Exam of "Quantum Fluids" M1 ICFP 2017-2018

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The exam consists of two independant exercises. The duration is 3 hours.

1 Fluctuations of the number of particles in a Bose-Einstein condensate

In this exercise we are interested in the fluctuations of the number of particles in a Bose-Einstein condensate, for an ideal gas, then for an interacting gas using the Bogoliubov theory. It will be an opportunity to find that the canonical ensemble and the grand canonical ensemble are equivalent only if the fluctuations of the number of particles are small in relative values, which is not the case in certain situations ...

1.1 Ideal Bose gas

Let's consider an ideal gas of bosons at thermal equilibrium in the grand canonical ensemble. The energy and the number of particles are fixed on average and the parameters $\beta = 1/k_B T$ and μ are fixed. We denote by $\{\phi_\lambda\}$ and ϵ_λ the eigenfunctions and eigenenergies specific to a particle. The one-particle state of minimal energy ϕ_0 ($\lambda = 0$) is assumed to be non degenerate.

1.1.1 Ideal gas of bosons in the grand canonical ensemble

(a) Let l be a microscopic state of the system of energy E_l and number of particles N_l. Write its probability of realization P_l in the grand canonical ensemble.

(b) Each microscopic state l corresponds to a set of occupation numbers of the different one-particle states

$$l \leftrightarrow \{n_\lambda^{(l)}\} \tag{1}$$

where $\{n_\lambda^{(l)}\}$ is the number of particles in the one-particle state ϕ_λ when the system is in the microscopic state l. Write the energy E_l and the number of particles N_l as a function of $\{n_\lambda^{(l)}\}$.

(c) Show that P_l, now $P_l(\{n_\lambda^{(l)}\})$ or more simply $P(\{n_\lambda\})$, is a product :

$$P(\{n_\lambda\}) = \Pi_\lambda P_\lambda(n_\lambda) \tag{2}$$

Give the functions $P_\lambda(n_\lambda)$. What does the fact that $P(\{n_\lambda\})$ is factored physically mean ?

(d) Qualitatively plot the probability $P_\lambda(n_\lambda)$ as a function of n_λ. What is the most probable value of n_λ ?

(e) From $P_\lambda(n_\lambda)$, calculate the average occupation numbers $\bar{n}_\lambda$ in the grand canonical ensemble.

(f) Again using $P_\lambda(n_\lambda)$, show that the variance of n_λ is

$$(\Delta n_\lambda)^2 \equiv \overline{n_\lambda^2} - (\bar{n}_\lambda)^2 = \bar{n}_\lambda(\bar{n}_\lambda + 1) \tag{3}$$

(g) Suppose that each state λ is weakly populated : $\bar{n}_\lambda \ll 1$. Show that the fluctuations in the mode are Poissonian (the variance is equal to the mean value).

(h) Suppose now that the one-particle ground state ϕ_0 is macroscopically populated, that is, we are dealing with a condensate. What can be said of $(\Delta n_0)^2$? Comment.

1.1.2 Ideal gas of bosons in the canonical ensemble

We will now set the total number of particles to a specific value N, which better describes the experimental situation.

(i) Let l be a microscopic state of the system of energy E_l (and number of particles N). Write its probability of realization P_l in the canonical ensemble.

(j) Each microscopic state l is represented by a set of occupation numbers of the different one-particle states

$$l \leftrightarrow \{n_\lambda\} \qquad \text{with} \qquad \sum_\lambda n_\lambda = N \tag{4}$$

where we have imposed the additional constraint of the conservation of the total number of particles. The gas is at a temperature below the critical temperature of Bose condensation. The number of particles in the condensate is given by :

$$n_0 = N - \sum_{\lambda \neq 0} n_\lambda \tag{5}$$

and it is not an independent variable. We thus have the one-to-one correspondence :

$$l \leftrightarrow \{n_\lambda\}_{\lambda \neq 0} \tag{6}$$

with the constraint $\sum_{\lambda \neq 0} n_\lambda < N$.

Express E_l as a function of the n_λ and show that the probability distribution of the occupation numbers of one-particle excited states can be written as

$$P(\{n_\lambda\}_{\lambda \neq 0}) = \Theta(N - \sum_{\lambda \neq 0} N_\lambda) \times \Pi_{\lambda \neq 0} P_\lambda(n_\lambda) \tag{7}$$

where Θ is the Heaviside function $\Theta(x) = 1$ for $x \geq 0$ and $\Theta(x) = 0$ for $x < 0$. Give the functions $P_\lambda(n_\lambda)$ up to a proportionality factor.

(k) We now introduce an approximation justified in the presence of a condensate. We neglect the possibility that the condensate is empty. This leads to

$$P(\{n_\lambda\}_{\lambda \neq 0}) \simeq \Pi_{\lambda \neq 0} P_\lambda(n_\lambda) \tag{8}$$

From the expression of $P_\lambda(n_\lambda)$, show that one finds formally a grand canonical ensemble for the non condensed particles with a chemical potential (equal to ϵ_0) fixed by the condensate that serves here as an infinite reservoir of particles.

(l) Show that, N being fixed, one has $(\Delta n_0)^2 = (\Delta n_\perp)^2$ where $N_\perp = \sum_{\lambda \neq 0} n_\lambda$.

1.1.3 Uniform case in $3D$

In this section, the atoms are in a cubic box of size L (3-dimensional) with periodic boundary conditions. So we have $\lambda = \mathbf{k}$ where $\mathbf{k}$ is a wave vector.

(m) Give the expression of ϕ_λ and ϵ_λ. Specify which values of the wave vector $\mathbf{k}$ are compatible with the periodic boundary conditions.

(n) Show that
$$(\Delta n_0)^2 = \sum_{\mathbf{k}\neq\mathbf{0}} \frac{1}{4\,\mathrm{sh}^2(\beta\epsilon_k/2)} \tag{9}$$

(o) Show that by replacing the discrete sum over $\mathbf{k}$ by an integral in the thermodynamic limit, we obtain a divergent integral.

(p) So we keep the discrete sum. The sum is dominated by the terms with $\beta\epsilon_k \ll 1$, one can thus linearize the hyperbolic sine function. Show that
$$(\Delta n_0)^2 = \left(\frac{k_B T}{\Delta}\right)^2 \sum_{\mathbf{n}\in\mathbb{Z}^{3*}} \frac{1}{(n_x^2+n_y^2+n_z^2)^2} = \left(\frac{k_B T}{\Delta}\right)^2 \times 16,53\ldots \tag{10}$$
and give the value of Δ as a function of the mass m of the particles and the size L of the box. What is the physical meaning of Δ ?

(q) Using the previous result and a result of the first subsection, show that, while remaining large in the thermodynamic limit ($N \to \infty$, $V \to \infty$, N/V = constant), the fluctuations of the number of particles in the condensate are smaller than in the grand canonical ensemble.

(r) Are the fluctuations of n_0 larger or smaller than Poissonian fluctuations ?

1.2 The interacting gas

We now consider an interacting Bose gas in the canonical ensemble, the goal being to see how the interactions will affect the result obtained in the previous subsection. We will use the Bogoboliubov theory and we will consider from the start the case of a homogeneous system (cubic box of volume $V = L^3$ with periodic boundary conditions). We introduce $\rho = N/V$ the density of particles and g the coupling constant that characterizes the interactions between particles.

In the lectures, we introduced the $\psi(\mathbf{r}) = \sqrt{N}\phi_0(\mathbf{r})$ field, where N is the number of particles and $\phi_0(x)$ the condensate wave function obeying the Gross-Pitaevskii equation. We have seen that a fluctuation $\delta\psi(\mathbf{r})$ of this field, developed on the eigenmodes of the linearized dynamics of the fluctuations, takes the form
$$\delta\psi(\mathbf{r}) = \sum_{\mathbf{k}\neq\mathbf{0}} \left(b_{\mathbf{k}} U_k + b^*_{-\mathbf{k}} V_k\right) \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}} \tag{11}$$
where the amplitudes U_k, V_k and the mode energy ϵ_k are given by :
$$U_k - V_k = \frac{1}{U_k + V_k} = \left(\frac{\epsilon_k}{\frac{\hbar^2 k^2}{2m}}\right)^{1/2} \qquad \text{and} \qquad \epsilon_k = \sqrt{\frac{\hbar^2 k^2}{2m}\left(\frac{\hbar^2 k^2}{2m} + 2\rho g\right)} \tag{12}$$

The modal amplitudes $b_{\mathbf{k}}$, $b^*_{\mathbf{k}}$ simply evolve as $b_{\mathbf{k}}(t) = e^{-\frac{i}{\hbar}\epsilon_k t}\, b_{\mathbf{k}}(0)$. In the quantum version of the theory, they are replaced by bosonic operators
$$b_{\mathbf{k}} \to \hat{b}_{\mathbf{k}} \quad ; \quad b^*_{\mathbf{k}} \to \hat{b}^\dagger_{\mathbf{k}} \quad ; \quad [\hat{b}_{\mathbf{k}}, \hat{b}^\dagger_{\mathbf{k}'}] = \delta_{\mathbf{k},\mathbf{k}'} \tag{13}$$

The field
$$\delta\hat{\psi}(\mathbf{r}) = \sum_{\mathbf{k}\neq\mathbf{0}} \left(\hat{b}_{\mathbf{k}} U_k + \hat{b}^\dagger_{-\mathbf{k}} V_k\right) \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}} \tag{14}$$

then represents the particle field in modes orthogonal to the condensate mode $\phi_0(\mathbf{r}) = \frac{1}{\sqrt{V}}$ and

$$\hat{N}_\perp = \int d^3r\, \delta\hat{\psi}^\dagger(\mathbf{r})\delta\hat{\psi}(\mathbf{r}) \tag{15}$$

represents the operator *number of non-condensed particles.*

(s) From the equations (14) and (15), show that

$$\hat{N}_\perp = \sum_{\mathbf{k}\neq\mathbf{0}} (U_k^2 + V_k^2)\hat{b}_\mathbf{k}^\dagger\hat{b}_\mathbf{k} + V_k^2 + U_kV_k(\hat{b}_\mathbf{k}^\dagger\hat{b}_{-\mathbf{k}}^\dagger + \hat{b}_{-\mathbf{k}}\hat{b}_\mathbf{k}) \tag{16}$$

In the quantum Bogoliubov theory, the system is described as a set of independent quasiparticles. The operators $\hat{a}_0$ and $\hat{a}_0^\dagger$ of creation and annihilation of a particle in the condensate mode can be eliminated from the Hamiltonian in favor of $\delta\hat{N}_\perp$ in the approximation of the "never empty condensate". Finally we get :

$$\hat{H}_{\text{Bog}} = E_0(N) + \sum_{\mathbf{k}\neq\mathbf{0}} \epsilon_k \hat{n}_\mathbf{k} \qquad \text{with} \qquad \hat{n}_\mathbf{k} = \hat{b}_\mathbf{k}^\dagger\hat{b}_\mathbf{k} \tag{17}$$

A microscopic state l of the system is then represented by the set of occupation numbers $\{n_\mathbf{k}\}_{\mathbf{k}\neq 0}$ of Bogoliubov modes (or Bogoliubov excitations) :

$$l \leftrightarrow \{n_\mathbf{k}\}_{\mathbf{k}\neq 0} \tag{18}$$

and the constraint on the total number of particles in the canonical ensemble imposes

$$\hat{n}_0 = N - \hat{N}_\perp \tag{19}$$

where $\hat{n}_0$ is the operator number of particles in the condensate. The system at equilibrium in the canonical ensemble (in the approximation of a "never empty condensate") is thus described by a density operator of the form

$$\hat{\rho}_{\text{Bog}} = \frac{1}{Z} e^{-\beta \sum_{\mathbf{k}\neq\mathbf{0}} \epsilon_k \hat{b}_\mathbf{k}^\dagger \hat{b}_\mathbf{k}} \tag{20}$$

(t) Using $\hat{\rho}_{\text{Bog}}$, calculate the average of the quasiparticle occupation numbers as a function of their eigenenergy ϵ_k.

(u) Show that for all $s \in \mathbb{N}^*$, $\langle(\hat{b}_\mathbf{k})^s\rangle = 0$, the average being taken in the state $\hat{\rho}_{\text{Bog}}$. You can take the trace in the Fock basis $|\{n_\mathbf{k}\}\rangle$ (we remind that $\hat{b}_\mathbf{k}|n_\mathbf{k}\rangle = \sqrt{n_\mathbf{k}}|n_\mathbf{k} - 1\rangle$). Express the average value of $\hat{N}_\perp$ in terms of the $\bar{n}_\mathbf{k}$.

(v) Show that the variance of $\hat{N}_\perp$ is :

$$(\Delta N_\perp)^2 = \sum_{\mathbf{k}\neq\mathbf{0}} (U_k^2 + V_k^2)^2 \bar{n}_\mathbf{k}(\bar{n}_\mathbf{k} + 1) + 2U_k^2V_k^2\left[\bar{n}_\mathbf{k}^2 + (1 + \bar{n}_\mathbf{k})^2\right] \tag{21}$$

You can use the following result (Wick's theorem) which states that for a density operator of the form (20), where the $\hat{b}_\mathbf{k}$ are bosonic operators, and for operators $\hat{A}_i$ equal to $\hat{b}_{\mathbf{k}_i}$ or $\hat{b}_{\mathbf{k}_i}^\dagger$, one has

$$\langle \hat{A}_1\hat{A}_2\hat{A}_3\hat{A}_4\rangle = \langle \hat{A}_1\hat{A}_2\rangle\langle \hat{A}_3\hat{A}_4\rangle + \langle \hat{A}_1\hat{A}_3\rangle\langle \hat{A}_2\hat{A}_4\rangle + \langle \hat{A}_1\hat{A}_4\rangle\langle \hat{A}_2\hat{A}_3\rangle \tag{22}$$

(w) We introduce the dimensionless variable q defined by

$$\frac{\hbar^2 k^2}{2m} = 2\rho g q^2 \qquad \text{or, in an equivalent way} \qquad \hbar c k = 2\rho g q \tag{23}$$

where $c = \sqrt{\rho g/m}$ is the speed of sound in the condensate. Show that at low k, for $k_B T \gg \epsilon_k$, we have

$$U_k \simeq \frac{1}{2}\frac{1}{q^{1/2}} \qquad , \qquad V_k \simeq -\frac{1}{2}\frac{1}{q^{1/2}} \qquad \text{and} \qquad \bar{n}_k \simeq \frac{k_B T}{2\rho g}\frac{1}{q} \tag{24}$$

The dispersion relation $k \mapsto \epsilon_k$ will be approximated by its low k expression.

(x) Show that if we replace the sum (21) by an integral over $\mathbf{k}$ in the thermodynamic limit, we obtain a divergent integral.

(y) We keep the discrete sum but only retain the dominant terms in the low k expansion of the summand. Show that

$$(\Delta N_\perp)^2 \simeq \frac{1}{2}\left(\frac{k_B T}{\Delta}\right)^2 \sum_{\mathbf{n}\in\mathbb{Z}^{3*}} \frac{1}{(n_x^2 + n_y^2 + n_z^2)^2} \tag{25}$$

(z) Deduce the value of $(\Delta n_0)^2$, compare it with the case of the ideal gas, and conclude.

2 Cooling fermions using an adiabatic process

A very efficient way to cool down a gas of bosons well below degeneracy is evaporative cooling. This technique consists in cutting the upper part of the energy distribution by removing the particles of highest energy. Then it relies on elastic collisions between atoms to reach a new thermal equilibrium at a lower temperature. Unfortunately it turns out not to be very efficient for a gas of fermions and allows to reach only temperatures of typically $0.2\,T_F$, where T_F is the Fermi temperature of the gas. The goal of this exercise is to show another method which could cool fermions in two spin states $|\uparrow\rangle$ and $|\downarrow\rangle$ down to very low temperatures.

The key idea is to use a Feshbach resonance to change the s-wave scattering length a from positive to negative. For $a > 0$, atoms form $\uparrow\downarrow$ molecules of size much smaller than the typical intermolecular distance. These molecules can then be considered as bosons. They can be cooled down efficiently using evaporation and be condensed. Then a is changed adiabatically (here with entropy remaining constant) towards negative values. Molecules dissociate and the condensate of molecules turns into a cold degenerate Fermi gas.

2.1 Entropy of a perfect gas of trapped fermions

Let's consider as ensemble of fermions of mass m in two spin states $|\uparrow\rangle$ and $|\downarrow\rangle$. The fermions are trapped in an isotropic harmonic potential in 3D. Therefore the one-particle Hamiltonian is

$$h_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2 \tag{26}$$

with $p^2 = p_x^2 + p_y^2 + p_z^2$ et $r^2 = x^2 + y^2 + z^2$. We neglect interactions between atoms. We use the grand canonical ensemble of temperature $T = 1/(k_B\beta)$ (k_B is the Boltzmann constant) and chemical potential μ to describe the gas. The grand potential is

$$J = -k_B T \sum_\lambda \ln\left(1 + e^{\beta(\mu - \epsilon_\lambda)}\right) \tag{27}$$

where the sum runs across all the eigenstates of the one-particle Hamiltonian h_0.

(a) Write down the eigenenergies ϵ_λ of h_0 and give the quantum numbers characterizing each eigenstate ϕ_λ. In the following we choose the origin of energies such that the minimal eigenenergie ϵ_0 is zero.

(b) Compute the density of states in the harmonic trap $\rho(\epsilon)$ and show that it is of the form

$$\rho(\epsilon) = A\epsilon^2 \tag{28}$$

where A is a constant to be expressed as a function of ω.

(c) Show that in the limit where $k_B T \gg \hbar\omega$, we can write

$$J = k_B T \int_0^\infty d\epsilon\, \rho(\epsilon) \ln\left(1 - n(\epsilon)\right) \tag{29}$$

where $n(\epsilon)$ is the average (fermionic) occupation number of a one particle state of energy ϵ, and $\rho(\epsilon)$ is the density of states previously computed.

(d) Integrate J by parts and perform a low temperature expansion of J including terms up to order four in T. Use the following relation

$$\int_0^\infty \frac{g(\epsilon)d\epsilon}{e^{\beta(\epsilon-\mu)}+1} \simeq \int_0^\mu g(\epsilon)d\epsilon + \frac{\pi^2}{6}g'(\mu)(k_B T)^2 + \frac{7\pi^4}{360}g'''(\mu)(k_B T)^4 + \ldots \tag{30}$$

where $g(\epsilon)$ is a regular function of ϵ.

(e) Use $S = -\partial_T J|_{\mu,\omega}$ to compute the entropy S of the gas as a function of μ, A and T.

(f) Use $N = -\partial_\mu J|_{T,\omega}$, where N is the total number of fermions, to express the chemical potential μ as a function of A and N, to lowest order (order zero in T).

(g) Compute the Fermi energy ϵ_F in the harmonic trap as a function of N and A, and show that

$$S = k_B N\pi^2\left(\frac{T}{T_F}\right) + \mathcal{O}(T^3) \tag{31}$$

where $T_F = \epsilon_F/k_B$.

2.2 Entropy of an ideal gas of bosons

Let's consider an ideal gas of spinless bosons. They are trapped and condensed ($T \ll T_c$ where T_c is the critical temperature). The goal of this section is to compute the entropy of the gas a function of temperature. The one-particle Hamiltonian is still h_0 (see (26)). The grand potential is this time

$$J = k_B T \sum_\lambda \ln\left(1 - e^{\beta(\mu-\epsilon_\lambda)}\right) \tag{32}$$

where the sum runs across all the eigenstates of the one-particle Hamiltonian h_0.

(h) Compute the density of states in the harmonic trap $\rho(\epsilon)$ for the gas of bosons and show that it is of the form

$$\rho(\epsilon) = A_B\epsilon^2 \tag{33}$$

where $A_B = A/2$ and A is the constant computed in (b).

(i) Give the value of the chemical potential μ in the presence of a condensate for $T \ll T_c$.

(j) Explain why the ground state h_0 can be neglected when computing the entropy.

(k) Show that in the limit $k_B T \gg \hbar\omega$, we can write

$$J = k_B T \int_0^\infty d\epsilon\, \rho(\epsilon) \ln\left(1 - e^{-\beta\epsilon}\right) . \tag{34}$$

(l) Integrate J by parts and express the entropy S of the gas as a function of A_B, T and $g_4(1) = \zeta(4)$, where g is the Bose function

$$g_\alpha(z) = \frac{1}{\Gamma(\alpha)} \int_0^\infty dy\, y^{\alpha-1} \frac{ze^{-y}}{1 - ze^{-}y} \tag{35}$$

and ζ is the Riemann Zeta function. We remind that $\Gamma(n+1) = n!$ for any integer n.

(m) Compute the critical temperature T_c in the harmonic trap as a function of the number of bosons N_B, the trapping frequency ω and $\zeta(3)$.

(n) Knowing that $\zeta(4) = \pi^4/90$, show that

$$S = N_B k_B \left(\frac{T}{T_c}\right)^3 \frac{2\pi^4}{45\,\zeta(3)} . \tag{36}$$

2.3 Transform at constant entropy

We now want to estimate the efficiency of the whole fermion cooling process.

(o) We start from a condensate of molecules ($a > 0$) cooled down to $T = 0.25\,T_c$ and we transform the system to a gas of fermions by changing the sign of a at constant entropy. Compute the final temperature of the fermions in unit of T_F ($\zeta(3) = 1.202...$).