731 Homework #4

Due October 2nd, 2006

1. A&M, problem 2.2 (30 pts)
2. A&M, problem 4.1 (15 pts) = 5 + 5 + 5
3. A&M, problem 4.2 (15 pts) = 8 + 7
4. A&M, problem 4.3 (10 pts)
5. A&M, problem 4.5 (20 pts) = 10 + 10
6. A&M, problem 4.6 (20 pts) = 5 + 5 + 5 + 5

Total 110

Solutions HW # 4.

1) (A & M 2.2)

a) $\frac{\partial s}{\partial T} = \frac{1}{T}\frac{\partial u}{\partial T}$; $f(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/k_BT}+1}$: $u = \int \frac{d\vec{k}}{4\pi^3}\, \varepsilon f(\varepsilon)$

$$\frac{\partial s}{\partial T} = \frac{1}{T}\int\frac{d\vec{k}}{4\pi^3}\,\varepsilon\,\frac{\partial f}{\partial T} \Rightarrow s = \int dT\,\frac{\partial f}{\partial T}\frac{\varepsilon}{T}\int\frac{d\vec{k}}{4\pi^3}$$

$$= \int df\cdot\frac{\varepsilon}{T}\int\frac{d\vec{k}}{4\pi^3} = k_B\int \ln\frac{1-f(\varepsilon)}{f(\varepsilon)}\,df\int\frac{d\vec{k}}{4\pi^3} \quad \left(\ln\left(\frac{1}{f}-1\right) = \frac{\varepsilon-\mu}{k_BT}\right)$$

$$s = -k_B\int\left[f\ln f + (1-f)\ln(1-f)\right]\frac{d\vec{k}}{4\pi^3} + \text{Const.}$$

$s \to 0$ when $T \to 0$ $\to$ Const $= 0$

$$s = -k_B\int\frac{d\vec{k}}{4\pi^3}\left[f\ln f + (1-f)\ln(1-f)\right]\frac{d\vec{k}}{4\pi^3}.$$

b) $P = -(u - Ts - \mu n) \Rightarrow$

$$P = -\left(\int\frac{d\vec{k}}{4\pi^3}\,\varepsilon f(\varepsilon) + T k_B\int\frac{d\vec{k}}{4\pi^3}\left[f\ln f + (1-f)\ln(1-f)\right] - \mu\int\frac{d\vec{k}}{4\pi^3} f(\varepsilon)\right)$$

$$P = +k_BT\left\{\int\frac{d\vec{k}}{4\pi^3}\left[-\frac{\varepsilon}{k_BT}f - f\ln f - (1-f)\ln(1-f) + \frac{\mu}{k_BT}f\right]\right\}$$

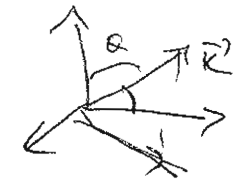
$$\boxed{f = \frac{1}{e^{(\varepsilon-\mu)/k_BT}+1} \Rightarrow \frac{\varepsilon-\mu}{k_BT} = \ln\frac{1-f}{f}}$$

$$P = k_BT\int\frac{d\vec{k}}{4\pi^3}\ln\left(1+e^{-\frac{\varepsilon-\mu}{k_BT}}\right)$$

$$P(\lambda\mu, \lambda T) = k_B \lambda T \int \frac{d\vec{k}}{4\pi^3} \ln\left(1 + e^{-\frac{\varepsilon - \lambda\mu}{\lambda k_B T}}\right)$$

$$\varepsilon = \frac{\hbar^2 k^2}{2m}$$

$$P(\lambda\mu,\lambda T) = \lambda k_B T \int \frac{d\vec{k}}{4\pi^3} \ln\left(1 + e^{-\left(\frac{\frac{\hbar^2}{2m}\left(\frac{k}{\sqrt{\lambda}}\right)^2 - \mu}{k_B T}\right)}\right)$$



$k' = k/\sqrt{\lambda}$; $dk = \sqrt{\lambda}\, dk'$. $d\vec{k} = k^2\, dk\, d\theta\, d\varphi$

$$= \sqrt{\lambda}\,\lambda\, \underbrace{k'^2\, dk'\, d\theta'\, d\varphi'}_{d\vec{k}'}$$

$$= \lambda^{3/2}\, d\vec{k}'$$

$$P = \lambda\cdot\lambda^{3/2} k_B T \int \frac{d\vec{k}'}{4\pi^3}\ln\left(1+e^{-\frac{\overbrace{\frac{\hbar^2}{2m}k'^2}^{=\varepsilon}-\mu}{k_B T}}\right)$$

$$P = \lambda^{5/2} P(\mu,T) \quad ; \quad \boxed{P(\lambda\mu,\lambda T) = \lambda^{5/2}P(\mu,T)}$$

c) $p = -u + TS + \mu n$

$$\boxed{T = \left(\frac{\partial u}{\partial n}\right)_u}$$

$$\left(\frac{\partial p}{\partial\mu}\right)_T = -\left(\frac{\partial u}{\partial \mu}\right)_T + T\left(\frac{\partial s}{\partial\mu}\right)_T + n$$

$$= \underbrace{-\frac{\partial u}{\partial\mu}\Big)_T + \frac{\partial u}{\partial s}\frac{\partial s}{\partial\mu}}_{0} + n = n$$

$$\frac{\partial p}{\partial T}\Big)_\mu = -\frac{\partial u}{\partial T}\Big)_\mu + S + \mu\left(\frac{\partial n}{\partial T}\right)_\mu = -\left(\frac{\partial u}{\partial T}\right)_\mu + S + \frac{\partial u}{\partial n}\frac{\partial n}{\partial T}$$

$$= S$$

(3)

d) $$P = k_BT \int \frac{dk}{4\pi^3} \ln\left(1 + e^{-\frac{\varepsilon-\mu}{k_BT}}\right)$$

$$= k_BT \int \frac{4\pi k^2 dk}{4\pi^3} \ln\left(1 + e^{-\frac{\varepsilon-\mu}{k_BT}}\right)$$

$$P = \left\{ \underbrace{\frac{k^3}{3} \ln\left(1 + e^{-\frac{\varepsilon-\mu}{k_BT}}\right)\bigg|_0^\infty}_{\to 0} - \int \frac{k^3}{3} \frac{e^{-\frac{\varepsilon-\mu}{k_BT}}\left(-1/k_BT\right)\left(-\frac{\hbar^2 k}{m}\right) dk}{1 + e^{-\varepsilon-\mu/k_BT}} \right.$$

$$= \frac{1}{\pi}\int \frac{\hbar^2 k^4}{3m} \cdot \left(\frac{1}{\left(e^{\frac{\varepsilon-\mu}{k_BT}} + 1\right)}\right) dk$$

$$P = \frac{2}{3}\left(\int \frac{d\vec{k}}{4\pi^3} \cdot \frac{\hbar^2 k^2}{2m} \cdot \frac{1}{e^{\frac{\varepsilon-\mu}{k_BT}}+1}\right) = 2/3\, u.$$

e) $$z = e^{\mu/k_BT} = e^{\beta\mu} \; ; \; \beta = 1/k_BT$$

$$\frac{C_p}{C_V} = \frac{(\partial z/\partial T)_P}{(\partial z/\partial T)_V} \; ; \; \frac{1}{z}\left(\frac{\partial z}{\partial T}\right)_V = -\frac{3}{2T} \frac{f_{3/2}(z)}{f_{1/2}(z)}$$

$$f_n(z) = \frac{1}{\Gamma(n)} \int_0^\infty \frac{x^{n-1}}{z^{-1}e^x+1} dx \; ; \; z\frac{\partial}{\partial z} f_n = f_{n-1}$$

$$\Rightarrow \frac{C_p}{C_V} = \frac{\frac{5}{2T}}{\frac{3}{2T}} \left(\frac{f_{5/2} f_{1/2}}{f_{3/2}}\right)^2 = 5/3 \frac{f_{5/2} f_{1/2}}{f_{3/2}}$$

at low T:

$$f_{1/2} = \frac{2}{\pi^{1/2}}(\ln z)^{1/2} - \frac{\pi^{3/2}}{12}[\ln(z)]^{-3/2} + \cdots$$

$$f_{3/2} = \frac{4}{3\pi^{1/2}}(\ln z)^{3/2} + \frac{\pi^{3/2}}{6}\ln(z)^{-1/2} + \cdots$$

$$f_{5/2} = \frac{8}{15\pi^{1/2}}(\ln z)^{5/2} + \frac{\pi^{3/2}}{3}\ln(z)^{1/2} + \cdots$$

$$\ln z = \mu/k_BT \approx \epsilon_F/k_BT \; ; \quad \mu \approx \epsilon_F \text{ when T low}$$

$$\Rightarrow \frac{C_p}{C_V} = 1 + \frac{\pi^2}{3}\left(\frac{k_BT}{\epsilon_F}\right)^2 + \Theta\left(\frac{k_BT}{\epsilon_F}\right)^4 \cdots$$

f) $$U = \int_0^{\mu} \varepsilon g(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6}(k_BT)^2[\mu g'(\mu) + g(\mu)] + \frac{7\pi^4}{360}(k_BT)^4(\mu g''' + 3g'') + \cdots$$

$$\mu = \varepsilon_F - \frac{\pi^2}{6}(k_BT)^2 * g'/g$$

$$U \Rightarrow \int_0^{\epsilon_F} \varepsilon g(\varepsilon)\, d\varepsilon + (\mu - \epsilon_F)\epsilon_F g(\epsilon_F) + \frac{1}{2}(\mu - \epsilon_F)^2(\epsilon_F g'(\epsilon_F) + g(\epsilon_F)) + \pi^2/6\,(k_BT)^2[\mu g' + g] + \frac{21\pi^2}{360}(k_BT)^4 g''$$

$$U = \int_0^{\epsilon_F} \varepsilon g(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6}(k_B T)^2 \frac{g'}{g} \epsilon_F\, g(\epsilon_F) + \frac{1}{2}\frac{\pi^4}{36}(k_B T)^4 \frac{g'^2}{g^2} \epsilon_F\, g'$$

$$+ \frac{1}{2}\frac{\pi^4}{36}(k_B T)^4 \frac{g'^2}{g^2} g +$$

$$+ \frac{\pi^2}{6}(k_B T)^2 \Big[\mu g'(\epsilon_F) + \mu(\mu - \epsilon_F) g''(\epsilon_F) + g(\epsilon_F) + (\mu - \epsilon_F) g'(\epsilon_F)$$

$$+ \dots$$

$$= \int_0^{\epsilon_F} \varepsilon g(\varepsilon)\, d\varepsilon + \frac{1}{2}\frac{\pi^2}{36}(k_B T)^4 \frac{g'}{g} - \left(\frac{\pi^2}{6} k_B^2 T^2\right)^2 \frac{g'}{g} +$$

$$\frac{\pi^2}{6} k^2 T^2 \times \left(-\pi^2/6\, k_B^2 T^2 \frac{g'}{g}\right)(\mu + g') + \frac{\pi^2}{6} k_B^2 T^2 g(\epsilon_F)$$

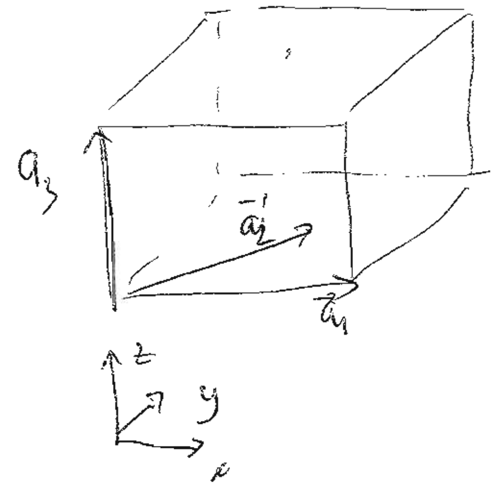
$$+ \frac{21}{360}\pi^4 k_B^4 T^4 g''$$

$$C_V = \frac{\partial u}{\partial T} = \frac{\pi^3}{3} k_B^2 T\, g(\epsilon_F) - \frac{\pi^4}{90} k_B^4 T^3 g \left[15 \frac{g'}{g} - 4 \frac{g''}{g} \right]$$

2) 4.1

Bravais

a)

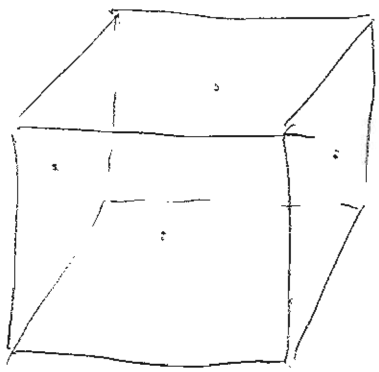


$a_1 = a\hat{x}$

$a_2 = a/2\,(\hat{x}+\hat{y})$

$a_3 = a\hat{z}$

b)



not a Bravais lattice.

Simple cubic + 3 point

(Basis : $\vec{0}$, $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ }.

c) No.

Bravais lattice : a_1, a_2, a_3

Basis = $\vec{0}$, $\frac{a}{2}\hat{x}$, $a/2\,\hat{y}$, $a/2\,\hat{z}$

2) 4.2

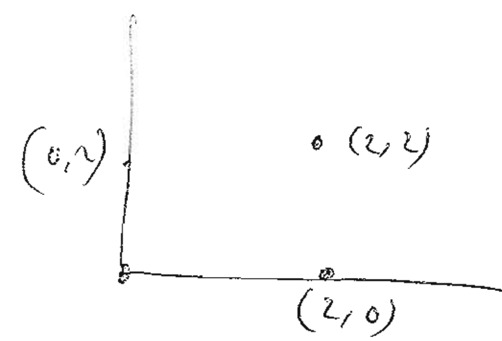
a) n_i are either all even or all odd

simple cubic.

$$\begin{cases} \vec{a_1} = 2\hat{x} \\ \vec{a_2} = 2\hat{y} \\ \vec{a_3} = 2\hat{z} \end{cases}$$

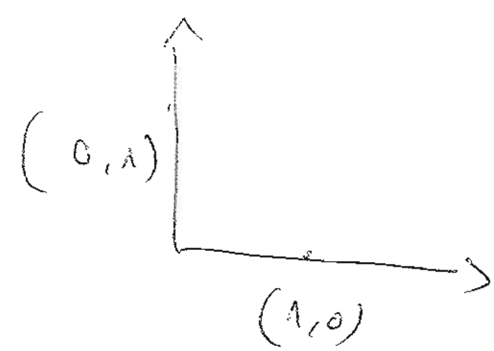
b)

$$\begin{cases} \vec{a_1} = \hat{y} + \hat{z} \\ \vec{a_2} = \hat{z} + \hat{x} \\ \vec{a_3} = \hat{x} + \hat{y} \end{cases}$$



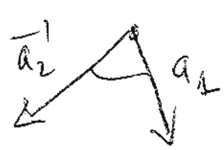
if n_3 is even $\Rightarrow$ $n_1 + n_2$ = event

if n_3 is odd $\rightarrow$ $n_1 + n_2$ = odd



face - centered cubic.

3). 4.3



$$\vec{a_1} = -\frac{a}{4}(\hat{x} + \hat{y} + \hat{z})$$

$$a_2 = \frac{a}{2}(\hat{x} + \hat{y}) - \frac{a}{4}(\hat{x} + \hat{y} + \hat{z})$$

$$= \frac{a}{4}(\hat{x} + \hat{y} - \hat{z})$$

$$\cos\hat{\theta} = \frac{\vec{a_1}\,\vec{a_2}}{|a_1||a_2|} = \frac{-1/16}{3 \times 1/16} = -1/3$$

$\theta = 105^\circ 28'$

4.5)

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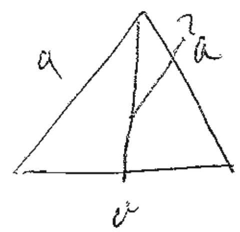
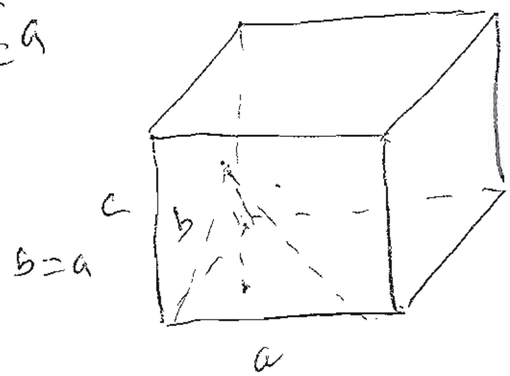
$\frac{2}{3}\frac{\sqrt{3}}{2}a$





$h = \sqrt{2/3}\cdot a$

$c = 2 h = 2\sqrt{2/3}\, a$

$\frac{c}{a} \approx 1.633$

b). cubic phase ; density = number of atoms per unit volume

$\vec{a_1} = a\hat{x}$

$\vec{a_2} = a\hat{y}$

$\vec{a_3} = a\hat{z}$

density $= 1/a^3$

hcp phase. There are 2 atoms in unit cell

$\vec{a_1} = a'\hat{x}$

$\vec{a_2} = a'/2\,\hat{x} + \sqrt{3}/2\, a'\hat{y}$

$a_3 = c'\hat{z}$

$$\text{density} = \frac{2}{a'\left(\frac{\sqrt{3}}{2}a'\right)\cdot c'}$$

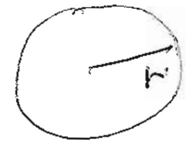
density does not change ; $\frac{2}{a^3} = \frac{2}{\frac{\sqrt{3}}{2}a'^2 c}$

$c' = 1.633\,a$.

$$\frac{1}{a^3} = \frac{1}{a'^3 \cdot \frac{\sqrt{3}}{2} \cdot 1.633} \rightarrow \boxed{a' \approx 3.168\ A^\circ}$$ 9

4.6.

$$1 = \frac{1}{\frac{4\pi}{3} r^3}$$ unit density.

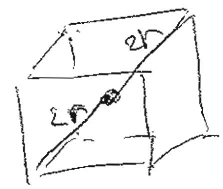


$$\Rightarrow r = \left(\frac{3}{4\pi}\right)^{1/3}$$

fcc: $2r = \frac{\sqrt{2}}{2} a \Rightarrow a = 2\sqrt{2}\, r$

$$\rho = \frac{4}{a^3} = \frac{4}{8\sqrt{3}^3 r^3} = \frac{\sqrt{2}}{6}\pi = 0.74$$

bcc: $\sqrt{3} a = 4r \rightarrow a = 4/3\, r$



$$\rho_{bcc} = \frac{2}{a^3} = \frac{2}{\frac{64}{3\sqrt{3}} r^3} = 0.68$$

sc: $a = 2r$, $\rho = 1/a^3 = \frac{1}{8r^3} = 0.52$

diamond: $\frac{\sqrt{3}}{4} a = 2r \rightarrow a = \frac{8}{\sqrt{3}} R.$

$$\rho = 0.34$$