1

Homework #~~6~~7 Solution

Statistical Mechanics.

1) Problem 1

Consider an ideal quantum gas of Fermi particles at a temperature T.

(a) Write the probability $p(n)$ that there are n particles in a given single particle state as a function of the mean occupation number, $\langle n\rangle$.

(b) Find the root-mean-square fluctuation $\langle (n-\langle n\rangle)^2\rangle^{1/2}$ in the occupation number of a single particle state as a function of the mean occupation number $\langle n\rangle$. Sketch the result.

Solution

(a) Let ϵ be the energy of a single particle state, μ be the chemical potential. The partition function is

$$z = \sum_n e^{n(\mu-\epsilon)/kT} = 1 + e^{(\mu-\epsilon)/kT}.$$

The mean occupation number is

$$\boxed{\langle n\rangle = kT\frac{\partial}{\partial\mu}\ln z} = \frac{1}{e^{(\epsilon-\mu)/kT}+1}.$$

The probability is

$$\begin{aligned} p(n) &= \frac{1}{z}e^{n(\mu-\epsilon)/kT} \\ &= \frac{(1-\langle n\rangle)^n}{\langle n\rangle^{n-1}}. \end{aligned}$$

(b) $\langle (n-\langle n\rangle)^2\rangle = kT\dfrac{\partial\langle n\rangle}{\partial\mu} = \langle n\rangle(1-\langle n\rangle)$.

So we have $\langle (n-\langle n\rangle)^2\rangle^{1/2} = \sqrt{\langle n\rangle(1-\langle n\rangle)}$.

The result is shown in the figure.

Problem 1, cont.

The density of states is

$$D(E) = \frac{4\pi V(2m)^{3/2}}{h^3} E^{1/2} .$$

(b) If $T = 0$, the total number of electrons is

$$N = \int_0^{E_F} D(E)dE = \frac{2}{3} D(E_F) E_F .$$

(d) If $T \neq 0$,

$$N = \int_0^{\infty} \frac{D(E)}{e^{(E-\mu)/kT} + 1} dE .$$

2)

Solution

(a) By the Fermi distribution, the probability for a level ϵ to be occupied is

$$F(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)}+1},$$

so the probability for finding an electron at $\epsilon = \mu + \Delta$ is

$$F(\mu+\Delta) = \frac{1}{e^{\beta\Delta}+1},$$

and the probability for not finding electrons at $\epsilon = \mu - \Delta$ is given by

$$1 - F(\mu - \Delta) = \frac{1}{e^{\beta\Delta}+1}.$$

The two probabilities have the same value as required.

(b) When $T > 0$ K, some electrons with $\epsilon < 0$ will be excited to states of $\epsilon > \epsilon_g$. That is to say, vacancies are produced in the some states of $\epsilon < 0$ while some electrons occupy states of $\epsilon > \epsilon_g$. The number of electrons with $\epsilon > \epsilon_g$ is given by

$$\begin{aligned} n_e &= \int_{\epsilon_g}^{\infty} D(\epsilon)\frac{1}{e^{\beta(\epsilon-\mu)}+1}d\epsilon \\ &= \int_{\epsilon_g}^{\infty} a(\epsilon-\epsilon_g)^{1/2}\frac{1}{e^{\beta(\epsilon-\mu)}+1}d\epsilon. \end{aligned}$$

The number of vacancies for $\epsilon < 0$ is given by

$$\begin{aligned} n_p &= \int_{-\infty}^{0} D(\epsilon)\left[1-F(\epsilon)\right]d\epsilon \\ &= \int_{-\infty}^{0} b(-\epsilon)^{1/2}\frac{1}{e^{-\beta(\epsilon-\mu)}+1}d\epsilon. \end{aligned}$$

By $n_e = n_p$, we have $\mu = \epsilon_g/2$ when $a = b$. We also obtain the equation to determine μ when $a \neq b$,

$$\frac{a}{b} = \frac{e^{\beta(\epsilon+\epsilon_g-\mu)}+1}{e^{\beta(\epsilon+\mu)}+1}.$$

For $a > b$, we have

$$\frac{e^{\beta(\epsilon+\epsilon_g-\mu)}+1}{e^{\beta(\epsilon+\mu)}+1} > 1,$$

so that $\epsilon + \epsilon_g - \mu > \epsilon + \mu$, i.e., $\mu < \epsilon_g/2$. Hence μ shifts to lower energies. For $a < b$, $\mu > \epsilon_g/2$, μ shifts to higher energies.

(c) When $T = 0$, by

$$\int_{\epsilon_g}^{\mu} a(\epsilon-\epsilon_g)^{1/2} d\epsilon = n_d,$$

we obtain

$$\mu = \epsilon_g + \left(\frac{3n_d}{2a}\right)^{2/3}.$$

μ shifts to lower energies as T increases.

HW~~6~~7, Problem 3 solution:

a) The number of states with energy less than ω is

$$\Sigma(\omega)=\iint_{|\vec{k}|<w/c}\frac{dr\,dk}{(2\pi)^3}=\frac{4\pi V}{(2\pi)^3}\int_{|\vec{k}|<w/c}k^2dk=\frac{4\pi V}{(2\pi)^3}\frac{1}{3}\frac{\omega^3}{c^3}$$

Thus, the number of states between ω and ω+dω is

$$g(\omega)=\frac{d\Sigma}{d\omega}=\frac{V}{2\pi^2c^3}\omega^2$$

b) From $\int_0^{\omega_c}d\omega\, g(\omega)=3N$, we get:

$$\omega_c=\left(18\pi^2Nc^3/V\right)^{1/3}$$

c) Since z=1, the occupation number is

$$<n_{\vec{k}}>=\frac{1}{\exp(\beta\hbar ck)-1}$$

d) The total energy is:

$$<E>=\int_0^{\omega_c}d\omega\, g(\omega)<\varepsilon(\omega)>=\int_0^{\omega_c}d\omega\, g(\omega)\hbar\omega\left(\frac{1}{2}+<n_\omega>\right)$$

$$=\int_0^{\omega_c}d\omega\frac{V\omega^2}{2\pi^2c^3}\hbar\omega\left(\frac{1}{2}+\frac{1}{\exp(\beta\hbar\omega)-1}\right)$$

$$=\frac{\hbar V}{2\pi^2c^3}\int_0^{\omega_c}d\omega\quad\omega^3\left(\frac{1}{2}+\frac{1}{\exp(\beta\hbar\omega)-1}\right)$$

The specific heat is

$$C_V=\left.\frac{dE}{dT}\right|_{V,N}=\frac{\hbar V}{2\pi^2c^3}\int_0^{\omega_c}d\omega\quad\hbar\omega^4\frac{\exp(\beta\hbar\omega)}{[\exp(\beta\hbar\omega)-1]^2}\frac{1}{kT^2}$$

$$=\frac{\hbar^2V}{2\pi^2c^3kT^2}\int_0^{\omega_c}d\omega\quad\omega^4\frac{\exp(\beta\hbar\omega)}{[\exp(\beta\hbar\omega)-1]^2}$$

$$=9Nk\left(\frac{kT}{\hbar\omega_c}\right)^3\int_0^{\omega_c}d(\beta\hbar\omega)\;(\beta\hbar\omega)^4\frac{\exp(\beta\hbar\omega)}{[\exp(\beta\hbar\omega)-1]^2}$$

$$=9Nk\left(\frac{kT}{\hbar\omega_c}\right)^3\int_0^{\beta\hbar\omega_c}dx\;\frac{x^4\exp(x)}{[\exp(x)-1]^2}$$

For small T, $\beta\hbar\omega\to\infty$, the integration gives a constant so $C_V\sim T^3$.

For large T, $\beta\hbar\omega\to 0$, exp(x)~1+x, the integration gives $(\beta\hbar\omega_c)^3/3$.

So $C_V\sim 3Nk$ as in classical gas.

If $\mu = 0$, the integral ... occur.

Problem 4

Consider a photon gas enclosed in a volume V and in equilibrium at temperature T. The photon is a massless particle, so that $\varepsilon = pc$.

~~(a) What is the chemical potential of the gas? Explain.~~

(a) Determine how the number of photons in the volume depends upon the temperature.

(b) One may write the energy density in the form

$$\frac{\overline{E}}{V} = \int_0^\infty \rho(\omega)\,d\omega\,.$$

Determine the form of $\rho(\omega)$, the spectral density of the energy.

(c) What is the temperature dependence of the energy $\overline{E}$?

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Solution:

(a) The density of states is $8\pi V p^2 dp/h^3$, or $V\omega^2 d\omega/\pi^2 c^3$. Then t number of photons is

$$\overline{N} = \int \frac{V}{\pi^2 c^3}\omega^2 \frac{1}{e^{\hbar\omega/kT}-1}d\omega = \frac{V}{\pi^2 c^3}\left(\frac{kT}{\hbar}\right)^3 \int_0^\infty \frac{\alpha^2 d\alpha}{e^\alpha - 1} \propto T^3\,.$$

(b), (c) $$\frac{\overline{E}}{V} = \int \frac{\omega^2}{\pi^2 c^3}\frac{\hbar\omega}{e^{\hbar\omega/kT}-1}d\omega = \frac{(kT)^4}{\pi^2 c^3 \hbar^3}\int \frac{\xi^3 d\xi}{e^\xi - 1}\,.$$

Hence

$$\rho(\omega) = \frac{\hbar}{\pi^2 c^3}\frac{\omega^3}{e^{\hbar\omega/kT}-1}\,,$$

and $\overline{E} \propto T^4$.

$$\rho(\varepsilon) = \frac{4\pi}{h^3 c^3}\varepsilon^3 \frac{1}{e^{\beta\varepsilon}-1}$$

Problem 4.1

The density of state is $g(\varepsilon) = \alpha V \varepsilon^2$

α is a constant.

Grand thermodynamic potential

$$\Omega(T,V,\mu) = -k_B T \ln \Xi$$

$$= +k_B T \int d\varepsilon \; g(\varepsilon) \ln\left(1 - e^{-\beta\varepsilon}\right)$$

$$= k_B T \, \alpha V \int d\varepsilon \; \varepsilon^2 \ln\left(1 - e^{-\beta\varepsilon}\right)$$

$$= k_B T \, \alpha V \int d\left(\frac{\varepsilon^3}{3}\right) \ln\left(1 - e^{-\beta\varepsilon}\right)$$

$$= -k_B T \, \alpha V \int d\varepsilon \; \frac{\beta e^{-\beta\varepsilon}}{1 - e^{-\beta\varepsilon}} \cdot \frac{\varepsilon^3}{3}$$

$$= - \alpha V \int d\varepsilon \; \frac{\varepsilon^3}{3} \frac{1}{e^{\beta\varepsilon} - 1}$$

$$P = -\left.\frac{\partial \Omega}{\partial V}\right|_{T,\mu} = +\alpha \int d\varepsilon \; \frac{\varepsilon^3}{3} \frac{1}{e^{\beta\varepsilon} - 1}$$

$$= \frac{1}{3V} \int d\varepsilon \; g(\varepsilon) \frac{\varepsilon}{e^{\beta\varepsilon} - 1}$$

$$= \frac{1}{3V} \cdot \langle E \rangle$$

$$P = \cancel{\frac{1}{3V}} \frac{\langle E \rangle}{3V}$$

since $\langle E \rangle \sim T^4$, $P \sim T^4$.

Homework 7. # Problem 5.

$$\mathcal{Z} = \sum_{N,i} e^{-\beta(E_i - \mu N)}$$

$$z = e^{\beta\mu} : \text{fugacity}$$

$$\left.\frac{\partial \ln \mathcal{Z}}{\partial \beta}\right|_{\mu,V} = \frac{1}{\mathcal{Z}} \left.\frac{\partial \mathcal{Z}}{\partial \beta}\right|_{\mu,V}$$

$$= \frac{1}{\mathcal{Z}} \frac{\partial}{\partial \beta} \left.\left(\sum_{N,i} e^{-\beta(E_i - \mu N)} \right)\right|_{\mu,V}$$

$$= \frac{1}{\mathcal{Z}} \sum (\mu N - E_i)\, e^{-\beta(E_i - \mu N)}$$

$$-\left.\frac{\partial \ln \mathcal{Z}}{\partial \beta}\right|_{z,V} = E$$

$$-\left.\frac{\partial \ln \mathcal{Z}}{\partial \beta}\right|_{\mu,V} = \frac{1}{\mathcal{Z}} \sum (E_i - \mu N)\, e^{-\beta(E_i - \mu N)}$$

$$= E - \mu \langle N \rangle$$

$$E = -\left.\frac{\partial \ln \mathcal{Z}}{\partial \beta}\right|_{\mu,V} + \mu \langle N \rangle$$