

# 8.08 Statistical Physics II — Spring 2019

## Recitation Note 8

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### Contents

<b>1</b>	<b>Non-interacting Bose Gas</b>	<b>2</b>
1.1	Chemical Potential and Bose-Einstein Condensation . . . . .	2
1.2	Internal Energy and Heat Capacity . . . . .	4
1.3	Pressure and Equation of State . . . . .	5
1.4	Entropy and BEC as Phase Transition . . . . .	6

# 1 Non-interacting Bose Gas

In the last recitation and in the class, we have derived the grand partition function of non-interacting Bose gas:

$$\Xi_{\mathbf{k}} = \frac{1}{1 - e^{-\beta(\epsilon_{\mathbf{k}} - \mu)}}, \quad (1)$$

and  $\Xi = \prod_{\mathbf{k}} \Xi_{\mathbf{k}}$ . The Bose-Einstein distribution comes from

$$\langle n_{\mathbf{k}} \rangle = \frac{\ln \Xi_{\mathbf{k}}}{\partial(\beta\mu)} = \frac{1}{e^{\beta(\epsilon_{\mathbf{k}} - \mu)} - 1}, \quad (2)$$

where  $\mu$  is determined from the total particle number constraint  $N = \sum_{\mathbf{k}} \langle n_{\mathbf{k}} \rangle$ .

We are going to study the property of non-interacting Bose gas in detail. First, we need to choose a dispersion relation for bosons. Here we use quadratic dispersion in three dimensions:  $E_{\mathbf{k}} = \hbar^2 k^2 / 2m$  and  $k = \sqrt{k_x^2 + k_y^2 + k_z^2}$ . It is straightforward to generalize the calculation to any dimensions with any dispersion relation, which you will do in the pset.

## 1.1 Chemical Potential and Bose-Einstein Condensation

We first determine the  $\mu \sim N$  relation. It is often convenient to convert the momentum integral to the energy integral. Note that the energy only depends on the magnitude of the wavevector:

$$\sum_{\mathbf{k}} = V \int \frac{d^3 \mathbf{k}}{(2\pi)^3} = V \int_0^{+\infty} \frac{4\pi k^2 dk}{(2\pi)^3} = V \int_0^{+\infty} \frac{k^2 dk}{2\pi^2}. \quad (3)$$

Combined with  $dE/dk = \hbar^2 k/m$ , we have

$$\frac{k^2 dk}{2\pi^2} = \frac{m}{2\pi^2 \hbar^2} k dE = \underbrace{\frac{m}{2\pi^2 \hbar^2} \sqrt{\frac{2mE}{\hbar^2}}}_{g(E)} dE, \quad (4)$$

where  $\sum_{\mathbf{k}} = V \int g(E) dE$  and  $g(E)$  is called the density of states. The particle number constraint becomes

$$n = \frac{m^{3/2}}{\sqrt{2\pi^2 \hbar^3}} \int_0^{+\infty} \frac{\sqrt{E} dE}{e^{-\beta(E-\mu)} - 1} = \frac{m^{3/2}}{\sqrt{2\pi^2 \hbar^3} \beta^3} \int_0^{+\infty} \frac{\sqrt{x} dx}{e^{x/z} - 1}, \quad (5)$$

where we have changed the variable  $x = \beta E$  and denote  $z \equiv e^{\beta\mu}$ , which is the fugacity of the system. Note that the integral is dimensionless because both  $x$  and  $z$  are dimensionless. The above expression can be simplified further by introducing the thermal wavelength  $\lambda_T \equiv \sqrt{2\pi \hbar^2 / m k_B T}$ .

$$n \lambda_T^3 = \frac{2}{\sqrt{\pi}} \int_0^{+\infty} \frac{\sqrt{x} dx}{e^{x/z} - 1} = g_{3/2}(z). \quad (6)$$

The closed-form solution of the integral in general does not exist.

$g_{\nu}(z)$  is often called the Bose-Einstein function by physicists and polylogarithm functions by mathematicians. It is often expressed as a series:

$$\begin{aligned} g_{3/2}(z) &= \frac{2}{\sqrt{\pi}} \int_0^{+\infty} \frac{\sqrt{x} dx}{e^{x/z} - 1} = \frac{2z}{\sqrt{\pi}} \int_0^{+\infty} \frac{e^{-x} \sqrt{x}}{1 - ze^{-x}} dx \\ &= \frac{2z}{\sqrt{\pi}} \int_0^{+\infty} dx e^{-x} \sqrt{x} \sum_{p=0}^{\infty} z^p e^{-px} = \frac{2}{\sqrt{\pi}} \sum_{p=1}^{\infty} z^p \int_0^{+\infty} dx \sqrt{x} e^{-px} = \sum_{p=1}^{\infty} \frac{z^p}{p^{3/2}}. \end{aligned} \quad (7)$$

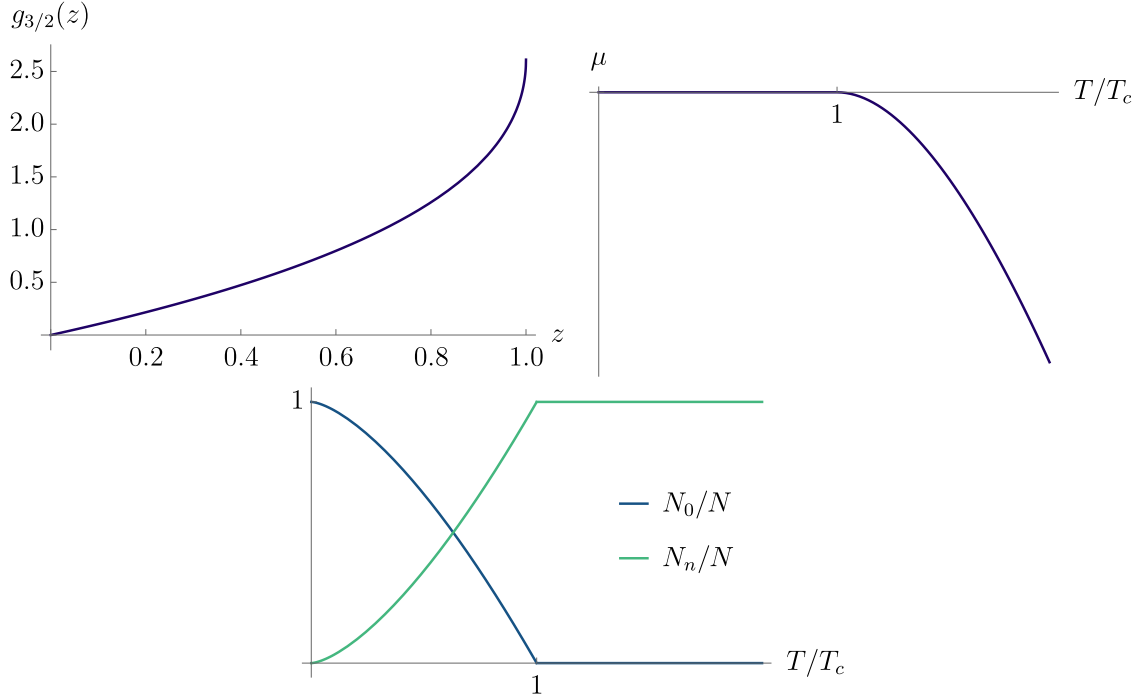


Figure 1: Plot of  $g_{3/2}(z)$ ; Chemical potential  $\mu$  for fixed density as a function of temperature  $T$ ; Number of bosons in the condensed phase  $N_0$  and in the normal phase  $N_n$  as functions of temperature  $T$ .

In general,  $g_\nu(z) \equiv \sum_{p=1}^{\infty} z^p/p^\nu$ .

$g_{3/2}(z)$  is plotted in Fig. 1, which increases monotonically with  $z$  and is finite only when  $|z| \leq 1$ .  $z = 1$  corresponds to  $\mu = 0$  and  $g_{3/2}(z) = \zeta(3/2) \approx 2.612$ . Since  $z$  increases monotonically with  $\mu$ , this is consistent with the fact that  $\mu \leq 0$  in non-interacting Bose gas (if you don't know why, check the last recitation note). However, this also sets an upper limit  $g_{3/2}(1)$  on  $n\lambda_T^3$ . What happens in reality if we have a system of Bose gas with density  $n\lambda_T^3 > g_{3/2}(1)$ , for example, by lowering the temperature under the critical temperature  $T_c$ ?

$$k_B T_c = \frac{2\pi\hbar^2}{m} \left( \frac{n}{2.612} \right)^{2/3}. \quad (8)$$

At zero temperature, it is rather obvious all the particle will occupy the lowest energy state, which is the zero momentum  $k = 0$  state. On the other hand, since  $g(E) \propto \sqrt{E}$  and  $g(E = 0) = 0$ , the contribution from the zero momentum state is completely ignored in the continuity assumption. Therefore, we need to consider the  $\mathbf{k} = 0$  state separately when  $T < T_c$ .

$$N_0 = \frac{1}{e^{-\beta\mu} - 1}, \quad (9)$$

or

$$\mu = -k_B T \ln \left( 1 + \frac{1}{N_0} \right) \sim -\frac{k_B T}{N_0}. \quad (10)$$

In the thermodynamic limit, a finite fraction of the bosons are at the zero momentum state, and both  $N$  and  $N_0$  tends to infinity. Thus  $\mu = 0$ . The temperature dependence of  $\mu$  is plotted in Fig. 1.

The conservation of particle number is then

$$N = N_0 + \sum_{\mathbf{k} \neq 0} \frac{1}{e^{\beta\epsilon_{\mathbf{k}}} - 1}, \quad (11)$$

and replace the  $\mathbf{k}$  summation by continuum integral

$$n = n_0 + n_n = 2.612\lambda_T^{-3}, \quad (12)$$

where  $n_0$  is the condensate density and  $n_n$  is the normal density. With the help of Eq. (6), Equation (12) can also be rewritten as

$$\frac{n_0}{n} = 1 - \left(\frac{T}{T_c}\right)^{3/2}, \quad (13)$$

which is plotted in Fig. 1. Note the similarity of the functional form to the magnetization of ferromagnetism transition near the critical point. There the critical exponent of magnetization is  $1/2$  instead of  $3/2$ .

It is often said a macroscopic number (i.e. proportional to system size) of bosons are condensed into the zero momentum state. This phenomenon is called the Bose-Einstein condensation (BEC).

One might question the validity of treating  $\mathbf{k} = 0$  state separately while treating all  $\mathbf{k} \neq 0$  states as a continuum. Suppose in a cubic box with side length  $L$ , the lowest excited state corresponds to the momentum state  $k = 2\pi/L$ . Therefore,  $\varepsilon_{\mathbf{k}} \sim \hbar^2/mL^2 \sim V^{-2/3}\hbar^2/m$ . It follows

$$N_1 = \frac{1}{e^{\beta(\varepsilon_{\mathbf{k}} - \mu)} - 1} \sim \frac{1}{e^{\beta\hbar^2 V^{-2/3}/m} - 1} = O(V^{2/3}), \quad (14)$$

in the  $V \rightarrow \infty$  limit. On the other hand  $N_0 = O(V)$ . Therefore  $N_1/N_0 = O(V^{-1/3}) \rightarrow 0$  in the thermodynamic limit, i.e., the occupation of any individual single particle state with  $\mathbf{k} \neq 0$  is negligible compared with the special  $\mathbf{k} = 0$  state.

## 1.2 Internal Energy and Heat Capacity

The internal energy of Bose gas can be computed directly by noting that condensed state does not contribute to the internal energy:

$$U = V \int_0^{+\infty} \frac{Eg(E)dE}{e^{\beta(E-\mu)} - 1} = \frac{3}{2}Vk_B T \lambda_T^{-3} g_{5/2}(z). \quad (15)$$

Therefore,

$$u = \frac{U}{N} = \begin{cases} \frac{3}{2}k_B T \frac{g_{5/2}(z)}{g_{3/2}(z)}, & T \geq T_c, \\ \frac{3}{2}k_B \frac{T^{5/2}}{T_c^{3/2}} \frac{g_{5/2}(1)}{g_{3/2}(1)}, & T < T_c. \end{cases} \quad (16)$$

When  $T \gg T_c$ , according to Eq. (7), both  $g_\nu(z) \sim z$  when  $z \ll 1$ ,

$$u \sim \frac{3}{2}k_B T, \quad (17)$$

which reduces to the result of monoatomic classical ideal gas. This is consistent with the fact that at high temperature  $\mu \ll 0$  and  $e^{-\beta\mu} \gg 1$ , and the Bose-Einstein distribution reduces to the Boltzmann distribution

$$\langle n_{\mathbf{k}} \rangle = \frac{1}{e^{\beta(\varepsilon_{\mathbf{k}} - \mu)} - 1} \sim e^{-\beta(\varepsilon_{\mathbf{k}} - \mu)}. \quad (18)$$

When  $T \ll T_c$ , we have  $u \sim T^{5/2}$ , which is a power law dependence. This reflects the fact that there is no energy gap existing in the system.

Knowing the internal energy, it is straightforward to compute the heat capacity from  $C_V = (\partial U/\partial T)_V$ . At low temperature  $T \ll T_c$ ,  $C_V \sim T^{3/2}$ ; at high temperature  $T \gg T_c$ ,  $C_V \sim 3k_B/2$ .

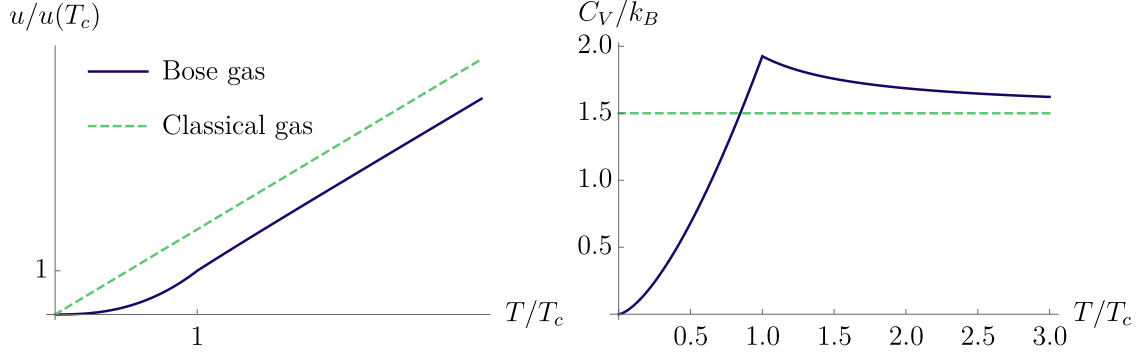


Figure 2: Internal energy per particle  $u$  and heat capacity  $C_V$  as functions of temperature  $T$  for Bose gas and classical ideal gas.

### 1.3 Pressure and Equation of State

There exists a general relation between the pressure and the internal energy in non-interacting systems. Suppose the dispersion relation is  $\varepsilon_{\mathbf{k}} \sim k^\alpha \sim V^{-\alpha/d}$ ,

$$p = - \left( \frac{\partial U}{\partial V} \right)_S \quad (19)$$

$$= - \left( \frac{\partial U}{\partial V} \right)_{n_i, \forall i} \quad (20)$$

$$= - \sum_i n_i \frac{\partial \varepsilon_i}{\partial V} \quad (21)$$

$$= \frac{\alpha}{d} \sum_i n_i \varepsilon_i / V \quad (22)$$

$$= \frac{\alpha}{d} \frac{U}{V}. \quad (23)$$

Equation (19) is equivalent to (20) because entropy is fully determined by the occupation of each state. This relation does not depend on the underlying statistics of the system, as long as the system is non-interacting such that  $U = \sum_i n_i \varepsilon_i$ .

As a consistency check, one can also derive the result using the grand partition function for Bose gas:

$$\Omega = k_B T \sum_{\mathbf{k}} \ln(1 - e^{-\beta(\varepsilon_{\mathbf{k}} - \mu)}). \quad (24)$$

It follows

$$p = - \left( \frac{\partial \Omega}{\partial V} \right)_{T, \mu} = - \sum_{\mathbf{k}} \frac{\frac{\partial \varepsilon_{\mathbf{k}}}{\partial V} e^{-\beta(\varepsilon_{\mathbf{k}} - \mu)}}{1 - e^{-\beta(\varepsilon_{\mathbf{k}} - \mu)}} = - \sum_{\mathbf{k}} n_{\mathbf{k}} \frac{\partial \varepsilon_{\mathbf{k}}}{\partial V}, \quad (25)$$

which reduces to Eq. (21). Note that this derivation is only true for Bose gas.

In our particular example,  $\alpha = 2$  and  $d = 3$ , it follows

$$pV = \frac{2}{3} U. \quad (26)$$

One can check the validity of this formula for classical monoatomic ideal gas, where  $U = 3Nk_B T/2$ . Equation (26) reduces to the familiar equation of state  $pV = Nk_B T$ .

For non-interacting Bose gas, with Eq. (15),

$$p = \frac{3}{2} k_B T \lambda_T^{-3} g_{5/2}(z). \quad (27)$$

## 1.4 Entropy and BEC as Phase Transition

When  $0 \leq T \leq T_c$ , the entropy of the system can be computed as

$$s(T) = \int_0^T \frac{C_V(T')}{T'} dT' = \frac{5}{2} k_B \frac{T^{3/2}}{T_c^{3/2}} \frac{g_{5/2}(1)}{g_{3/2}(1)}. \quad (28)$$

On the other hand, note that  $N_n \sim (T/T_c)^{3/2}$ ,  $s(T)$  can be rewritten as

$$s(T) = N_n s(T_c) = N_0 s(0) + N_n s(T_c). \quad (29)$$

The last equality is because  $s(0) = 0$ . Equation (29) can be interpreted as that the system is a statistical mixture of the condensed phase and the normal phase.

The BEC for non-interacting bosons are usually regarded as a first-order phase transition. (Note that this is true only for non-interacting bosons. BEC of interacting bosons are more complicated. ) There are at least two evidences that suggest this interpretation:

- No discontinuity of specific heat;
- At any nonzero temperature below  $T_c$ , the full thermodynamic property of the system can be described as a two-phase mixture just like the mixture of vapor and liquid.