T})$ times this grandcanonical partition function, the fluctuations of N' being neglected. The formal expression of $Q^B(\mu)$ is the exponential of a quadratic form

in the creation–annihilation operators:

$$Q^B(\mu) = \text{Tr} \exp \left[-\frac{1}{k_B T} \left(\sum_p' (\epsilon(p) - \mu) a_p^\dagger a_p + \frac{2\pi\hbar^2 f}{m} \sum_p' (\Psi_0^2 a_p^\dagger a_{-p}^\dagger + \Psi_0^{*2} a_p a_{-p} + 2|\Psi_0|^2 a_p^\dagger a_p) \right) \right]. \quad (10)$$

We have included the chemical potential term $\mu N' = \mu \sum_p' a_p^\dagger a_p$ together with the standard kinetic energy term, whence the combination $\epsilon(p) - \mu$ in the term diagonal in the occupation numbers $n_p = a_p^\dagger a_p$. On the other hand, the Bogoliubov transformation will require a factor 2 only in the diagonal part of the interaction term, the remaining term $\frac{4\pi\hbar^2 f}{m} |\Psi_0|^2 \sum_p' a_p^\dagger a_p$ is a constant at N' fixed and so will be included in the full free energy at the end in the form $\frac{4\pi\hbar^2 f}{m\Omega} n_0(N - n_0)$.

The full energy operator is not diagonal in the representation on the basis of states with a fixed number of particles at each momentum: it is diagonal in states at a fixed number of quasiparticles. Therefore, this Bogoliubov theory cannot consider as a first-order perturbation the interaction operator diagonal in states at a fixed number of particles, which was the starting point of the calculation in the previous section. Another consequence of this noncommutation between the quasiparticles' and particles' operators is that one has to be careful when taking into account the Lagrange constraint of a fixed number of particles (*not* of quasiparticles) when computing the contribution of the thermally excited states to the partition function. Let us point out that [5] assumes that the total number of particles and of quasiparticles are the same (equation (19) in [5]), something that does not follow from the operator algebra. We have just shown that the Lagrange constraint for the number of particles amounts formally to add $-\mu$ to the energy per particle. Now the resulting operator (that is the energy minus $\mu N'$) can be diagonalized as done by Bogoliubov, but by replacing everywhere $\epsilon(p)$ by $\epsilon(p) - \mu$ in the final expression. We shall compute the trace in the grand canonical ensemble and in the basis where the Hamiltonian is diagonal, that is after a Bogoliubov transformation. Formally this last trace is over an arbitrary number of quasiparticles. The result is

$$Q^B(\mu) = \exp \left[-\frac{\mu(N - n_0)}{k_B T} - \frac{\Omega}{(2\pi\hbar)^3} \int d^3 p \ln(1 - e^{-\epsilon_B(p, \mu, \rho_s)/k_B T}) \right]$$

where

$$\epsilon_B(p, \mu, \rho_s) = \sqrt{\left(\frac{p^2}{2m} - \mu\right)^2 + 2\left(\frac{p^2}{2m} - \mu\right) \frac{4\pi f \hbar^2 \rho_s}{m}}. \quad (11)$$

In this expression for $Q_{N'}^B(\mu)$, we have neglected the contribution coming from the change in the ground state energy arising from the Bogoliubov transformation, as it would yield higher-order corrections only. This kind of correction is responsible for the term of order $\alpha^{3/2}$ (in our notation) in the expansion of the ground state energy (see the second-order term in equation (17) of [5] for instance, with a proportional to our α), and would similarly yield corrections, though smaller than the one used in this paper. The density of thermal particles follows by deriving the free energy with respect to μ :

$$\rho'(\mu) = -\frac{1}{(2\pi\hbar)^3} \int d^3 p \frac{1}{e^{\frac{\epsilon_B(p, \mu, \rho_s)}{k_B T}} - 1} \frac{\partial \epsilon_B(p, \mu, \rho_s)}{\partial \mu}. \quad (12)$$

It is important to notice at this point that the thermodynamical expression we are using may look different from what is in the literature because the chemical potential enters in a nontrivial way in quantities related to the quasiparticles. It is true that if the quasiparticles

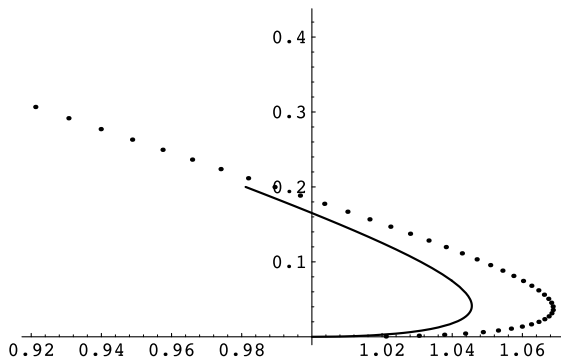


Figure 2. The condensate density ρ_s/ρ_c as a function of the specific volume $v = \frac{\rho_c}{\rho}$. The full curve is the calculation up to first order (equation (6)), while the dotted curve is the numerical solution of (14) and (16). We have taken $\alpha = 0.1$.

were phonons in a solid they would be associated to the conservation of energy only, whence their thermodynamics would depend on the temperature only, and no chemical potentials would be involved. However, the quasiparticles in a condensed Bose gas are not independent of the true particles: changing the occupation number of quasiparticles changes the occupation number of particles themselves. Therefore, the thermodynamics of quasiparticles involve both the temperature (related to the energy conservation) and in a nontrivial way the chemical potential related to the conservation of the number of particles. The total partition function at this Bogoliubov approximation is

$$Q_N^B = \sum_{n_0} \exp \left\{ -\frac{1}{k_B T} \left[\mu(N - n_0) + \frac{2\pi\hbar^2 f}{m\Omega} [(N - n_0)^2 + N^2] + \frac{k_B T \Omega}{(2\pi\hbar)^3} \int d^3 p \ln(1 - e^{-\frac{\epsilon_B(p, \mu, \rho_s)}{k_B T}}) \right] \right\}. \quad (13)$$

As in the previous section one gets \bar{n}_0 by looking for the saddle point of the sum (note that $\epsilon_B(p, \mu, \rho_s)$ depends explicitly on n_0 because $n_0 = \rho_s \Omega$):

$$\mu + \frac{4\pi\hbar^2 f}{m} (\rho - \rho_s) = \frac{1}{(2\pi\hbar)^3} \int d^3 p \frac{1}{e^{\frac{\epsilon_B(p, \mu, \rho_s)}{k_B T}} - 1} \frac{\partial \epsilon_B}{\partial \rho_s}. \quad (14)$$

Equations (12) and (14) solve, in principle, the problem. Obtaining $\frac{\partial \epsilon_B}{\partial \mu}$ and $\frac{\partial \epsilon_B}{\partial \rho_s}$ from (11) and putting the result into (12) one transforms (14) into

$$\tilde{\mu} \equiv \frac{\mu}{k_B T} = -\alpha^2 \tilde{\rho}_s \frac{4}{\sqrt{\pi} \zeta(3/2)} \int_0^\infty \frac{1}{e^{\hat{\epsilon}(x)} - 1} \frac{x^2 dx}{\hat{\epsilon}(x)} \quad (15)$$

where $\hat{\epsilon}(x) = \sqrt{(x^2 - \tilde{\mu})^2 + 2\alpha(x^2 - \tilde{\mu})\tilde{\rho}_s}$. Equation (12) becomes

$$\tilde{\rho} = \tilde{\rho}_s + \frac{\tilde{\mu}}{\alpha} + \frac{4}{\sqrt{\pi} \zeta(3/2)} \int_0^\infty \frac{1}{e^{\hat{\epsilon}(x)} - 1} \frac{(x^2 - \tilde{\mu})x^2 dx}{\hat{\epsilon}(x)}. \quad (16)$$

We have solved numerically these coupled equations for $\alpha = 0.1$. The relation between $\tilde{\rho}_s$ and $\tilde{\mu}$ is derived from (15).

Then one gets directly $\tilde{\rho}$ as a function of $\tilde{\mu}$. We have plotted $\tilde{\rho}_s$ versus $1/\tilde{\rho}$ as a parametric plot of $\tilde{\mu}$ in figure 2.

Near the BE transition ρ_s and μ vanish. Their relation follows from the singular behaviour of the integral (15) near $x = 0$:

$$\int_0^\infty \frac{x^2 dx}{(x^2 - \tilde{\mu})(x^2 - \tilde{\mu} + 2\alpha\tilde{\rho}_s)} = \frac{\pi}{2} \frac{\sqrt{2\alpha\tilde{\rho}_s - \tilde{\mu}} - \sqrt{-\tilde{\mu}}}{2\alpha\tilde{\rho}_s}.$$

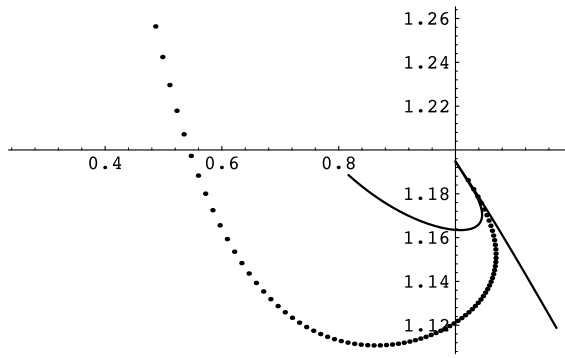


Figure 3. The equilibrium pressure P/P_c as a function of the specific volume $v = \frac{\rho_c}{\rho}$. As before, the full curve was drawn with equation (8), and the dotted curve with (18). We have taken $\alpha = 0.1$.

Near the transition (ρ_s and μ close to zero) one has

$$(-\tilde{\mu})^{3/2} = \frac{\sqrt{\pi}}{\zeta(3/2)} \alpha^2 \rho_s \quad (17)$$

therefore up to Bogoliubov order one gets that $\tilde{\mu} \sim -\tilde{\rho}_s^{2/3} \gg \tilde{\rho}_s$ near the transition, showing that in this range the dominant order is not the one found by the calculation of section 2. Under the same assumptions, one approximates (16) by

$$\delta\tilde{\rho} = \tilde{\rho} - 1 = \tilde{\rho}_s + \tilde{\mu}/\alpha - \frac{\sqrt{\pi}}{\zeta(3/2)} \sqrt{2\alpha\tilde{\rho}_s - \tilde{\mu}}.$$

One sees from here that $\delta\tilde{\rho}$ and $\tilde{\rho}_s$ scales as α .

Finally, we obtain the equation of state

$$P/P_c = \alpha \frac{\zeta(3/2)}{2\zeta(5/2)} ((\tilde{\rho} - \tilde{\rho}_s)^2 + \tilde{\rho}^2) - \frac{4}{\sqrt{\pi}\zeta(5/2)} \int_0^\infty \ln(1 - e^{-\hat{\epsilon}(x)}) x^2 dx \quad (18)$$

which is plotted in figure 3.

4. Conclusions

Once the Bogoliubov transformation has been made, we obtain that at the dominant order (that is for f or α small), the condition that the total partition function is stationary under exchange of particles between the condensate and the thermal particles near $\rho_s = 0$ is $\mu \sim -\alpha^{4/3} \rho_s^{2/3}$, different from the result in section 2.

The result of these considerations is a consistent derivation of the first correction to the thermodynamic parameters of the BE gas, arising from the short-range interaction, in the dilute gas limit.

To summarize:

- (1) The chemical potential μ is given near $\rho_s = 0$ at the dominant order by $\mu \sim -\alpha^{4/3} \rho_s^{2/3}$, a quantity much larger than $\alpha\rho_s$ as ρ_s vanishes with α fixed. The above relation for the chemical potential is valid if ρ_s is small, but much larger than $\alpha\rho$. If ρ_s becomes less than $\alpha\rho_s$, then other terms than the ones we have considered here to get the energy operator of equation (9) become relevant.
- (2) Among the important effects of the Bogoliubov renormalization is to change the momentum distribution for small momenta. The momentum distribution of quasiparticles at small momenta, has the form

$$-\frac{1}{(2\pi\hbar)^3} \frac{1}{e^{\frac{\epsilon_B(p, \mu, \rho_s)}{k_B T}} - 1} \frac{\partial \epsilon_B(p, \mu, \rho_s)}{\partial \mu}$$

where the various quantities are explained in the body of the text. This momentum distribution cannot be cast in the form of a simple Bose factor, which means probably that a kinetic theory consistent with the present equilibrium distribution should have a structure far more complex than the classical Boltzmann–Nordheim kinetic theory [16], a question we plan to investigate actively.

References

- [1] Bogoliubov N N 1947 *J. Phys.* **11** 23
- [2] Lee T D, Huang K and Yang C N 1957 *Phys. Rev.* **106** 1135
- [3] Huang K and Yang C N 1957 *Phys. Rev.* **105** 767
- [4] Huang K, Yang C N and Luttinger J M 1957 *Phys. Rev.* **105** 776
- [5] Lee T D and Yang C N 1958 *Phys. Rev.* **112** 1419
- [6] Huang K 1963 *Statistical Mechanics* (New York: Wiley) section 13.5
- [7] Anderson M H *et al* 1995 *Science* **269** 198
Bradley C C *et al* 1995 *Phys. Rev. Lett.* **75** 1687
Davis K B *et al* 1995 *Phys. Rev. Lett.* **75** 3969
- [8] Huang K 1999 *Phys. Rev. Lett.* **83** 3770 and references therein
- [9] Baym G *et al* 1999 *Phys. Rev. Lett.* **83** 1703
- [10] Bru J B and Zagrebnov V A 1998 *J. Phys. A: Math. Gen.* **31** 9377
- [11] van den Berg M, Lewis J T and Pulé J V 1988 *Commun. Math. Phys.* **118** 61
- [12] Dorlas T C, Lewis J T and Pulé J V 1991 *Phys. Acta* **64** 1200
Dorlas T C, Lewis J T and Pulé J V 1993 *Commun. Math. Phys.* **156** 37
- [13] Angelescu N, Verbeure A and Zagrebnov V A 1992 *J. Phys. A: Math. Gen.* **25** 3473
- [14] Landau L D 1941 *J. Phys. (USSR)* **5** 71
- [15] Robinson J E 1951 *Phys. Rev.* **83** 678
- [16] Pomeau Y *et al* 1999 *C.R. Acad. Sci., Paris B* **327** 791