11/10

Last time: Ideal Bose-Einstein gas

$$N_e \le \frac{V(2\pi m k T)^{3/2}}{h^3} I_{max}$$

$$I = \int_0^\infty \frac{x^{1/2}}{z^{-1}e^x - 1}\,dx \xrightarrow[z\to 1]{I\to I_{max}} I_{max} = \int_0^\infty \frac{x^{1/2}}{e^x - 1}\,dx$$

$$\approx 2.3$$

When $z \to 1$

$$N_e = \frac{V(2\pi m k T)^{3/2}}{h^3} I_{max} = N_e^{max}(T)$$

Notice that if $T \to 0$ then $N_e \to 0$

also $N_0 = N - N_e = N - \frac{V(2\pi m k T)^{3/2}}{h^3} I_{max}$.

When does $N_0 \sim N$?

1) If $N > N_e^{max}$ then the extra particles have to go to be part of N_0.

if $N > N_e^{max} = \frac{V (2\pi m k T)^{3/2}}{h^3} I_{max}$

this happens for large $\frac{N}{V}$ while $z \to 1$.

2) We have to calculate the temperature T_c for which $N_e^{max} = N$.

$$N = \frac{V(2\pi m k T_c)^{3/2}}{h^3} I_{max} \Rightarrow T_c = \frac{h^2}{2\pi m k}\left[\frac{N}{V I_{max}}\right]^{2/3}$$

Then for $T < T_c$ there will be a sizeable number of particles in the ground state.

Then for $T < T_c$:

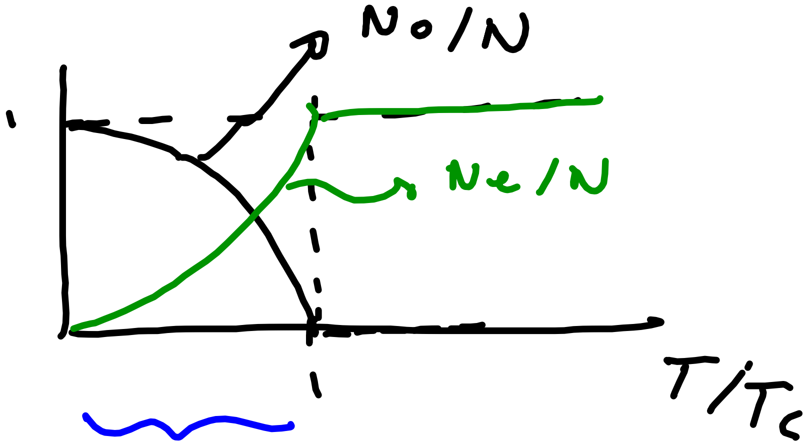
$$N_e = \frac{V(2\pi m k T)^{3/2}}{h^3} I_{max} < N$$

and

$$N = \frac{V(2\pi m k T_c)^{3/2}}{h^3} I_{max}$$

Then $\frac{N_e}{N} = \left(\frac{T}{T_c}\right)^{3/2}$ and $N_0 = N - N_e$

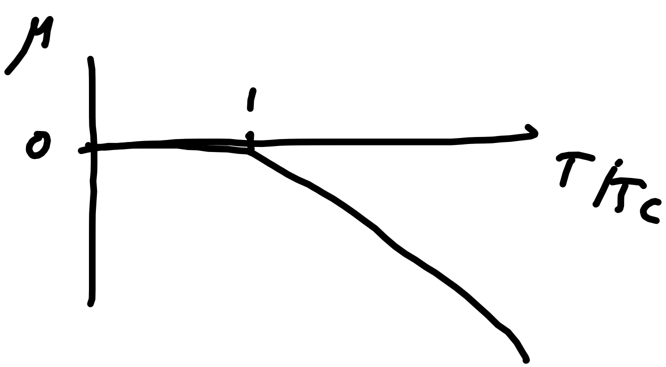
$$\frac{N_0}{N} = 1 - \frac{N_e}{N} = 1 - \left(\frac{T}{T_c}\right)^{3/2}$$



mixed phase state.

For $0 < T < T_c$: mixed phases: • normal N_e particles.

• Bose-Einstein condensate N_0 particles.



Heat capacity:

For $T < T_c$ $\mu \simeq 0$:

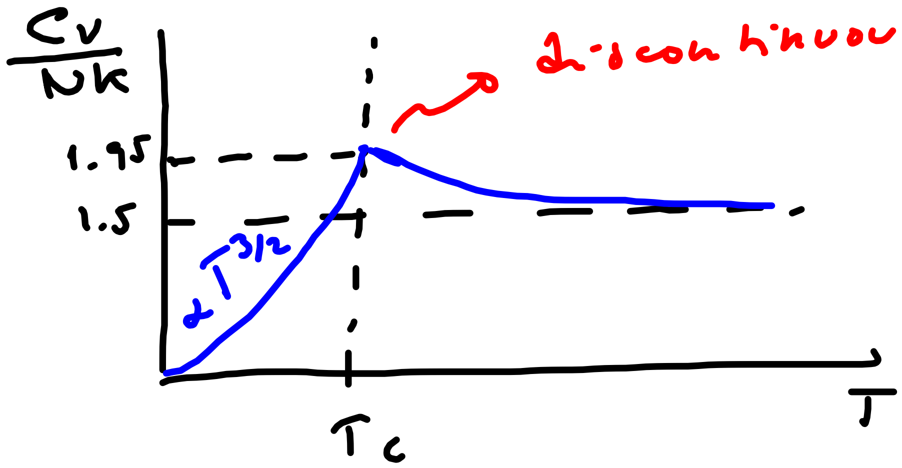
$$\langle E \rangle = \frac{2\pi V (2m)^{3/2}}{h^3} (kT)^{5/2} \underbrace{\int_0^\infty \frac{x^{3/2}\,dx}{z^{-1}e^x - 1}}_{\text{a number}}$$

~ 1 (no T dependence)

$$\propto T^{5/2}$$

$$C_V = \left.\frac{\partial E}{\partial T}\right|_V \propto T^{3/2}.$$

At $T = T_c$ solving the integrals for $\langle \bar{E} \rangle$ you can find that $\frac{C_V(T_c)}{kT} \simeq 1.95 > 1.5$



discontinuous first derivative at the Bose - Einstein critical temperature.

The cumulant expansion (or cluster expansion).

Kardar (Ch. 5):

In the lecture of 8/27 we saw that (Kardar Ch. 2):

$$\langle F(x) \rangle = \int_{-\infty}^{\infty} dx\, p(x)\, F(x)$$

where $p(x)$ is a probability distribution.

then the moments of $p(x)$ are given by

$$m_n = \langle x^n \rangle = \int dx\, p(x)\, x^n$$

We also found the characteristic function of $p(x)$ given by its Fourier transform.

$$\tilde{p}(x) = \langle e^{-ikx} \rangle = \int dx\, p(x)\, e^{-ikx} \quad (1)$$

Since

$$p(x) = \frac{1}{2\pi} \int dk\, \tilde{p}(k)\, e^{ikx} \quad \text{(antitransform)}$$

We see that

$$\tilde{p}(k) \overset{(1)}{=} \langle e^{-ikx} \rangle = \langle \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} x^n \rangle =$$

$$(2) \quad = \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} \underbrace{\langle x^n \rangle}_{m_n}$$

$\tilde{p}(k)$ can be expanded in terms of m_n.

Also:

$$e^{ikx_0}\tilde{p}(k) = \langle e^{-ik(x-x_0)} \rangle =$$

$$= \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} \underbrace{\langle (x-x_0)^n \rangle}$$

$\langle x^n \rangle_c$: cumulants.

Notice that

$\langle (x-x_0)^2 \rangle = \langle x^2 \rangle_c$ for example.

Also:

$$\ln \tilde{p}(k) \overset{②}{=} \ln\left(1+\sum_{n=1}^{\infty}\frac{(-ik)}{n!}\langle x^n\rangle\right) =$$

$$\ln(1+\varepsilon)=\sum_{n=1}^{\infty}\frac{(-1)^{n+1}\varepsilon^n}{n}$$

$$= \sum_{n=1}^{\infty}\frac{(-ik)^n}{n!}\langle x^n\rangle_c$$

Shown in 8/27 lecture.

Now let's apply this concept to the problem of the non-ideal classical gas.

Non-ideal Gas

$$\mathcal{H}_N = \sum_{i=1}^{N} \frac{\bar{p}_i^2}{2m} + V(\bar{r}_1, \ldots, \bar{r}_N)$$

$$Z = \frac{1}{N!} \int \prod_{i=1}^{N} \left(\frac{d^3p_i \, d^3r_i}{h^3} \right) e^{-\beta \sum_{i=1}^{N} \frac{\bar{p}_i^2}{2m}} e^{-\beta V(\{\bar{r}_i\})}$$

$$\equiv \underbrace{Z_0(T,V,N)}_{\text{partition function of the ideal gas}} \underbrace{\left\langle e^{-\beta V(\bar{r}_1, \ldots \bar{r}_N)} \right\rangle^0}_{Z_U}$$

partition function of the ideal gas

Z_U : average value of $e^{-\beta U}$ using Z_0 as probability.

Where we have defined

$$\langle G \rangle^0 = \frac{\int \cdots \int G \; Z_0 \, d^3r_1 \ldots d^3r_N}{Z_0}$$

expectation value of operator G with the probability distribution $e^{-\beta \sum \frac{\vec{p}_i^{\,2}}{2m}}$ of the non-interacting ideal gas.

then

$$Z = Z_0 \langle e^{-\beta U(\bar{r}_1 \ldots \bar{r}_N)} \rangle^0$$

$$\ln Z = \ln Z_0 + \ln \langle e^{-\beta U(\bar{r}_1, \ldots, \bar{r}_N)} \rangle^0 =$$

$$\stackrel{3}{=} \ln Z_0 + \sum_{n=1}^{\infty} \frac{(-\beta)^n}{n!} \langle U^n \rangle_c$$

Notice that the moments of U are given by:

$$\langle U^n \rangle^0 = \int \left(\prod_{i=1}^{N} \frac{d^3 r_i}{V} \right) U^n(\bar{r}_1, \ldots \bar{r}_N)$$

Then the expectation value of any operator O can be obtained as:

$$\langle O \rangle = \frac{1}{N!\,Z} \int \prod_{i=1}^{N} \left(\frac{d^3 p_i \, d^3 r_i}{h^3} \right) e^{-\beta \sum_i \frac{\bar{p}_i^2}{2m}}$$

$$e^{-\beta V(\bar{r}_1 \ldots \bar{r}_N)}\, O = \frac{\langle O\, e^{-\beta V(\bar{r}_1 \ldots \bar{r}_N)} \rangle^0}{\langle e^{-\beta V(\bar{r}_1 \ldots \bar{r}_N)} \rangle^0}$$

Notice that $\langle O \rangle$ is evaluated for the non-ideal gas.

Cluster expansion.

Non-ideal gas:

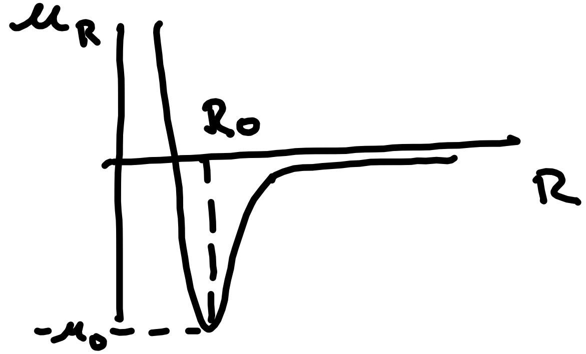
$$Z = \underbrace{\frac{1}{N!\,h^3}\int \prod_{i=1}^{N} d^3p_i\, e^{-\beta \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m}}}_{\frac{Z_0}{V^N}} \int \prod_{i=1}^{N} d^3r_i\, e^{-\beta U(\{\vec{r}_i\})}$$

$$= Z_0 \underbrace{\frac{1}{V^N}\int \prod_{i=1}^{N} d^3r_i\, e^{-\beta U(\{\vec{r}_i\})}}_{Z_U}$$

We will assume that

$R = |\bar{r}_i - \bar{r}_j|$

$$U = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} u_{ij}$$



$$\therefore \quad Z_U = \frac{1}{V^N} \int \prod_{i=1}^{N} d^3 r_i \prod_{\substack{\text{pairs} \\ \langle ij \rangle}} e^{-\beta u_{ij}} \qquad (4)$$

Since $u_{ij} \ll 1 \Rightarrow e^{-\beta u_{ij}} \approx 1 + \underbrace{f_{ij}}_{\text{deviations from 1 of the exponential}}$

Now

$$\prod_{\langle i,j\rangle} e^{-\beta u_{ij}} \simeq \prod_{\langle i,j\rangle} (1 + f_{ij}) =$$

$$= 1 + \sum_{\langle i,j\rangle} f_{ij} + \sum_{\substack{\langle i,j\rangle \neq \langle k,l\rangle \\ \text{different pairs}}} f_{ij} f_{kl} + \cdots \quad (5)$$

Plugging (5) in (4):

$$Z_v = \frac{1}{V^N} \int \prod_i d^3 r_i \left(1 + \sum_{\langle i,j \rangle} f_{ij} + \sum_{\langle i,j \rangle \neq \langle k,l \rangle} f_{ij} f_{kl} + \dots \right.$$

$$\simeq \frac{1}{V^N} \overbrace{\int \prod_i d^3 r_i}^{V^N} + \frac{1}{V^N} \int \prod_i d^3 r_i \sum_{\langle i,j \rangle} f_{ij} +$$

$$+ \frac{1}{V^N} \int \prod_i d^3 r_i \sum_{\langle i,j \rangle \neq \langle k,l \rangle} f_{ij} f_{kl} + \dots$$

$$\simeq 1 + \frac{1}{V^N} \underbrace{\int \prod_i d^3 r_i \sum_{\langle i,j \rangle} f_{ij}}_{*} + \dots$$

Let's consider (*) :

$$\frac{1}{V^N}\int \prod_k d^3r_k \sum_{\langle i,j\rangle} f_{ij} = \frac{V^{N-2}}{V^N}\sum_{\langle i,j\rangle}\int d^3r_i\, d^3r_j\, f_{ij}$$

$$= \frac{1}{V^2}\,\frac{N(N-1)}{2}\underbrace{\int d^3r_i\, d^3r_j\, f_{ij}}_{\text{independent of } i,j} =$$

$$= \frac{1}{V^2}\,\frac{N(N-1)}{2}\int d^3r_1\, d^3r_2\, f_{12}$$

Graphic representation:

 $\equiv \frac{1}{2}\frac{N(N-1)}{V^2}\int d^3r_1\, d^3r_2\, f_{12}$

Also

 $\equiv \frac{1}{V}\int d^3r_1 = \frac{V}{V} = 1$

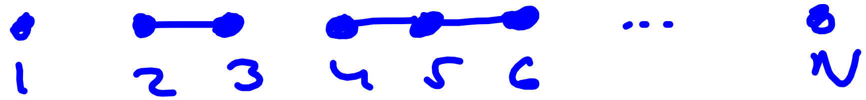
Rules to translate a graph to an integral:

- 1) Number the dots starting with 1 for each dot i, up to N (can be very large!).
- 2) Write down the expression $\frac{1}{V}\int d^3r_i$ for each dot.

- 3) Multiply N for the first dot, $(N-1)$ for the second, etc.

- 4) For a line connecting dots i and j write down a factor f_{ij}.

Example:



$$\frac{N!}{V^N}\left(\int d^3r_1\right)\int d^3r_2\, d^3r_3\, f_{23}\cdot$$

$$\cdot\left(\int d^3r_4\, d^3r_5\, d^3r_6\, f_{45}\, f_{56}\right)\left(\int d^3r_7\right)\cdots\left(\int d^3r_N\right)$$

- 5) Correct by a symmetry factor (to be continued).