KING FAHD UNIVERSITY OF PETROLUIM AND MINERALS
DEPARTMENT OF PHYSICS
PHYS 530 STATISTICAL PHYSICS
FALL 2005
FIRST MAJOR(18/12/2005)
TIME (12:00 P.M. ----- 3:00P.M.)

Answer the following problems. (SHOW YOUR WORK)

1- For Fermi-Dirac statistics:

i- show that the partition function for an ideal electron gas is given by:

$$Z = \prod_{i=1}^{\infty} 1 + e^{-\beta(\varepsilon_i - \mu)} \ ,$$

ii- A simple quantum model of thermionic emission of electrons from a metal surface is to assume a Fermi-Dirac distribution for the electrons in the metal in the form:

$$\langle n_s \rangle = \frac{1}{e^{+\beta\varepsilon_s} + 1}$$

and potential energy step of height (work function φ), which the electrons must surmount in order to escape. Show that this model leads to a thermionic current proportional to $T^{1/2} e^{-\beta\varphi}$.)

2- A system is composed of a large number N of one-dimensional quantum harmonic oscillators whose angular frequencies are distributed over the range $\omega_a \le \omega \le \omega_b$ with a frequency distribution function $f(\omega) = \frac{A}{\omega}$. Calculate the following:

i- The constant A .

ii- The partition function of the system.

iii- The average energy, and find the limit in the high temperature case, i.e. $2k_B T > \hbar\omega$.

iv- The specific heat in above limit.

3- For an ideal Fermi gas, let T_o be the temperature at which the chemical potential of the gas is zero. Find T_o in terms of T_F , the Fermi temperature of the gas..

4- The canonical partition function of an ideal monatomic gas of N non-interacting particles of mass m, enclosed in a container of volume V, is given by: $Z = \frac{V^N}{N!}\lambda^{-3N}$, where $\lambda = \frac{h}{\sqrt{2\pi m k_B T}}$ is the de Broglie wavelength. The equation of the state for a dilute gas of interacting particle is

$$P \approx \frac{Nk_BT}{V}\left[1+\frac{N}{V}B(T)\right]$$

where $B(T)$ is the second Virial coefficient. The partition function of such a gas can be written as:

$$Z_N = \frac{Z}{V^N}Q_N, \qquad Q_N = \int\cdots\int e^{-\beta U} dr_1 \cdots dr_N$$

where Q_N is the configurational integral and U is the sum of all pair interaction potentials, each pair interaction being $u(\boldsymbol{r})$, where $\boldsymbol{r}$ is the relative spacing. All triple and higher order collisions, and also correlations between pairs are ignored.

i- Show that the partition function is:

$$Z_N = Z\left\{1+\frac{N(N-1)}{2V}\int\left(e^{-\beta u(\boldsymbol{r})}-1\right)d\boldsymbol{r}\right\}$$

ii- Derive the equation of state with the Virial coefficient

$$B(T) = -\frac{1}{2}\int\left(e^{-\beta u(\boldsymbol{r})}-1\right)d\boldsymbol{r}$$

and briefly discuss the validity of the various steps.

iii- Consider the interaction potential u for the model of hard sphere is given by:

$$u = \begin{cases} \infty, & 0 \le r \le r_o \\ 0, & r > r_o \end{cases}$$

where r_o is the radius of the molecule. Sketch the Mayer *f*-function and calculate the second Virial coefficient. Briefly discuss your result.

Solve one of the following two problems:

1- Consider a system of two non-interacting, identical particles which may occupy any of the three energy levels

$$\varepsilon_n = n\varepsilon, \qquad\qquad n = 0, 1, \text{ and } 2.$$

The lowest energy level, $\varepsilon_0 = 0$, is doubly degenerate. Suppose that the system is in thermal equilibrium at temperature T. Determine the partition function and the mean energy of the system if:

i- the particles obey Fermi-Dirac statistics,

ii- the particles obey Bose-Einstein statistics.

iii- Determine the high temperature $\lim_{T \to \infty}$ of the mean energy for each of the above two cases. Comparing the final results, what can you conclude about the behavior of the fermions and bosons in this limit?

2- Consider a system of ***two*** non-interacting and identical particles in a volume V. Each particle has three accessible energy levels $\varepsilon_1 = 0$, $\varepsilon_2 = 1\varepsilon$, and $\varepsilon_3 = 2\varepsilon$. If the particles obey Bose-Einstein statistics:

i- determine the **partition function,**

ii- determine **the mean occupation number** $\overline{n_1}$ of the first quantum state,

iii- determine the low temperature limit of $\overline{n_1}$.

Physics 530 Second major

Formula sheet

<u>Fall Semester 2005-2006 (Term 051)</u>

$$S = -\left(\frac{\partial F}{\partial T}\right)_{V,N}, \quad T = \left(\frac{\partial F}{\partial S}\right)_{V,N}, \quad P = -\left(\frac{\partial F}{\partial V}\right)_{N,T}, \quad C_v = \left(\frac{\partial U}{\partial T}\right)_{N,V}$$

$$S = Nk\left[\ln\left(\frac{V}{N}\right) + \frac{3}{2}\ln\left(\frac{2\pi mkT}{h^2}\right) + \frac{5}{2}\right] \qquad g(\varepsilon)d\varepsilon = g_s\frac{2\pi V}{h^3}(2m)^{3/2}\varepsilon^{1/2}d\varepsilon$$

$$S = k\ln w, \quad P_r = \frac{1}{Z}e^{-\beta E_{er}}, \quad <n_i> = -\frac{1}{\beta}\frac{\partial \ln Z}{\partial \varepsilon_i} \qquad <\varepsilon> = -\frac{\partial \ln Z}{\partial \beta} \qquad Z_{sp} = \sum_{n=0}^{\infty} g_i e^{-\beta\varepsilon_i}$$

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}, \quad -1 < x < 1 \qquad \text{Stirling's formula: } N! = N\ln N - N$$

Integrals

$$\int_0^\infty x^n e^{-ax}dx = \frac{n!}{a^{n+1}}, \qquad n > 1, 2, 3, \cdots, \quad a > 0$$

$$\int_0^\infty e^{-ax}dx = \frac{1}{a}, \quad \int_0^\infty xe^{-ax}dx = \frac{1}{a^2}, \quad \int_0^\infty x^2e^{-ax}dx = \frac{2}{a^3}, \quad \int_{-\infty}^\infty e^{-ax^4}dx = \frac{2\Gamma(5/2)}{a^{1/4}}$$

$$\int_0^\infty x^{2n+1}e^{-ax^2}dx = \frac{n!}{2a^{n+1}}, \qquad n > 1, 2, 3, \cdots, \quad a > 0$$

$$\int_0^\infty x^{2n}e^{-ax^2}dx = \frac{1.3.5....(2n-1)}{2^{n+1}a^n}\sqrt{\frac{\pi}{a}}. \qquad n > 1, 2, 3, \cdots, \quad a > 0$$

$$\int_0^\infty \frac{x^{1/2}}{e^x - 1}dx = 2.612\frac{\sqrt{\pi}}{2}, \quad \int_0^\infty \frac{x^{1/2}}{e^x + 1}dx = 0.678, \quad \int_0^\infty \frac{x^3}{e^x - 1}dx = \frac{\pi^4}{15}, \quad \int_0^\infty \frac{x^4e^x}{(e^x - 1)^2}dx = \frac{4\pi^4}{15}$$

$\int_{-\infty}^\infty e^{-ax^2}dx = \sqrt{\frac{\pi}{a}}$	$\int_0^\infty xe^{-ax^2}dx = \frac{1}{2a}$
$\int_{-\infty}^\infty x^2e^{-ax^2}dx = \frac{1}{2a}\sqrt{\frac{\pi}{a}}$	$\int_0^\infty x^3e^{-ax^2}dx = \frac{1}{2a^2}$
$\int_{-\infty}^\infty x^4e^{-ax^2}dx = \frac{3}{4a^2}\sqrt{\frac{\pi}{a}}$	$\int_0^\infty x^5e^{-ax^2}dx = \frac{1}{a^3}$

1-i-

Consider the situation where the mean occupation number of a given state is independent on the mean occupation numbers of the other states. In particular, we consider the situation where the states obey the Pauli exclusion principle. That is, a particular possible state will be either occupied or unoccupied, so that $N_s = 0$ or 1.

$$Z = \sum_{N_1=0}^{1} \sum_{N_2=0}^{1} \cdots e^{-\beta \sum_s N_s \varepsilon_s} = \sum_{N_1=0}^{1} \sum_{N_2=0}^{1} \cdots e^{-\beta (N_1 \varepsilon_1 + N_2 \varepsilon_2 + \cdots)}$$

$$= \left\{ \sum_{N_1=0}^{1} e^{-\beta N_1 \varepsilon_1} \right\} \left\{ \sum_{N_2=0}^{1} e^{-\beta N_2 \varepsilon_2} \right\} \cdots = \prod_{s=0}^{\infty} \left\{ 1 + e^{-\beta \varepsilon_s} \right\},$$

ii- See Pathria 8.3 A.

2

A system is composed of a large number N of one-dimensional quantum harmonic oscillators whose angular frequencies are distributed over the range $w_a \le w \le w_b$ with a frequency distribution function $f(w) = \frac{A}{w}$. Calculate the following:

a. The constant A.
b. The partition function of the system.
c. The average energy, and find the limit in the high temperature case, i.e. $2kT >> \hbar w$.
d. The specific heat in above limit.

Answer:

(a).

$$N = \int_{w_a}^{w_b} f(w)dw = A\int_{w_a}^{w_b} \frac{dw}{w} = A\ln(\frac{w_a}{w_b}) \Rightarrow A = \frac{N}{\ln(\frac{w_a}{w_b})}$$

(b) In quantum mechanics, since the energy levels is $\epsilon_n = (n + \frac{1}{2})h\nu$, the partition function is given by

$$Z_1 = \sum_{n=0}^{\infty} e^{-\beta\epsilon_n} = e^{-a}\sum_{n=0}^{\infty}\left\{e^{-2a}\right\}^n$$

$$= \frac{e^{-a}}{1-e^{-2a}} = \frac{1}{e^{a}-e^{-a}} = (2\sinh a)^{-1}$$

where $a = \frac{\hbar w}{2kT}$.

(c).

$$E_w = -\frac{\partial \ln Z_1}{\partial \beta} = \frac{\hbar w}{2}\coth(a)$$

$$E = \int_{w_a}^{w_b} f(w)E_w dw = \frac{A\hbar}{2}\int_{w_a}^{w_b} \coth(\frac{\beta\hbar w}{2})dw = \frac{A}{\beta}\ln[\frac{\sinh(\frac{\beta\hbar w_a}{2})}{\sinh(\frac{\beta\hbar w_b}{2})}]$$

$$\overline{E} = \frac{E}{N} = \frac{1}{\beta\ln(\frac{w_a}{w_b})}\ln[\frac{\sinh(\frac{\beta\hbar w_a}{2})}{\sinh(\frac{\beta\hbar w_b}{2})}]$$

$$\cong kT \qquad\qquad (2kT >> \hbar w)$$

(d).

$$C_v = k$$

$$N = \int_0^\infty \frac{2\pi g_s (2m)^{3/2} v}{h^3} \frac{\epsilon^{1/2} \, d\epsilon}{e^{\beta(\epsilon-\mu)} + 1}$$

where $\beta = \frac{1}{kT}$, and $z = e^{\beta\mu}$, and μ is the chemical potential.

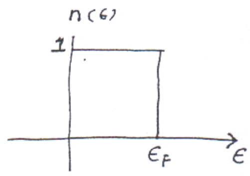
Suppose at $T = T_0 = \frac{1}{k\beta_0}$, $\mu = 0$, Then

$$N = \int_0^\infty \frac{2\pi g_s v (2m)^{3/2}}{h^3} \frac{\epsilon^{1/2} \, d\epsilon}{e^{\beta_0 \epsilon} + 1}$$

$$= \frac{2\pi g_s v (2m)^{3/2}}{h^3} \int_0^\infty \frac{\epsilon^{1/2} d\epsilon}{e^{\beta_0 \epsilon} + 1}$$

$$= \frac{2\pi g_s v (2m)^{3/2}}{h^3 \beta_0^{3/2}} \underbrace{\int_0^\infty \frac{x^{1/2} dx}{e^x + 1}}_{0.678}$$

$$\therefore \boxed{N = \frac{2\pi g_s v (2m)^{3/2}}{h^3 \beta_0^{3/2}} 0.678} \quad (1)$$



On the other hand consider the Fermi gas at $T = 0$ where it is completely degenerate

$$n(\epsilon) = \begin{cases} 1 & \epsilon < \epsilon_F \\ 0 & \epsilon > \epsilon_F \end{cases}$$

$$\therefore N = \int_0^{\epsilon_F} \frac{2\pi g_s v (2m)^{3/2}}{h^3} \epsilon^{1/2} \, d\epsilon$$

$$\boxed{N = \frac{2\pi g_s v (2m)^{3/2}}{h^3} \frac{2}{3} \epsilon_F^{3/2}} \quad (2)$$

T_F is defined such that $\epsilon_F = kT_F \equiv 1/\beta_F$

By comparing (1) and (2), we have.

$$\frac{2}{3} \epsilon_F^{3/2} = 0.678 / \beta_0^{3/2}$$

$$\therefore \frac{2}{3} T_F^{3/2} = 0.678 \, T_0^{3/2}$$

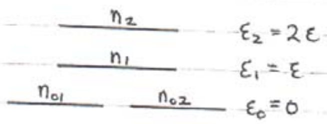
$$\therefore \left(\frac{T_0}{T_F}\right)^{3/2} = 0.983 \quad \sim \quad \frac{T_0}{T_F} = (0.983)^{2/3}$$

$$\therefore \boxed{T_0 = 0.9886 \, T_F}$$

4- See my notes

5-

Energy levels:



Occupation #'s : $\sum_r n_r = n_{01} + n_{02} + n_1 + n_2 = 2$

Consider a canonical ensemble of systems. The partition function is given by

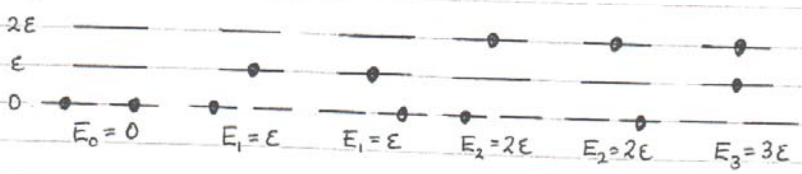
$$Z(V,T) = \sum_{n_{01}, n_{02}, n_1, n_2} e^{-\beta(n_{01}\varepsilon_0 + n_{02}\varepsilon_0 + n_1\varepsilon_1 + n_2\varepsilon_2)}$$

$$= \sum_{E_r} g(E_r)\, e^{-\beta E_r}$$

↑ Degeneracy of energy level E_r

↑ Sum over energy levels E_r of the system

a) Fermi-Dirac statistics:



⇒ The partition function:

$$Z(V,T) = e^{-\beta E_0} + 2e^{-\beta E_1} + 2e^{-\beta E_2} + e^{-\beta E_3}$$

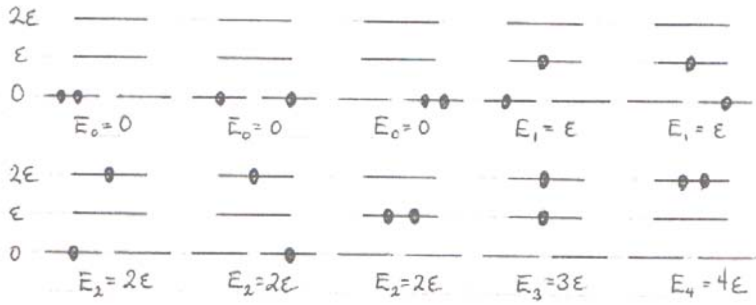
$$= 1 + 2e^{-\beta\varepsilon} + 2e^{-2\beta\varepsilon} + e^{-3\beta\varepsilon}$$

The mean energy: $\bar{E} = -\frac{\partial}{\partial\beta}\ln Z = -\frac{1}{Z}\frac{\partial Z}{\partial\beta}$

$$\Rightarrow \bar{E} = \frac{2\varepsilon e^{-\beta\varepsilon} + 4\varepsilon e^{-2\beta\varepsilon} + 3\varepsilon e^{-3\beta\varepsilon}}{1 + 2e^{-\beta\varepsilon} + 2e^{-2\beta\varepsilon} + e^{-3\beta\varepsilon}}$$

$$\Rightarrow \quad \bar{E} = \frac{\varepsilon e^{-\beta\varepsilon}(2+4e^{-\beta\varepsilon}+3e^{-2\beta\varepsilon})}{1+2e^{-\beta\varepsilon}+2e^{-2\beta\varepsilon}+e^{-3\beta\varepsilon}}$$

b) Bose-Einstein statistics:



$\Rightarrow$ The partition function:

$$Z(V,T) = 3e^{-\beta E_0} + 2e^{-\beta E_1} + 3e^{-\beta E_2} + e^{-\beta E_3} + e^{-\beta E_4}$$

$$= 3+2e^{-\beta\varepsilon}+3e^{-2\beta\varepsilon}+e^{-3\beta\varepsilon}+e^{-4\beta\varepsilon}$$

$$\Rightarrow \quad \bar{E} = -\frac{\partial}{\partial\beta}\ln Z = -\frac{1}{Z}\frac{\partial Z}{\partial\beta}$$

$$= \frac{2\varepsilon e^{-\beta\varepsilon}+6\varepsilon e^{-2\beta\varepsilon}+3e^{-3\beta\varepsilon}+4e^{-4\beta\varepsilon}}{3+2e^{-\beta\varepsilon}+3e^{-2\beta\varepsilon}+e^{-3\beta\varepsilon}+e^{-4\beta\varepsilon}}$$

$$= \frac{\varepsilon e^{-\beta\varepsilon}(2+6e^{-\beta\varepsilon}+3e^{-2\beta\varepsilon}+4e^{-3\beta\varepsilon})}{3+2e^{-\beta\varepsilon}+3e^{-2\beta\varepsilon}+e^{-3\beta\varepsilon}+e^{-4\beta\varepsilon}}$$

d) High temperature limit: $T \to \infty \Rightarrow \beta \to 0$
$\Rightarrow e^{-\beta\varepsilon} \to 1$

Fermions: $\bar{E} \xrightarrow[\beta\to 0]{} \frac{9\varepsilon}{6} = \frac{3}{2}\varepsilon$

Bosons: $\bar{E} \xrightarrow[\beta\to 0]{} \frac{15\varepsilon}{10} = \frac{3}{2}\varepsilon$

Boltzmann particles: $\bar{E} \xrightarrow[\beta\to 0]{} \frac{24\varepsilon}{16} = \frac{3}{2}\varepsilon$

In the high temperature limit fermions and bosons behave as classical Boltzmann particles.

Energy levels:

n_3 — $\varepsilon_3 = 2\varepsilon$
n_2 — $\varepsilon_2 = \varepsilon$
n_1 — $\varepsilon_1 = 0$

Occupation #'s: $\sum_r n_r = n_1 + n_2 + n_3 = 2$

Bose-Einstein statistics:

n_1	2	1	1	0	0	0
n_2	0	1	0	2	1	0
n_3	0	0	1	0	1	2

$\Rightarrow$ Partition function:

$$Z(T,V,N) = \sum_{n_1,n_2,n_3} e^{-\beta(n_1\varepsilon_1 + n_2\varepsilon_2 + n_3\varepsilon_3)}$$
$$= e^{-2\beta\varepsilon_1} + e^{-\beta(\varepsilon_1+\varepsilon_2)} + e^{-\beta(\varepsilon_1+\varepsilon_3)} + e^{-2\beta\varepsilon_2} + e^{-\beta(\varepsilon_2+\varepsilon_3)} + e^{-2\beta\varepsilon_3}$$
$$= 1 + e^{-\beta\varepsilon} + e^{-2\beta\varepsilon} + e^{-2\beta\varepsilon} + e^{-3\beta\varepsilon} + e^{-4\beta\varepsilon}$$
$$= 1 + e^{-\beta\varepsilon} + 2e^{-2\beta\varepsilon} + e^{-3\beta\varepsilon} + e^{-4\beta\varepsilon}$$
$$= \left(1 + e^{-2\beta\varepsilon}\right)^2 + e^{-\beta\varepsilon}\left(1 + e^{-2\beta\varepsilon}\right)$$
$$= \underline{\left(1 + e^{-2\beta\varepsilon}\right)\left(1 + e^{-\beta\varepsilon} + e^{-2\beta\varepsilon}\right)}$$

a) $$\bar{n}_1 = -\frac{1}{\beta}\left(\frac{\partial \ln Z}{\partial \varepsilon_1}\right)_{T,\varepsilon_2,\varepsilon_3}$$
$$= \frac{2e^{-2\beta\varepsilon_1} + e^{-\beta(\varepsilon_1+\varepsilon_2)} + e^{-\beta(\varepsilon_1+\varepsilon_3)}}{Z}$$
$$= \underline{\frac{2 + e^{-\beta\varepsilon} + e^{-2\beta\varepsilon}}{\left(1+e^{-2\beta\varepsilon}\right)\left(1+e^{-\beta\varepsilon}+e^{-2\beta\varepsilon}\right)}}$$

c) Low temperature limit: $T \to 0 \Rightarrow e^{-\beta\varepsilon} \to 0$

$\Rightarrow \underline{\bar{n}_1 \to 2, \ \bar{n}_2 \to 0, \ \bar{n}_3 \to 0}$