

Worksheet 11 - Solutions

1) Fermi-Dirac Distribution $T \rightarrow \infty$

we have that the Fermi-Dirac distribution

$$\langle n_i \rangle = \frac{1}{e^{\beta(\epsilon_i - \mu)} + 1}$$

So, in the limit $T \rightarrow \infty ; \beta \rightarrow 0$

$$\langle n_i \rangle \Big|_{\beta \rightarrow 0} = \frac{1}{e^0 + 1} = \frac{1}{1 + 1} = \frac{1}{2}$$

In this limit, we have that the system is in the maximum ignorance limit. As the fermions occupation can only be 0 or 1, the system density matrix has 50% of statistical weight on each state (0 and 1). Saying that the two states have the same probability is equivalent to the statement of maximum ignorance.

2) Fermi-Dirac Distribution.

The number of ways to distribute N_e identical particles among G_e states with no more than 1 particle per state

$$W_e = \frac{G_e!}{N_e! (G_e - N_e)!} \quad S = k_B \ln (W_e)$$

Simply, using the Stirling formula, we can get

$$S = k_B \sum_e \left[G_e \ln (G_e) - N_e \ln (N_e) - (G_e - N_e) \ln (G_e - N_e) \right].$$

The occupation number goes as $N_e/G_e = \langle n_e \rangle$.

$$S = k_B \sum_e \left[G_e \left(\ln (G_e) - \frac{N_e \ln (N_e)}{G_e} - \left(1 - \frac{N_e}{G_e}\right) \ln \left(G_e \left(1 - \frac{N_e}{G_e}\right)\right) \right) \right]$$

$$S = k_B \sum_e \left[G_e \left(\ln (G_e) - \langle n_e \rangle \ln (\langle n_e \rangle) - \left(1 - \langle n_e \rangle\right) \ln \left(1 - \langle n_e \rangle\right) \right. \right. \\ \left. \left. - \left(1 - \langle n_e \rangle\right) \ln (G_e) \right) \right]$$

$$= -k_B \sum_i \left[G_C (\langle n_i \rangle \ln(n_i) + (1-\langle n_i \rangle) \ln(1-\langle n_i \rangle)) - \langle n_i \rangle \ln(G_C) \right]$$

$$= -k_B \sum_i \left[G_C (\langle n_i \rangle \ln(\langle n_i \rangle) + (1-\langle n_i \rangle) \ln(1-\langle n_i \rangle)) \right]$$

in the case of ignoring spins, then $G_C = 1$.

3) Identical particle pair.
A two particle wave function is constructed from one particle states k_1, k_2
Given symmetries due to the statistics:

Bosons

$$|k_1, k_2\rangle = \begin{cases} (|k_1\rangle |k_2\rangle + |k_2\rangle |k_1\rangle)/\sqrt{2} & \text{for } k_1 \neq k_2 \\ |k_1\rangle |k_2\rangle & \text{for } k_1 = k_2 \end{cases}$$

So, the partition function for Bosons goes

$$Z_{2\text{-particles}}^{\text{Bosons}} = \text{Tr} (e^{-\beta H}) = \sum_{k_1, k_2} \langle k_1, k_2 | e^{-\beta H} | k_1, k_2 \rangle$$

$$\begin{aligned} &= \sum_{k_1 \neq k_2} \frac{\langle k_1 | \langle k_2 | + \langle k_2 | \langle k_1 |}{\sqrt{2}} e^{-\beta H} \frac{|k_1\rangle |k_2\rangle + |k_2\rangle |k_1\rangle}{\sqrt{2}} \\ &\quad + \sum_{k_1 = k_2} \langle k_1 | \langle k_1 | e^{-\beta H} | k_1 \rangle | k_1 \rangle \\ &= \frac{1}{2} \sum_{k_1 \neq k_2} \exp \left(-\frac{\beta \hbar^2}{2m} (k_1^2 + k_2^2) \right) + \sum_{k_1} \exp \left(-\frac{2\beta \hbar^2 k^2}{2m} \right) \\ &= \frac{1}{2} \sum_{k_1, k_2} \exp \left(-\frac{\beta \hbar^2}{2m} (k_1^2 + k_2^2) \right) + \frac{1}{2} \sum_{k_1} \exp \left(-\frac{2\beta \hbar^2 k^2}{2m} \right) \\ &= \frac{1}{2} \left[Z_1(m) + Z_1 \left(\frac{m}{2} \right) \right]. \end{aligned}$$

And for Fermions

$$\begin{aligned}
 Z_{2\text{-particles}}^{\text{Fermions}} &= \text{Tr} \left(e^{-\beta H} \right) = \sum_{k_1 k_2} \langle k_1, k_2 | e^{-\beta H} | k_1, k_2 \rangle_F \\
 &= \sum_{k_1 k_2} \frac{\langle k_1 | \langle k_2 | - \langle k_2 | \langle k_1 |}{\sqrt{2}} e^{-\beta H} \frac{| k_1 \rangle | k_2 \rangle - | k_2 \rangle | k_1 \rangle}{\sqrt{2}} \\
 &= \frac{1}{2} \sum_{k_1 k_2} \left[\langle k_1 | \langle k_2 | e^{-\beta H} | k_1 \rangle | k_2 \rangle - \cancel{\langle k_1 | \langle k_2 | e^{-\beta H} | k_2 \rangle | k_1 \rangle} \right. \\
 &\quad \left. - \cancel{\langle k_2 | \langle k_1 | e^{-\beta H} | k_1 \rangle | k_2 \rangle} + \cancel{\langle k_2 | \langle k_1 | e^{-\beta H} | k_2 \rangle | k_1 \rangle} \right] \\
 &= \frac{1}{2} \sum_{k_1, k_2} \exp \left(-\frac{\beta \hbar^2}{2m} (k_1^2 + k_2^2) \right) - \frac{1}{2} \sum_n \exp \left(-\frac{2\beta \hbar^2 k^2}{2m} \right) \\
 &= \frac{1}{2} \left[Z_1^2(m) - Z_1 \left(\frac{m}{2} \right) \right].
 \end{aligned}$$

2) If the system is non-degenerate, the correction term is way smaller than the classical one,

$$\begin{aligned}
 \ln(Z_2^\pm) &= \ln \left\{ \left[Z_1^2(m) \pm Z_1 \left(\frac{m}{2} \right) \right] / 2 \right\} \\
 &= 2 \ln(Z_1^2(m)) + \underbrace{\ln \left[1 \pm \frac{Z_1(m/2)}{Z_1^2(m)} \right]}_{\ln(1 \pm x) \xrightarrow{x \rightarrow 0} \pm x - \frac{x^2}{2} \pm \frac{x^3}{3} \dots} - \ln(2)
 \end{aligned}$$

Taking the Taylor expansion around 0 to first order

$$\approx 2 \ln(Z_1^2(m)) \pm \frac{Z_1(m/2)}{Z_1^2(m)} - \ln(2)$$

Now, using

$$Z_1(m) = \frac{V}{\lambda(m)^3} \rightarrow \lambda(m) = \frac{h}{\sqrt{2\pi m k_B T}}$$

And using that

$$Z_2^{\text{classical}} = \frac{1}{2} Z_1(m)^2 \rightarrow \ln(Z_2^{\text{classical}}) = 2 \ln(Z_1(m)) - \ln(2)$$

we can write

$$\ln Z_2^{\pm} \approx \ln Z_2^{\text{classical}} \pm \frac{\lambda(m)}{V} \left(\frac{\lambda(m)}{\lambda(m/2)} \right)^3$$

$$= \ln Z_2^{\text{classical}} \pm 2^{-3/2} \frac{\lambda^3(m)}{V}$$

$$\downarrow$$

$$\Delta \ln Z^{\pm} = \ln Z_2^{\pm} - \ln Z_2^{\text{classical}} = \pm 2^{-3/2} \frac{\lambda^3(m)}{V} = \pm 2^{-3/2} \frac{h^3 \rho^{3/2}}{\sqrt{(2\pi m)^{3/2}}}$$

Thus, the change in energy

$$\Delta E^{\pm} = -\partial_{\beta} \Delta \ln Z_2^{\pm} = \pm \frac{2^{-3/2} h^3}{\sqrt{(2\pi m)^{3/2}}} \partial_{\beta} \beta^{3/2}$$

$\underbrace{}_{\frac{3}{2} \beta^{3/2-1}}$

$$= \pm \frac{3}{2^{5/2}} \frac{1}{\beta} \frac{\lambda^3(m)}{V}$$

and the corrections on the heat capacity

$$\Delta C_V^{\pm} = \frac{\partial E}{\partial T} \Big|_V = \pm \frac{3}{2^{5/2}} \frac{h^3}{\sqrt{(2\pi m)^{3/2}}} \partial_T \left(\left(\frac{1}{k_B T} \right)^{1/2} \right)$$

$$\partial_T \left(\frac{1}{k_B T} \right)^{1/2} = \frac{1}{k_B^{1/2}} \partial_T T^{-1/2}$$

$$= \frac{1}{k_B^{1/2}} (-1/2) T^{-1/2-1}$$

$$= \pm \frac{3}{2^{7/2}} k_B \frac{h^3 \beta^{3/2}}{\underbrace{\sqrt{(2\pi m)^{3/2}}}_{\lambda^3(m)/V}}$$

3) The approximation breaks if the corrections are comparable to the first term.

That happens when $\lambda_r \sim \text{size of the Box}$.

$$\lambda_r = \frac{n}{\sqrt{2\pi m k_B T}} \geq L \sim V^{1/3}$$

$$\frac{\hbar^2}{L^2} \geq 2\pi m k_B T$$

$$k_B T \leq \frac{\hbar^2}{2\pi m L^2}$$

4 Generalized ideal Gas.

1) The Grand Potential

let us start from the partition functions.

Fermions:

$$Q_F = \sum_{N=0}^{\infty} e^{\beta \mu N} \sum_{\{n_\nu\}} e^{-\beta \sum_\nu n_\nu \epsilon_\nu} = \prod_\nu \sum_{n_\nu=0}^1 e^{\beta(\mu - \epsilon_\nu)n_\nu} = \prod_\nu [1 + e^{\beta(\mu - \epsilon_\nu)}]$$

Bosons:

$$Q_B = \sum_{N=0}^{\infty} e^{\beta \mu N} \sum_{\{n_\nu\}} e^{-\beta \sum_\nu n_\nu \epsilon_\nu} = \prod_\nu \sum_{\{n_\nu\}} e^{\beta(\mu - \epsilon_\nu)n_\nu} = \prod_\nu [1 - e^{\beta(\mu - \epsilon_\nu)}]^{-1}$$

so, if we take $\eta = 1$ for bosons and $\eta = -1$ for fermions

$$\ln(Q_\eta) = -\eta \sum_\nu \ln[1 - \eta e^{-\beta(\mu - \epsilon_\nu)}]$$

To evaluate this expression, we can change the summation for an integral in d dimensions

$$\sum_N \rightarrow \int d^d N \rightarrow \frac{V}{(2\pi)^d} \int d^d k = \frac{V S_d}{(2\pi)^d} \int k^{d-1} dk$$

where

$$S_d = \frac{2\pi^{d/4}}{(d/2 - 1)!}$$

Then

$$\ln(Q_\eta) = -\eta \frac{\sqrt{S_d}}{(2\pi)^d} \int dk k^{d-1} \ln \left[1 - \eta z e^{\beta(\mu - \epsilon_d)} \right]$$

$$= -\eta \frac{\sqrt{S_d}}{(2\pi)^d} \int dk k^{d-1} \ln \left[1 - \eta z e^{\beta k^s} \right]$$

where $z = e^{-\beta\mu}$ and $\epsilon = |\beta|/k^s$

we can now make a change in variables

$$x = \beta k^s \rightarrow k = \left(\frac{x}{\beta} \right)^{1/s} \quad \text{and} \quad dk = \frac{1}{s} \left(\frac{x}{\beta} \right)^{1/s-1} \frac{dx}{\beta}$$

Hence

$$\ln(Q_\eta) = -\eta \frac{\sqrt{S_d}}{(2\pi)^d} \frac{\beta^{-d/s}}{s} \int dx x^{d/s-1} \ln \left(1 - \eta z e^{-x} \right)$$

$$u = \ln \left(1 - \eta z e^{-x} \right) \quad du = x^{d/s-1} dx$$

$$du = \frac{dx}{1 - \eta z e^{-x}} \times \cancel{\left(/ \eta z e^{-x} \right)} \quad u = s \frac{x}{d} \Big|_0^\infty$$

$$= - \cancel{\eta} \frac{\sqrt{S_d}}{(2\pi)^d} \frac{\beta^{-d/s}}{d} \int dx \frac{x^{d/s}}{1 - \eta z e^{-x}}$$

$$= - \frac{\sqrt{S_d}}{(2\pi)^d} \frac{\beta^{-d/s}}{d} \int dx \frac{x^{d/s}}{\frac{e^{-x}}{z} - \eta}$$

or

$$\ln(Q_\eta) = \frac{\sqrt{S_d}}{(2\pi)^d} \beta^{-d/s} \Gamma\left(\frac{d}{s} + 1\right) f_{\frac{d}{s}+1}^\eta(z)$$

with

$$f_n^\eta(z) = \frac{1}{\Gamma(n)} \int dx \frac{x^{n-1}}{z^{-1} e^x - \eta}$$

In the same context,

$$N = \frac{\partial}{\partial(\beta\mu)} \ln(Q_\eta) \Big|_{\beta} = -\eta \frac{\sqrt{Sd}}{(2\pi)^d} \frac{\beta^{\frac{d}{2}S}}{S} \frac{\partial}{\partial\beta\mu} \int dx x^{\frac{d}{2}S-1} \ln(1-\eta e^{-x})$$

$$= \frac{\sqrt{Sd}}{(2\pi)^d} \frac{\beta^{\frac{d}{2}S}}{S} \int dx \frac{x^{\frac{d}{2}S-1} z e^{-x}}{1-\eta + e^{-x}} = \frac{\sqrt{Sd}}{(2\pi)^d} \frac{\beta^{\frac{d}{2}S}}{S} 2 \int dx \frac{x^{\frac{d}{2}S-1}}{z^{-1}e^{-x}-\eta}$$

so

$$\eta = \frac{N}{V} = \frac{Sd}{(2\pi)^d S} (k_B T)^{\frac{d}{2}S} \Gamma\left(\frac{d}{2}\right) \cdot f_{\frac{d}{2}S}(z)$$

2) The Gas Pressure is given by

$$PV = -k_B T \ln(Q_\eta) = \underbrace{\frac{\sqrt{Sd}}{(2\pi)^d} \frac{(k_B T)^{\frac{d}{2}+1}}{d}}_{\propto \beta^{-\frac{d}{2}S}} \Gamma\left(\frac{d}{2}+1\right) \cdot f_{\frac{d}{2}S+1}(z)$$

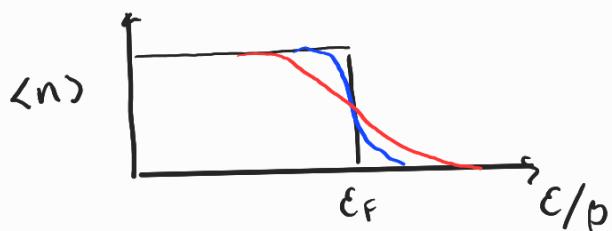
$$E = -\frac{\partial}{\partial\beta} \ln(Q_\eta) \Big|_z = -\frac{d}{S} \frac{\ln(Q_\eta)}{\beta} = -\frac{d}{S} k_B T \ln(Q_\eta)$$

$$\frac{PV}{E} = \frac{S}{d} \rightarrow \text{Same Result}$$

Classically
Obtained.

3) Fermions at low T

$$\frac{1}{e^{\beta(\epsilon-\epsilon_F)+1}} \approx \Theta(\epsilon - \epsilon_F) \rightarrow f_n(z) \approx \frac{(\beta\epsilon_F)^n}{n! \Gamma(n)}$$



So

$$E \approx \frac{\sqrt{S_d}}{(2\pi)^d} \cdot \frac{E_F^{\frac{d}{s}+1}}{d}, \quad PV \approx \frac{\sqrt{S_d}}{(2\pi)^d} \cdot \frac{E_F^{\frac{d}{s}+1}}{S}$$

$$n = \frac{S_d}{(2\pi)^d} \cdot \frac{E_F^{\frac{d}{s}}}{S}$$

So

$$\frac{E}{N} \approx \frac{\sqrt{S_d}}{N(2\pi)^d} \cdot \frac{E_F^{\frac{d}{s}+1}}{d} = \frac{1}{n} \cdot \frac{S_d}{(2\pi)^d} \cdot \frac{E_F^{\frac{d}{s}+1}}{d} \approx \frac{S}{d} E_F \propto n^{\frac{s}{d}}$$

and

$$P \propto E_F^{\frac{d}{s}+1} \propto n^{\frac{s}{d}+1}$$

Bosons

To see if Bose-Einstein Condensation Occurs, we need to check if $z = z_{\max} = 1$, and as $f_{\frac{d}{s}}^+(z)$ is monotonic for $0 \leq z \leq 1$ the maximum value for the right hand side equation for $n = N/V$, goes

$$\frac{S_d}{(2\pi)^{\frac{d}{s}}} (k_B T)^{\frac{d}{s}} \Gamma\left(\frac{d}{s}\right) f_{\frac{d}{s}}^+(1).$$

if this value is larger than n , we can always find $z < 1$ so the equation is satisfied.

So, let us compute $f_{\frac{d}{s}}^+(1)$

$$f_{\frac{d}{s}}^+(z_{\max}=1) = \frac{1}{\Gamma(d/s)} \int dx \frac{x^{d/s}-1}{e^x - 1}$$

The integrand diverges for $x \rightarrow 0$

$$\int_0^c dx \frac{x^{d/s} - 1}{e^x - 1} \approx \underbrace{\int_0^c dx x^{d/s - 2}}$$

converges for $\frac{d}{s} - 1 > -1$
or $d > s$

The condensation occurs for $d > s$

For $d = s = 2$ (2d Gas) the integral diverges log
then No Condensation occurs