MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Physics Department

8.044 Statistical Physics I — Spring Term 2013

Final Exam, Solutions

Problem 1 (20 points) Binary Alloy

a) Find the number of different ways of choosing the n α-sites to be vacated and occupied by β atoms.

$$\#_\alpha = \underline{\frac{N!}{n!(N-n)!}}$$

b) Find the number of different ways of choosing the n β-sites from which to take the β atoms.

$$\#_\beta = \underline{\frac{N!}{n!(N-n)!}}$$

c) Find the entropy of the system as a function of n.

$$S(n) = k_B \ln \Omega = k_B \ln(\#_\alpha \times \#_\beta) = \underline{2k_B \ln\left(\frac{N!}{n!(N-n)!}\right)}$$

d) Find $U(T, N)$.

$$S(n) = 2k_B\left[N\ln N - n\ln n - (N-n)\ln(N-n) - N + n + (N-n)\right]$$

$$\frac{1}{T} = \left(\frac{\partial S}{\partial U}\right)_N = \left(\frac{\partial S}{\partial n}\right)_N \underbrace{\left(\frac{\partial n}{\partial U}\right)_N}_{1/\epsilon} = \frac{2k_B}{\epsilon}\left[-1 - \ln n + 1 + \ln(N-n)\right]$$

$$\frac{\epsilon}{2k_BT} = -\ln\left(\frac{n}{N-n}\right) \to \frac{n}{N-n} = e^{-\epsilon/2k_BT}$$

Solving for n gives

$$n = \frac{N}{1+e^{\epsilon/2k_BT}} \quad \to \quad \underline{U(T,N) = \frac{N\epsilon}{1+e^{\epsilon/2k_BT}}}$$

Problem 2 (20 points) DNA Model

a) This is a classical system with N non-degenerate states with energies $E_n = n\epsilon$.

$$Z_1 = \sum_{n=0}^{N} e^{-n\epsilon/k_BT}$$

b) When $kT \ll \epsilon$ one need consider only the lowest two energy states; this becomes an energy gap dominated situation.

$$\begin{aligned}
\langle n \rangle &= \sum_{n=0}^{N} n \frac{e^{-n\epsilon/k_BT}}{Z} \\
&\approx \frac{0\, e^{-0} + 1\, e^{-\epsilon/k_BT}}{e^{-0} + e^{-\epsilon/k_BT}} = \frac{e^{-\epsilon/k_BT}}{1 + e^{-\epsilon/k_BT}} \\
&\approx \underline{e^{-\epsilon/k_BT}}
\end{aligned}$$

c) When $k_BT \gg \epsilon$ one can approximate sums over n by integrals. For example

$$Z = \sum_{n=0}^{N} e^{-n\epsilon/k_BT} = \left(\frac{k_BT}{\epsilon}\right) \sum_{n=0}^{N} e^{-n\epsilon/k_BT} \left(\frac{\epsilon}{k_BT}\right) \approx \frac{k_BT}{\epsilon} \underbrace{\int_0^\infty e^{-x}\, dx}_{1} = \frac{k_BT}{\epsilon}$$

d) In a similar manner

$$\begin{aligned}
\langle n \rangle &= \sum_{n=0}^{N} n \frac{e^{-n\epsilon/k_BT}}{Z} \\
&= \sum_{n=0}^{N} \frac{n\epsilon}{k_BT} e^{-n\epsilon/k_BT} = \left(\frac{k_BT}{\epsilon}\right) \sum_{n=0}^{N} \frac{n\epsilon}{k_BT} e^{-n\epsilon/k_BT} \left(\frac{\epsilon}{k_BT}\right) \\
&\approx \frac{k_BT}{\epsilon} \underbrace{\int_0^\infty x e^{x}\, dx}_{1} \\
&\approx \underline{\frac{k_BT}{\epsilon}}
\end{aligned}$$

Alternatively use $Z_1 = 1/(\beta\epsilon)$.

$$\langle n \rangle = \frac{< U >}{\epsilon} = \frac{1}{\epsilon}\left(\frac{-1}{Z}\frac{\partial Z}{\partial \beta}\right) = \frac{1}{\epsilon}\left(\frac{-1}{Z}\right)\left(\frac{-Z}{\beta}\right) = \underline{\frac{k_BT}{\epsilon}}$$

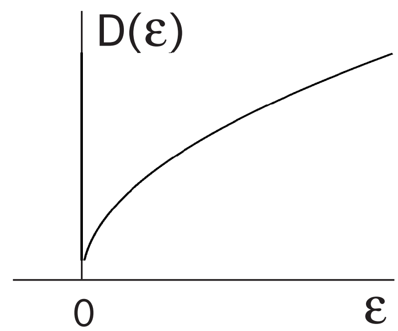
Problem 3 (20 points) Spin Waves

a)

$$D(\vec{k}) = \frac{L_x}{2\pi}\frac{L_y}{2\pi}\frac{L_z}{2\pi} = \underline{\frac{V}{(2\pi)^3}}$$

b)

$$\begin{aligned}
\#(\omega) &= \text{(volume of sphere in k-space)} \times D(\vec{k}) \\
&= \frac{4}{3}\pi k^3(\omega)\frac{V}{(2\pi)^3} \quad \text{use} \quad k = (\omega/a)^{1/2} \\
&= \frac{V}{6\pi^2}\left(\frac{\omega}{a}\right)^{3/2} \\
D(\omega) &= \frac{d\#(\omega)}{d\omega} = \underline{\frac{V}{(2\pi)^2} a^{-3/2}\,\omega^{1/2}}
\end{aligned}$$



c)

$$\begin{aligned}
U &= \int_0^\infty \langle \epsilon(\omega)\rangle\, D(\omega)\, d\omega \\
&= \frac{V}{(2\pi)^2} a^{-3/2} \int_0^\infty \frac{\hbar\omega}{(e^{\hbar\omega/k_BT}-1)}\,\omega^{1/2}\, d\omega \ + \text{Z.P. contribution} \\
&= \frac{V}{(2\pi)^2}\left(\frac{1}{\hbar a}\right)^{3/2}(k_BT)^{5/2}\underbrace{\int_0^\infty \frac{x^{3/2}}{e^x-1}\,dx}_{\equiv I} \ + \text{Z.P. contribution}
\end{aligned}$$

$$C_V(T,V) = \left(\frac{\partial U}{\partial T}\right)_V = \underline{\frac{5}{8\pi^2}\,k_BV\left(\frac{k_BT}{\hbar a}\right)^{3/2} I}$$

d) There is no energy gap behavior ($C_V \propto T^n e^{-\Delta/k_BT}$) because of the integration over a continuous distribution of gaps ($\Delta = \hbar\omega$), some of which are less than k_BT for any physical T.

Problem 4 (20 points) Graphene

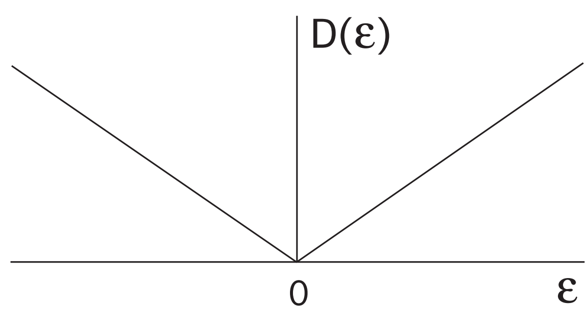
a)

$$D(\vec{k}) = \frac{L_x}{2\pi}\frac{L_y}{2\pi} = \underline{\frac{A}{(2\pi)^2}}$$

b)

$$\begin{aligned} \#(\epsilon) &= 2 \times (\text{area of disk in k-space}) \times D(\vec{k}) \\ &= 2 \times \pi k^2(\epsilon) \frac{A}{(2\pi)^2} \quad \text{use} \quad k = \frac{\epsilon}{\hbar v} \\ &= \frac{A}{2\pi}\left(\frac{1}{\hbar v}\right)^2 \epsilon^2 \\ D_c(\epsilon) &= \frac{d\#(\epsilon)}{d\epsilon} = \underline{\frac{A}{\pi}\left(\frac{1}{\hbar v}\right)^2 \epsilon} \end{aligned}$$

c)



d)

$\mu(T = 0)$ rests at the last filled state at $T = 0$ which is at the top of the valence band, so $\underline{\mu(T = 0) = 0}$.

$D(\epsilon)$ is symmetric about $\epsilon = 0$. If μ stays at $\epsilon = 0$ the symmetry of $\langle n(\epsilon, T)\rangle$ assures that as T increases the number of electrons lost from the valence band is exactly equal to the number of electrons appearing in the conduction band. Thus $\underline{\mu(T) = 0}$ for all T covered by this model.

e)

$$
\begin{aligned}
U &= \int_{-\infty}^{\infty} \epsilon \, \langle n(\epsilon, T) \rangle \, D(\epsilon) \, d\epsilon \\
&= 2 \int_{0}^{\infty} \epsilon \, \langle n(\epsilon, T) \rangle \, D_c(\epsilon) \, d\epsilon \\
&= \frac{A}{\pi} \left(\frac{1}{\hbar v} \right)^2 \int_0^{\infty} \frac{1}{(e^{\epsilon/k_B T} + 1)} \, \epsilon^2 \, d\epsilon \\
&= \frac{A}{\pi} \left(\frac{1}{\hbar v} \right)^2 (k_B T)^3 \underbrace{\int_0^{\infty} \frac{x^2}{(e^x + 1)} \, dx}_{\equiv I} \\
&= \underline{\frac{A}{\pi} \left(\frac{1}{\hbar v} \right)^2 (k_B T)^3 \, I}
\end{aligned}
$$

f)

$C_A(T) = (\partial U / \partial T)_A$ so $\underline{C_A(T) \text{ will be proportional to } T^2 \text{, that is the temperature exponent } n = 2}$.

Problem 5 (20 points) BEC

a)

$$\begin{aligned}
N &= \int_0^\infty < n > D(\epsilon)\, d\epsilon \\
&= \int_0^\infty \frac{1}{e^{(\epsilon-\mu)/k_BT}-1}\left[\frac{V}{(2\pi)^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\epsilon}\right] d\epsilon \\
&= \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty \frac{\sqrt{\epsilon}}{e^{(\epsilon-\mu)/k_BT}-1}\, d\epsilon \\
&= \frac{V}{4\pi^2}\left(\frac{2mk_BT}{\hbar^2}\right)^{3/2}\underbrace{\int_0^\infty \frac{\sqrt{x}}{e^{(x-y)}-1}\, dx}_{\equiv I(y)} \\
n &= \underline{\frac{V}{4\pi^2}\left(\frac{2mk_BT}{\hbar^2}\right)^{3/2} I(y)}
\end{aligned}$$

b) Bose-Einstein condensation begins when the above condition is satisfied with $\mu = 0$ which also means our dimensionless parameter $y = 0$.

$$n_c = \underline{\frac{V}{4\pi^2}\left(\frac{2mk_BT_c}{\hbar^2}\right)^{3/2} I(y=0)}$$

c)

$dU = TdS - PdV + \mu dN$; change independent variables to T, V, N:

$$dS = \left.\frac{\partial S}{\partial T}\right|_{T,V} dT + \left.\frac{\partial S}{\partial V}\right|_{T,N} dV + \left.\frac{\partial S}{\partial N}\right|_{T,V} dN$$

So $\partial U/\partial N|_{V,T} = \mu + T\,\partial S/\partial N|_{T,V}$.

Now use Maxwell relation derivable from $dF = ...$ on the information sheet: $\partial S/\partial N|_{T,V} = -\partial\mu/\partial T|_{T,N}$. so

$$\left.\frac{\partial U}{\partial N}\right|_{V,T} = \mu - T\left.\frac{\partial \mu}{\partial T}\right|_{N,V} = -T^2\left.\frac{\partial}{\partial T}\frac{\mu}{T}\right|_{N,V} = \left.\frac{\partial(\beta\mu)}{\partial\beta}\right|_{N,V}$$

In the Bose condensed phase $\mu = 0$ and is independent of the temperature, so both terms in $\partial U/\partial N$ are zero.

d)

From answer to part a)

$$n = \frac{1}{4\pi^2}\left(\frac{2mk}{\hbar^2}\right)^{3/2} T^{3/2}\int_0^\infty \frac{\sqrt{x}\,dx}{e^{(x-y)}-1} \qquad\qquad C\times\frac{N}{V}\beta^{3/2} = \int_0^\infty \frac{\sqrt{x}\,dx}{e^{(x-y)}-1}$$

where C is a collection of constants.

Differentiate this equation implicitly w.r.t. β and $y = \mu\beta$,

$$\frac{3}{2}\times\frac{N}{V}\beta^{1/2} = \left(\int_0^\infty \sqrt{x}dx\frac{e^{(x-y)}}{(e^{(x-y)}-1)^2}\right)\frac{dy}{d\beta}$$

Both the term on the left and the term in () are positive definite. Thus $dy/d\beta > 0$.

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