Condensation and superfluidity in a one-dimensional gas of bosons

Exam for the course “Fluides quantiques" M1 ICFP 2013-2014

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Time : 3 hours

Throughout the whole exam we consider a 1D gas of N non-relativistic spinless bosons of mass m. The gas is confined in a box $[0, L]$ and we consider periodic boundary conditions.
The system is described by the Hamiltonian

$$\hat{H}_0 = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2} \sum_{1\le i\neq j\le N} V(\hat{x}_i - \hat{x}_j) \tag{1}$$

where $\hat{p}_i$ is the momentum operator of the i-th particle, $\hat{x}_i$ is the position operator and $V(\hat{x}_i - \hat{x}_j)$ the interaction potential. We assume that the system is in thermal equilibrium.

1 Effect of dimensionality on Bose-Einstein condensation

We will show that the dimensionality of space has an important impact on the phenomenon of Bose-Einstein condensation. More specifically, for one-dimensional systems there is no condensation in the thermodynamic limit.
In this section, we consider an ideal gas, $V(\hat{x}_i - \hat{x}_j) = 0$, described by the Hamiltonian

$$\hat{H}_0 = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} \tag{2}$$

We will describe the system in equilibrium in the grand canonical ensemble with chemical potential μ and temperature T.

1.1 Saturation of the population of the excited states

1. The eigenstates of the single-particle Hamiltonian are plane waves with wave vector k :

$$\phi_k(x) = \frac{e^{ikx}}{\sqrt{L}} \tag{3}$$

   What are the allowed values for k given the periodic boundary conditions ? What are the single-particle eigen energies ϵ_k as a function of k ?
2. Write down the single-particle ground-state wave function ϕ_0 and its energy.
3. Let N' denote the total population of all excited states. Express N' as a sum of the mean occupation numbers N_k of the states ϕ_k. We remind that $N_k = [e^{\beta(\epsilon_k-\mu)} - 1]^{-1}$.
4. Explain why the value

$$N'_{\max} = \sum_{k\neq 0} \frac{1}{e^{\beta(\epsilon_k-\epsilon_0)} - 1} \tag{4}$$

   is an upper bound of N'.
5. For a large enough system size the introduction of the density of states $\rho(\epsilon)$ allows one to replace the sum over states by an integral

$$\sum_k f(\epsilon_k) \ \rightarrow \ \int d\epsilon\, \rho(\epsilon)\, f(\epsilon) \tag{5}$$

Show that for our one-dimensional system

$$\rho(\epsilon) = \frac{L}{\pi}\sqrt{\frac{m}{2\hbar^2}}\frac{1}{\sqrt{\epsilon}} \tag{6}$$

6. Show that the integral for $N'_{\max}$ obtained in this way diverges. Is this an ultraviolet or an infrared divergence ?
7. We thus need to keep the sum in the calculation of $N'_{\max}$. To calculate the dominant contribution to the sum we use the approximation

$$N_k \simeq \frac{k_B T}{\epsilon_k - \mu} \tag{7}$$

(so-called classical field approximation) valid for $N_k \gg 1$. Show that one then obtains

$$N'_{\max} = \frac{L^2}{\lambda_{dB}^2}\frac{\pi}{3} \tag{8}$$

where $\lambda_{dB} = \sqrt{\frac{2\pi\hbar^2}{mk_BT}}$ is the thermal de Broglie wavelength, and where we have used the identity $\sum_{n=1}^{\infty}\frac{1}{n^2} = \frac{\pi^2}{6}$.

8. Let $\rho = N/L$ be the total number density and ρ' the number density for all the bosons in excited states. Express $\rho'_{\max}\lambda_{dB}$ as a function of L and explain why there is no Bose-Einstein condensation in the thermodynamic limit, defined by $L \to \infty$, $N \to \infty$, $\rho =$ constant, $T =$ constant.
9. Write down the mean occupation number N_0 of the lowest energy state ϕ_0 and N_1 of the first excited state ϕ_1 in the classical field limit as a function of k_BT, $|\mu|$ and ϵ_1.
10. Show that $N_0 \gg N_1 \Leftrightarrow |\mu| \ll \epsilon_1 \Leftrightarrow \rho\lambda_{dB} \gg \rho'_{\max}\lambda_{dB}$. One can thus have BEC condensation in a 1D system with finite size.

1.2 Spatial correlation function

We remind the expression for the correlation function :

$$g^{(1)}(x,x') = \langle \mathcal{A} \rangle \quad \text{with} \quad \mathcal{A} = \sum_{i=1}^{N} |i:x\rangle\langle i:x'| = \sum_{i=1}^{N} A(i)$$

which gives the coherence between x and x'. We have seen that one has in the grand-canonical ensemble :

$$\langle \mathcal{A} \rangle = \sum_k N_k \langle k|A|k\rangle = \sum_k N_k \phi_k^*(x)\phi_k(x')$$

with $|k\rangle$ an eigenstate of the single-particle Hamiltonian, $\hat{h}_1|k\rangle = \epsilon_k|k\rangle$.

11. Express $g^{(1)}(x,x')$ as a sum over k, as a function of ϵ_k, μ, x, x' and k_BT.
12. For $L \gg \lambda_{dB}$ and in the classical field limit we give the result (you are not asked to prove it)

$$g^{(1)}(x,x') = \rho e^{-|x-x'|/l_C} \quad \text{with} \quad l_C = \frac{\rho\lambda_{dB}^2}{2\pi} \tag{9}$$

Deduce from this result that the coherence length l_C is infinitely small compared to the size of the system in the thermodynamic limit.

13. Show that for a degenerate system, $\rho\lambda_{dB} \gg 1$, one has a coherence length $l_C \gg \lambda_{dB}$. How does then l_c in this regime compare to the coherence length of a non-degenerate gas.
14. Show that for a finite-sized system $\rho\lambda_{dB} \gg \rho'_{\max}\lambda_{dB}$ implies $l_C \gg L$.

2 Superfluidity and condensation of the ideal gas

In this section we consider the ideal gas (2) and we study the response of the system to a moving perturbation. We wish to point out the difference between the superfluid fraction and the condensed fraction. We focus on the degenerate regime $\rho\lambda_{dB} \gg 1 \Leftrightarrow e^{\beta\mu} \to 1^-$. We consider again the "classical field approximation" for the occupation numbers which is good in the limit $N_k \gg 1$:

$$N_k \simeq \frac{k_BT}{\epsilon_k - \mu}. \tag{10}$$

Again, sums cannot be replaced by integrals.

2.1 Calculation of the normal fraction f_n

We add a stirring potential to the Hamiltonian (2) that breaks translational invariance and moves with a velocity v_{rot} :

$$\hat{W}(t) = \sum_{i=1}^{N} \mathcal{W}(\hat{x}_i - v_{\text{rot}} t). \tag{11}$$

The normal fraction f_n for the system with finite size is defined as :

$$f_n = \lim_{v_{\text{rot}} \to 0} \lim_{\mathcal{W} \to 0} \frac{\langle \hat{P} \rangle}{N m v_{\text{rot}}} \tag{12}$$

where we have introduced the total momentum operator of the gas :

$$\hat{P} = \sum_{i=1}^{N} \hat{p}_i. \tag{13}$$

and the thermal average $\langle \hat{P} \rangle$ is taken in the presence of the perturbation.
To eliminate the time dependence of the stirring potential, it is convenient to introduce a change of reference frame. We introduce the time-dependent unitary transformation

$$\hat{U}(t) = e^{i\hat{P} v_{\text{rot}} t/\hbar} \tag{14}$$

This unitary transformation causes the state vector of the system $|\tilde{\psi}(t)\rangle \equiv \hat{U}(t)|\psi(t)\rangle$ to evolve according to the Hamiltonian

$$\tilde{H} = \hat{H}_0 + \hat{W}(t=0) - \hat{P} v_{\text{rot}} \tag{15}$$

where $\hat{H}_0$ is defined by (2) and $\hat{W}(t)$ is defined by (11).
The equilibrium state of the gas in the presence of the perturbation is described by the density operator in the grand-canonical ensemble :

$$\hat{\sigma} = \frac{1}{Z_{GC}} e^{-\beta(\tilde{H} - \mu \hat{N})} \quad \text{with } \tilde{H} \text{ given by (15) and} \quad Z_{GC} = \operatorname{Tr} e^{-\beta(\tilde{H} - \mu \hat{N})} \tag{16}$$

In the calculation of f_n we can directly take the limit $\mathcal{W} \to 0$ in $\hat{\sigma}$ and hence in $\tilde{H}$.

15. Write down the single-particle wave functions $\langle x|k\rangle$ for the eigenstates of the Hamiltonian $\tilde{H}$.
16. Write down the corresponding single-particle energies ϵ_k.
17. What are the allowed values of the wave vector k that satisfy the periodic boundary conditions ?
18. Express the mean value $\langle \hat{P} \rangle$ as a function of the mean occupation numbers N_k of the single-particle eigenstates.
19. Use the classical field approximation (10) to express the mean particle numbers $\langle \hat{N} \rangle \equiv N$ as a sum over all states. Show that

$$N = \frac{m L^2 k_B T}{2\pi^2 \hbar^2} \sum_{n \in \mathbb{Z}} \frac{1}{(n - \tilde{v})^2 + \nu_0^2}, \tag{17}$$

with $\tilde{v} = v_{\text{rot}}/v_1$ and $\nu_0^2 = -\mu/E_1 - \tilde{v}^2$ with v_1 and E_1 respectively the velocity and energy of a particle in the first excited state of $\hat{H}_0$ in the box.

20. Use the Poisson summation formula :

$$\sum_{n \in \mathbb{Z}} f(n) = \sum_{n \in \mathbb{Z}} \hat{f}(2\pi n), \tag{18}$$

where $f(x)$ is a function and $\hat{f}(q)$ its Fourier transform, and show that

$$N = \frac{m L^2 k_B T}{\hbar^2} \frac{1}{2\pi\nu_0} \frac{\sinh(2\pi\nu_0)}{\cosh(2\pi\nu_0) - \cos(2\pi\tilde{v})} \tag{19}$$

We remind that the Fourier transform of

$$f(x) = \frac{1}{\pi} \frac{a}{a^2 + x^2} \tag{20}$$

is

$$\hat{f}(q) = e^{-a|q|}. \tag{21}$$

for $a > 0$.

21. In a similar way one can obtain following result (don't prove this) :

$$\langle \hat{P} \rangle = Nm\, v_{\text{rot}} - \frac{mLk_BT}{\hbar}\, \frac{\sin(2\pi\tilde{v})}{\cosh(2\pi\nu_0) - \cos(2\pi\tilde{v})}. \tag{22}$$

Show that the normal fraction f_n defined in (12) is given by

$$f_n = 1 - \frac{\nu_0}{\sinh(2\pi\nu_0)}. \tag{23}$$

2.2 Comparison with the non-condensed fraction f_{nc}

22. Use the previous result (19) for N to calculate the non-condensed fraction in the limit $v_{\text{rot}} = 0$

$$f_{\text{nc}} = \frac{N - N_0}{N} \tag{24}$$

23. In view of the results of the first part, what is the physical meaning of the limit $\nu_0 \ll 1$?
24. Show that in this limit to second order in ν_0 one finds a very simple relation between f_n and f_{nc} which indicates that the condensate of the 1D ideal gas is not entirely superfluid.

3 The interacting gas

We consider an inter-particle interaction potential V with zero range

$$V(x_i - x_j) = g\delta(x_i - x_j) \tag{25}$$

where δ is the Dirac distribution and $g > 0$ is the coupling constant.
We will calculate the normal fraction of the interacting gas in a regime in which one can use the Bogoliubov approach. We admit that the Bogoliubov approach remains valid in the absence of a true condensate provided that the system is (i) in the weakly interacting regime :

$$\rho\xi = \sqrt{\frac{\hbar^2\rho}{mg}} \gg 1 \quad \text{where } \xi \text{ is the healing length} \tag{26}$$

and (ii) at a low enough temperature for the density fluctuations to be small.

$$k_BT \ll k_BT_{\text{fd}} = \rho g \times \rho\xi = \sqrt{\frac{\hbar^2\rho^3 g}{m}} \tag{27}$$

25. Show that in the regime of weak interactions (26) one always has $k_BT_{\text{fd}} \ll k_BT_{\text{deg}}$ where k_BT_{deg} is the temperature for degeneracy which corresponds to $\rho\lambda_{\text{dB}} = 1$. The fact whether there is a real condensate or not depends on the system size (see first part of this exam).

We will show that the 1D case is very peculiar because the statistical weight in equilibrium of having a spontaneously moving condensate (i.e. even in the absence of the stirring potential) is not negligible.
To calculate the normal fraction we use a result which was proven in one the tutorials

$$f_n = \frac{\langle \hat{P}^2 \rangle_0}{NmkT} \tag{28}$$

where the index 0 indicates that the mean is taken in the thermal state in absence of the stirring potential. In what follows we will calculate this mean value (28). We will calculate it first for a moving condensate with wave vector k_0 (the condensate wave function is a plane of wave vector k_0), and then take the average over all possible values of k_0.

3.1 Calculation of the main value of $\hat{P}^2$ for a moving condensate

In this part we use the Bogoliubov approach which is obtained for a moving condensate with wave vector k_0.

$$k_0 = \frac{2\pi n}{L} = \ \text{wave vector of the moving condensate} \tag{29}$$

After introducing the appropriate quasi-particle modes the Hamiltonian takes the form [1]

$$\hat{H}_{\mathrm{Bog}} = E[\phi] + \sum_{k\neq 0} \epsilon_k \hat{b}_k^\dagger \hat{b}_k, \tag{30}$$

where $\hat{b}_k$ and $\hat{b}_k^\dagger$ are bosonic quasi-particle operators such that $[\hat{b}_k, \hat{b}_k^\dagger] = 1$, $\hat{n}_k \equiv \hat{b}_k^\dagger \hat{b}_k$ is the number operator for quasi-particles, and $E[\phi]$ is the Gross-Pitaevskii energy functional.

$$E[\phi] = N \int dx \left[\frac{\hbar^2}{2m} \left| \frac{d\phi}{dx} \right|^2 + \frac{g}{2} N |\phi|^4 \right]. \tag{31}$$

The quasi-particle energies ϵ_k differ from the energies $\epsilon_k^{(0)}$ obtained for the case when the condensate is at rest. In particular one has

$$\epsilon_k = \epsilon_k^{(0)} + \hbar k v_0 \quad \text{with} \quad v_0 = \frac{\hbar k_0}{m} \tag{32}$$

In thermal equilibrium the system is described by the density operator

$$\hat{\sigma}_{\mathrm{Bog}}^{k_0} = \frac{e^{-\beta \hat{H}_{\mathrm{Bog}}}}{Z_{k_0}} \tag{33}$$

26. Calculate the partition function $Z_{k_0} = \mathrm{Tr}\left[e^{-\beta \hat{H}_{\mathrm{Bog}}}\right]$ as a function of β, ϵ_k and $E[\phi]$.
27. Show that
$$\langle \hat{b}_k^\dagger \hat{b}_k \rangle \equiv n_k = f(\epsilon_k) \quad \text{with} \quad f(\epsilon) = \frac{1}{e^{\beta\epsilon_k} - 1}. \tag{34}$$
Hint : consider the derivate of the partition function Z_{k_0} with respect to $A_k \equiv \beta\epsilon_k$.
28. Show that
$$\begin{aligned} \langle \hat{n}_k^2 \rangle - n_k^2 &= n_k(n_k+1) & (35)\\ \langle \hat{n}_k \hat{n}_{k'} \rangle - n_k n_{k'} &= 0 \quad \text{for} \quad k \neq k' & (36) \end{aligned}$$
Hint : consider the second derivatives of the partition function Z_{k_0} with respect to $A_k \equiv \beta\epsilon_k$ and $A_{k'} \equiv \beta\epsilon_{k'}$.
29. In case the condensate is at rest we have shown in one of the tutorials that the total momentum operator of the gas in the Bogoliubov approximation is given by
$$\hat{P}^{(0)} = \sum_{k\neq 0} \hbar k \hat{b}_k^\dagger \hat{b}_k \tag{37}$$
Show by using Galilean invariance that the total momentum operator of the gas with a condensate moving with wave vector k_0 (29) takes the form
$$\hat{P}^{(k_0)} = \hbar k_0 N + \sum_{k\neq 0} \hbar k \hat{b}_k^\dagger \hat{b}_k \tag{38}$$
30. Express the mean value of $(\hat{P}^{(k_0)})^2$ over the thermal distribution (33) as a function of n_k of (34).
31. We assume now that $v_0 \ll c$, with c the sound velocity $c^2 = \frac{\rho g}{m}$. Expand the n_k in the expression for $\langle (\hat{P}^{(k_0)})^2 \rangle$ obtained in the previous question up to first order in v_0. Use the relation
$$f'(\epsilon_k^{(0)}) = -\beta n_k^{(0)}(1 + n_k^{(0)}) \tag{39}$$
where the function $f(\epsilon)$ is defined by (34), f' is its derivative and
$$n_k^{(0)} = f(\epsilon_k^{(0)}) \tag{40}$$
32. Rewrite the result of the previous question in such a way that following quantity appears :
$$f_n^{(0)} \equiv \frac{\sum_{k\neq 0} n_k^{(0)}(n_k^{(0)}+1)\hbar^2 k^2}{N m k_B T} \tag{41}$$

1. We have left out a constant, which is a quantum correction to the ground-state energy, but which does not depend on k_0 and thus does not play any role here.

33. Up to terms of order $O[(f_n^{(0)})^2]$ show that the result can be written as

$$\langle (P^{(k_0)})^2 \rangle = N m k_B T f_n^{(0)} + N_s^2 \hbar^2 k_0^2. \tag{42}$$

where we have introduced the number of bosons in the superfluid fraction for the condensate at rest

$$N_s = N(1 - f_n^{(0)}) \tag{43}$$

34. By taking $k_0 = 0$ in (42) give the physical meaning of $f_n^{(0)}$ defined in (41).
35. Would it be compatible with Bogoliubov theory to include higher order terms in $f_n^{(0)}$?

3.2 Statistical mixture of moving condensate and calculation of the 'real' mean value of $\hat{P}^2$

In the so-called multi-valley Bogoliubov approach one approximates the true density operator of the gas in thermal equilibrium with a *statistical mixture* of moving condensates, each moving condensate being dressed by its Bogoliubov modes in thermal equilibrium. The statistical weight of the condensate with wave vector k_0 is given by the partition function Z_{k_0} calculated in the previous subsection (question 26).

34. We remind that the wave function of the condensate is a normalised plane wave with wave vector k_0. Calculate the Gross-Pitaevskii energy $E[\phi]$ (31) of the condensate as a function of N, $\hbar$, k_0, m, the coupling constant g and the density ρ.
35. Express the ratio Z_{k_0}/Z_0 of the wave functions of a moving condensate and a condensate at rest as a function of k_0, β, ϵ_k and $\epsilon_k^{(0)}$.
36. Show that this ratio can be written as :

$$\frac{Z_{k_0}}{Z_0} = e^{-\beta N \hbar^2 k_0^2/(2m)} \exp\left\{ -\sum_{k\neq 0} \ln\left[1 + n_k^{(0)}\left(1 - e^{-\beta \hbar k v_0}\right)\right]\right\} \tag{44}$$

37. Expand the expression *between curly brackets* $\{\ldots\}$ in (44) up to second order in v_0. We remind that $\ln(1+x) = x - x^2/2 + O(x^3)$ for $x \to 0$. Verify that the first order contribution is zero after summing over k and that the inclusion of the second order contribution leads to

$$\frac{Z_{k_0}}{Z_0} = e^{-\beta N_s \hbar^2 k_0^2/(2m)}, \tag{45}$$

by using the result (41) and the definition (43).

38. We now go to the thermodynamic limit, $N \to +\infty$ while $\rho = N/L^d$ constant with d the dimensionality of space. Show (in an easy way) that in one dimension the statistical weight of the moving condensates is not negligible in this limit. This shows that the condensate can spontaneously be moving in thermodynamical equilibrium.
39. Does the previous reasoning also work in three dimensions ?
40. We now return to 1D. Average the result (42) over the statistical weight (45). We now take the thermodynamic limit so that we can replace the sum over k_0 by an integral. We remind that

$$\frac{\int_{-\infty}^{+\infty} dx\, x^2 e^{-x^2/(2\sigma^2)}}{\int_{-\infty}^{+\infty} dx\, e^{-x^2/(2\sigma^2)}} = \sigma^2 \tag{46}$$

for $\sigma > 0$. Derive the 'true' value of $\langle \hat{P}^2 \rangle$, and the 'true' value of the normal fraction in 1D according to the definition (28). This result is very simple..