Quantum statistics and interactions

Final Exam 2022 - C. Winkelmann - UGA/Phelma

Bose-Einstein condensation

We study here the properties of a gas of a large number N of identical and spinless bosons, with mass m and dispersion relation $\epsilon_{\mathbf{k}} = (\hbar\mathbf{k})^2/2m$. At thermal equilibrium the different energy states are occupied according to the Bose-Einstein distribution

$$f(E) = \left(e^{\beta(E-\mu)} - 1\right)^{-1},$$

where $\beta = 1/(k_B T)$, μ is the chemical potential, T is the temperature and k_B the Boltzmann constant. Depending on the questions, we will consider the gas to be confined in a cubic box of volume L^3, or a three-dimensional harmonic trap.

1 Bose-Einstein condensation without interactions

We neglect interactions between the particles in this part of the problem.

1.1

To start with, consider a single such particle, trapped in a three-dimensional isotropic harmonic potential

$$V_{tr}(\mathbf{r}) = \frac{1}{2} m\omega_0^2 |\mathbf{r}|^2. \tag{1}$$

We take the bottom of the potential as the origin of energies. The energy levels in this potential are given by $E_n = \hbar\omega_0(n + 3/2)$. In this potential the particle has a ground state wave function

$$\psi_0(\mathbf{r}) \propto \exp\left(-\frac{1}{2}\frac{|\mathbf{r}|^2}{d^2}\right). \tag{2}$$

Relate the value of d to the parameters of the problem within numerical prefactors of order 1, from simple energetic arguments.

1.2

Describe (graphically) the energy distribution of the gas of N bosons in the trap. What is the sign of $\mu - E_0$? Assuming $T \gg \hbar\omega_0/k_B$, give an estimate of the spatial extent of the cloud confined in the trap.

1.3

Describe qualitatively how μ evolves as the temperature is lowered and the number N is kept fixed. You may write the sum/integral of occupations over energies to discuss this.

1.4

It can be shown that below a certain critical temperature T_c, $f(E_0)$ suddenly becomes very large $\to N$. This phenomenon is called Bose-Einstein condensation, and corresponds to the condensation of a macroscopic fraction of the N particles into the ground state. Assuming no interactions, write the zero-temperature ground state $|\Psi_0\rangle$ of in second quantized formalism in which all particles are condensed in ψ_0, starting from the vacuum state $|0\rangle$ and using the creation operator $a_0^\dagger$ of a particle in the single-particle ground state. Make sure $|\Psi_0\rangle$ has the correct prefactor, which guarantees that this state is normalised for bosons.

2 Hamiltonian of N weakly interacting bosons

We now consider a gas of N bosons confined in a cubic box of volume L^3. For describing the interactions of neutral atoms, we can assume that the two-particle interaction potential $V(\mathbf{r})$ is short-ranged and repulsive. The simplest way of modelling this potential is $V(\mathbf{r}) = g \times \delta(\mathbf{r})$, with $g > 0$.

2.1

Define the *non-interacting* N-particle ground state $|\Psi_0\rangle$ is defined in the present case of particles confined in a cubic box.

2.2

Recall the general form of the N-particle Hamiltonian in the presence of interactions from the lecture, and explain the action of the different creation and annihilation operators. Justify that in the present case the Hamiltonian can be written

$$H = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{g}{2L^3} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} a^\dagger_{\mathbf{k}} a^\dagger_{\mathbf{k}'} a_{\mathbf{k}'+\mathbf{q}} a_{\mathbf{k}-\mathbf{q}}. \tag{3}$$

2.3

Due to interactions, not all particles will be in state $\mathbf{k} = \mathbf{0}$ in the ground state of the gas. Our aim is to estimate the effect of weak interactions on the ground state population. The operator $\hat{n}_0 = a^\dagger_0 a_0$ counts the number of particles in state $\mathbf{k} = \mathbf{0}$, while $\hat{n}_e = \sum_{\mathbf{k}\neq\mathbf{0}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}}$ counts the number of particles in $\mathbf{k} \neq \mathbf{0}$ states. We note n_0 and n_e the corresponding expectation values, and obviously $N = n_0 + n_e$. Because the interactions are weak, we have $n_0 \approx N$ and $n_e \ll n_0, N$. Show that $\hat{n}_0^2$ can be approximated as

$$\hat{n}_0^2 \approx N^2 - 2N \sum_{\mathbf{k}\neq\mathbf{0}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}}. \tag{4}$$

2.4

Since the expectation value of $\hat{n}_0$ is a large number, we can neglect $\left[a_0, a^\dagger_0\right] = 1$ with respect to $\hat{n}_0$. This is equivalent to considering a_0 and $a^\dagger_0$ as simple numbers $\approx \sqrt{n_0}$. All other $a_{\mathbf{k}\neq\mathbf{0}}$ and $a^\dagger_{\mathbf{k}\neq\mathbf{0}}$ are still considered as operators.

Separate the sum in the interaction term in Eq. (3) according to three cases:

- i) all four momentum indices are 0,
- ii) two momentum indices are 0, the two other being $\neq 0$. The six different sub-cases of case ii) should be discussed in detail. Show that these introduce a term $4a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + a_{-\mathbf{k}} a_{\mathbf{k}} + a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}}$.
- iii) more than two indices are $\neq 0$.

Neglecting the terms $\ll n_0$ arising from case iii), show that one is eventually left with

$$H \approx \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{g}{2L^3} \left\{ n_0^2 + n_0 \sum_{\mathbf{k}\neq 0} \left(4a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + a_{-\mathbf{k}} a_{\mathbf{k}} + a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}} \right) \right\}. \tag{5}$$

2.5

Substituting back n_0 and n_0^2 by their operator expressions, as for instance in Eq. (4), show that

$$H \approx N^2 \frac{g}{2L^3} + \sum_{\mathbf{k}\neq 0} \left\{ \left(\varepsilon_{\mathbf{k}} + \frac{Ng}{L^3} \right) a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{Ng}{2L^3} (a_{-\mathbf{k}} a_{\mathbf{k}} + a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}}) \right\}. \tag{6}$$

3 Bogoliubov transformation

It will be convenient to define $b = Ng/L^3$. We will now show that the Hamiltonian in Eq. (6) can be diagonalised using a clever change of variables. Following Bogoliubov, we define a new set of operators

$$\alpha_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} a^{\dagger}_{-\mathbf{k}}, \tag{7}$$

where $u_{\mathbf{k}}, v_{\mathbf{k}}$ are a priori freely chosen real numbers.

3.1

Write also $\alpha^{\dagger}_{\mathbf{k}}$ and show that the new operators $\alpha_{\mathbf{k}}$ and $\alpha^{\dagger}_{\mathbf{k}}$ obey the standard bosonic commutation relations, under the condition that $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are chosen such that $u_{\mathbf{k}} = u_{-\mathbf{k}}$, $v_{\mathbf{k}} = v_{-\mathbf{k}}$, and $u^2_{\mathbf{k}} - v^2_{\mathbf{k}} = 1$, which we will assume from here on.

3.2

Revert the relation between a's and α's defined by Eq. (7) and its hermitian conjugate.

3.3

Rewrite Eq. (6) in terms of these new operators. Separate the $\sum_{\mathbf{k}\neq\mathbf{0}}$ into three parts, with one containing no α or $\alpha^{\dagger}$, the second containing only terms proportional to $\alpha^{\dagger}_{\mathbf{k}}\alpha_{\mathbf{k}}$, and the third one containing terms proportional to $\left(\alpha_{-\mathbf{k}}\alpha_{\mathbf{k}} + \alpha^{\dagger}_{\mathbf{k}}\alpha^{\dagger}_{-\mathbf{k}}\right)$.

3.4

Justify that there is a (unique) mathematical solution allowing to chose $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ such that

$$u^2_{\mathbf{k}} - v^2_{\mathbf{k}} = 1, \quad (\varepsilon_{\mathbf{k}} + b)u_{\mathbf{k}}v_{\mathbf{k}} + \frac{b}{2}(u^2_{\mathbf{k}} + v^2_{\mathbf{k}}) = 0. \tag{8}$$

For this, it is possible to use the following hyperbolic trigonometry relations

$$\cosh^2 x - \sinh^2 x = 1, \quad \cosh^2 x + \sinh^2 x = \cosh(2x), \quad 2\cosh x \sinh x = \sinh(2x).$$

3.5

Show that this choice allows considerably simplifying the Hamiltonian in Eq. (6). Discuss its new form.

3.6

Defining $\zeta_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}(\varepsilon_{\mathbf{k}} + 2b)}$, show that the Hamiltonian reduces to

$$H \approx H_0 + \sum_{\mathbf{k}\neq 0} \zeta_{\mathbf{k}}\, \alpha^{\dagger}_{\mathbf{k}}\alpha_{\mathbf{k}}, \tag{9}$$

where H_0 does not contain any $\alpha^{\dagger}_{\mathbf{k}}$ or $\alpha_{\mathbf{k}}$ operators.

3.7

We recognise thus that the $\alpha^{\dagger}_{\mathbf{k}}$ or $\alpha_{\mathbf{k}}$ operators create and annihilate excitations (called quasiparticles), which are composite in $\pm\mathbf{k}$. The lowest energy state of the weakly interaction Bose gas is given by the absence of any such excitation. We define the new ground state, in the presence of weak interactions, by $\alpha_{\mathbf{k}}|\Psi_0\rangle = 0$ for any $\mathbf{k} \neq \mathbf{0}$. Show that in this state, the number of particles with wavevector $\mathbf{k} \neq \mathbf{0}$ is $\langle\Psi_0|a^{\dagger}_{\mathbf{k}}a_{\mathbf{k}}|\Psi_0\rangle = v^2_{\mathbf{k}}$.

3.8

Evaluate the total number of uncondensed particles $n_e = \langle \Psi_0 | \hat{n}_e | \Psi_0 \rangle$.