Worksheet 11 - Solutions

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

we have that the Fermi-Dirac distribution

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

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

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

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). This probability is equivalent to the statement 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_l identical particles among G_l states with no more than 1 particle per state

$$W_l = \frac{G_l!}{N_l!(G_l - N_l)!} \qquad S = k_B \ln(W)$$

Simply, using the Stirling formula, we can get

$$S = k_B \sum_l \left[G_l \ln(G_l) - N_l \ln(N_l) - (G_l - N_l) \ln(G_l - N_l) \right].$$

The occupation number goes as $N_l / G_l = \langle n_l \rangle$.

$$S = k_B \sum_l \left[G_l \left(\ln(G_l) - \frac{N_l}{G_l} \ln(N_l) - \left(1 - \frac{N_l}{G_l}\right) \ln\left(G_l \left(1 - \frac{N_l}{G_l}\right)\right)\right)\right]$$

$$S = k_B \sum_l \left[G_l \left(\cancel{\ln(G_l)} - \langle n_l \rangle \ln(N_l) - (1 - \langle n_l \rangle) \ln(1 - \langle n_l \rangle) - (\cancel{1} - \langle n_l \rangle) \ln(G_l) \right] \right.$$

$$= -k_B \sum_l \left[G_l \left(\langle n_l \rangle \ln (N_l) + (1 - \langle n_l \rangle) \ln (1 - \langle n_l \rangle) - \langle n_l \rangle \ln (G_l) \right] \right.$$

$$= -k_B \sum_l \left[G_l \left(\langle n_l \rangle \ln (\langle n_l \rangle) + (1 - \langle n_l \rangle) \ln (1 - \langle n_l \rangle) \right) \right]$$

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

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

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

So, the partition function for Bosons goes

$$Z^{\text{Bosons}}_{2\text{-particles}} = \mathrm{Tr}\left(e^{-\beta H} \right) = \sum_{k_1, k_2} {}_B\langle k_1, k_2 | e^{-\beta H} | k_1, k_2 \rangle_B$$

$$= \sum_{k_1 \neq k_2} \frac{\langle k_1 | \langle k_2 | + \langle k_2 | \langle k_1 |}{\sqrt{2}} e^{-\beta H} \frac{|k_1\rangle |k_2\rangle + |k_2\rangle |k_1\rangle}{\sqrt{2}}$$

$$+ \sum_{k_1 = k_2 = k} \langle k | \langle k | e^{-\beta H} |k\rangle |k\rangle$$

$$= \frac{1}{2} \sum_{k_1 \neq k_2} \exp\left(-\frac{\beta \hbar^2}{2m} (k_1^2 + k_2^2) \right) + \sum_k \exp\left(-\frac{2\beta \hbar^2 k^2}{2m} \right)$$

$$= \frac{1}{2} \sum_{k_1, k_2} \exp\left(-\frac{\beta \hbar^2}{2m} (k_1^2 + k_2^2) \right) + \frac{1}{2} \sum_k \exp\left(-\frac{2\beta \hbar^2 k^2}{2m} \right)$$

$$= \frac{1}{2} \left[Z_1^2 (m) + Z_1 \left(\frac{m}{2} \right) \right].$$

And for Fermions

$$Z_{2\text{-particles}}^{\text{Fermions}} = Tr\left(e^{-\beta H}\right) = \sum_{k_1 k_2} {}_F\langle k_1, k_2 | e^{-\beta H} | k_1, k_2 \rangle_F$$

$$= \sum_{k_1 \neq k_2} \frac{\langle k_1 | \langle k_2 | - \langle k_2 | \langle k_1 |}{\sqrt{2}} \, e^{-\beta H} \, \frac{| k_1 \rangle | k_2 \rangle - | k_2 \rangle | k_1 \rangle}{\sqrt{2}}$$

$$= \frac{1}{2} \sum_{k_1 \neq k_2} \langle k_1 | \langle k_2 | e^{-\beta H} | k_1 \rangle | k_2 \rangle - \langle k_1 | \langle k_2 | e^{-\beta H} | k_2 \rangle | k_1 \rangle - \langle k_2 | \langle k_1 | e^{-\beta H} | k_1 \rangle | k_2 \rangle + \langle k_2 | \langle k_1 | e^{-\beta H} | k_2 \rangle | k_1 \rangle$$

$$= \frac{1}{2} \sum_{k_1, k_2} \exp\left(-\frac{\beta \hbar^2}{2m} \left(k_1^2 + k_2^2\right)\right) - \frac{1}{2} \sum_{k} \exp\left(-\frac{2\beta \hbar^2 k^2}{2m}\right)$$

$$= \frac{1}{2} \left[Z_1^2(m) - Z_1\left(\frac{m}{2}\right) \right].$$

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

$$\ln(Z_2^{\pm}) = \ln\left\{ \left[z_1^2(m) \pm z_1\left(\frac{m}{2}\right) \right] / 2 \right\}$$

$$= 2\ln(z_1(m)) + \underbrace{\ln\left[1 \pm \frac{z_1(m/2)}{z_1^2(m)}\right]}_{\ln(1 \pm x) \xrightarrow{x \to 0} \pm x - \frac{x^2}{2} \pm \frac{x^3}{3} \ldots} - \ln(2)$$

Taking the Taylor expansion around 0 to first order

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

Now, using

$$z_1(m) = \frac{V}{\lambda(m)^3} \longrightarrow \lambda(m) = \frac{h}{\sqrt{2\pi m k_B T}}$$

And using that

$$z_2^{\text{classical}} = \frac{1}{2} z_1(m)^2 \longrightarrow \ln\left(z_2^{\text{classical}}\right) = 2\ln(z_1(m)) - \ln(2)$$

we can write

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

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

$$\downarrow$$

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

Thus, the change in energy

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

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

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

and the corrections on the heat capacity

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

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

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

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

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

That happens when $\lambda_T \sim$ Size of the Box.

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

$$\downarrow$$

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

$$\downarrow$$

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

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4 Generalized ideal Gas.

1) The Grand Potential

let us start from the partition functions.

Fermions:

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

Bosons:

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

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

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

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

$$\sum_\nu \longrightarrow \int d^d n \longrightarrow \frac{V}{(2\pi)^d} \int d^d k = \frac{V S_d}{(2\pi)^d} \int k^{d-1} dk$$

where

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

Then

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

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

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

we can now make a change in variables

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

Hence

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

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

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

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

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

or

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

with

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

In the same context,

$$N = \frac{\partial}{\partial(\beta\mu)} \ln(Q_n)\Big|_\beta = -\eta \frac{V S_d}{(2\pi)^d} \frac{\beta^{d/s}}{s} \frac{\partial}{\partial\beta\mu} \int dx\, x^{d/s-1} \ln(1-\eta z e^{-x})$$

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

so

$$n = \frac{N}{V} = \frac{S_d}{(2\pi)^d s} (k_B T)^{d/s} \Gamma\left(\frac{d}{s}\right) \cdot f^{\eta}_{d/s}(z)$$

2) The Gas Pressure is given by

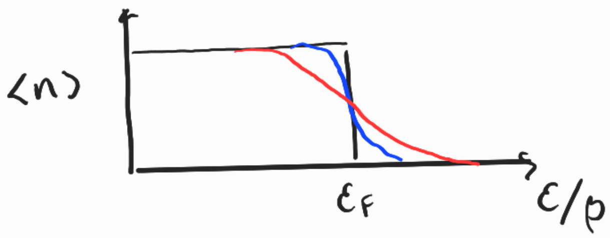
$$PV = \underbrace{-k_B T \ln(Q_\eta)}_{\propto \beta^{-d/s}} = \frac{V S_d}{(2\pi)^d} \frac{(k_B T)^{\frac{d}{s}+1}}{d} \Gamma\left(\frac{d}{s}+1\right) \cdot f_{d/s+1}(z)$$

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

$$\frac{PV}{E} = \frac{s}{d} \longrightarrow \text{Same Result Classically Obtained.}$$

3) Fermions at low T

$$\frac{1}{e^{\beta(\varepsilon-\varepsilon_f)}+1} \approx \Theta(\varepsilon - \varepsilon_F) \longrightarrow f_n(z) \approx \frac{(\beta\varepsilon_F)^n}{n\,\Gamma(n)}$$



So

$$E \approx \frac{V S_d}{(2\pi)^d} \frac{\epsilon_F^{d/s+1}}{d}, \qquad PV \approx \frac{V S_d}{(2\pi)^d} \frac{\epsilon_F^{d/s+1}}{s}$$

$$n = \frac{S_d}{(2\pi)^d} \frac{\epsilon_F^{d/s}}{s}$$

So

$$\frac{E}{N} \approx \frac{\overset{\frac{1}{n}}{V} S_d}{N (2\pi)^d} \frac{\epsilon_F^{d/s+1}}{d} = \frac{1}{n} \frac{S_d}{(2\pi)^d} \frac{\epsilon^{d/s+1}}{d} \approx \frac{s}{d} \epsilon_F \propto n^{s/d}$$

and

$$P \propto \epsilon_F^{d/s+1} \propto n^{s/d+1}$$

Bosons

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

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

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

So, let us compute $f^{+}_{d/s}(1)$

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

The integrand diverges for $x \to 0$

$$\int_0^{\epsilon} dx \, \frac{x^{d/s} - 1}{e^x - 1} \simeq \underbrace{\int_0^{\epsilon} dx \, x^{d/s - 2}}$$

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