Physics 431 - Homework 4

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September 2022

Problem 1

Part A

$$\begin{aligned}
\vec{r}_1 &= 0\hat{a_1} + 0\hat{a_2} + 0\hat{a_3} \\
\vec{r}_2 &= 0\hat{a_1} + \frac{1}{2}\hat{a_2} + \frac{1}{2}\hat{a_3} \\
\vec{r}_3 &= \frac{1}{2}\hat{a_1} + 0\hat{a_2} + \frac{1}{2}\hat{a_3} \\
\vec{r}_4 &= \frac{1}{2}\hat{a_1} + \frac{1}{2}\hat{a_2} + 0\hat{a_3} \\
\vec{r}_5 &= \frac{1}{4}\hat{a_1} + \frac{1}{4}\hat{a_2} + \frac{1}{4}\hat{a_3} \\
\vec{r}_6 &= \frac{1}{4}\hat{a_1} + \frac{3}{4}\hat{a_2} + \frac{3}{4}\hat{a_3} \\
\vec{r}_7 &= \frac{3}{4}\hat{a_1} + \frac{1}{4}\hat{a_2} + \frac{3}{4}\hat{a_3} \\
\vec{r}_8 &= \frac{3}{4}\hat{a_1} + \frac{3}{4}\hat{a_2} + \frac{1}{4}\hat{a_3}
\end{aligned}$$

Atoms are identical $\therefore \; f_j = f$

$$\vec{G} = h\vec{b_1} + k\vec{b_2} + l\vec{b_3} \tag{1}$$

$$S_G = \sum_{j=1}^{8} f e^{-i\vec{G}\cdot\vec{r}_j} \tag{2}$$

S ince we know we are going to be taking many dot products, we can simplify by below

$$\begin{aligned}
\vec{b_1} \cdot \hat{a_1} &= 2\pi \\
\vec{b_2} \cdot \hat{a_2} &= 2\pi \\
\vec{b_3} \cdot \hat{a_3} &= 2\pi
\end{aligned} \tag{3}$$

All other dot products will be 0

$$
\begin{aligned}
\vec{G}\cdot\vec{r}_1 &= 1\\
\vec{G}\cdot\vec{r}_2 &= \pi(k+l)\\
\vec{G}\cdot\vec{r}_3 &= \pi(h+l)\\
\vec{G}\cdot\vec{r}_4 &= \pi(h+k)\\
\vec{G}\cdot\vec{r}_5 &= \frac{\pi}{2}(h+k+l)\\
\vec{G}\cdot\vec{r}_6 &= \frac{\pi}{2}(h+3l+3k)\\
\vec{G}\cdot\vec{r}_7 &= \frac{\pi}{2}(3h+l+3k)\\
\vec{G}\cdot\vec{r}_8 &= \frac{\pi}{2}(3h+3l+k)
\end{aligned}
\tag{4}
$$

$$
\begin{aligned}
S_G &= \sum_{j=1}^{8} f e^{-i\vec{G}\cdot\vec{r}_j}\\
&= f\Big[1+e^{-i\pi(k+l)}+\\
e^{-i\pi(h+l)}&+\\
e^{-i\pi(h+k)}&+\\
e^{-i\frac{\pi}{2}(h+k+l)}&+\\
e^{-i\frac{\pi}{2}(h+3l+3k)}&+\\
e^{-i\frac{\pi}{2}(3h+l+3k)}&+\\
e^{-i\frac{\pi}{2}(3h+3l+k)}&\Big]
\end{aligned}
\tag{5}
$$

Part B

D efinitely had a little trouble understanding exactly how to answer this, so I just calculated a few to illustrate I know whats going on, just Kittels wording was tough.

$(h,k,l) = 4n$

$$
\begin{aligned}
(h,k,l) &= 4n\\
2n &= (\frac{h}{2},\frac{k}{2},\frac{l}{2})
\end{aligned}
\tag{6}
$$

(1,1,0)

$$\begin{aligned} S_G = f1 + -1+ \\ -1+ \\ 1+ \\ 1+ \\ 1+ \\ 1+ \\ -i \\ = f3 - i \end{aligned} \tag{7}$$

(2,2,0)

$$\begin{aligned} S_G = f1 + 1+ \\ 1+ \\ 1+ \\ 1+ \\ 1+ \\ 1+ \\ 1 \\ = 8f \end{aligned} \tag{8}$$

(1,1,1)

$$\begin{aligned} S_G = f[1 + e^{-i\pi 2}+ \\ e^{-i\pi 2}+ \\ e^{-i\pi 2}+ \\ e^{-i\frac{\pi}{2}3}+ \\ e^{-i\frac{\pi}{2}(7)}+ \\ e^{-i\frac{\pi}{2}(7)}+ \\ e^{-i\frac{\pi}{2}(7)}] \\ = f[4 - 4i] \end{aligned} \tag{9}$$

(2,2,2)

$$\begin{aligned} S_G = f[1 + 1+ \\ 1+ \\ 1+ \\ -1+ \\ -1+ \\ -1+ \\ -1] \\ = f[0] \end{aligned} \tag{10}$$

Problem 2

T he melting point is proportional to the cohesive energy. It seems like there was a small correction based on the structure type of the atom, generally however they increased together with a linear relationship. This makes sense as cohesive energy is what is keeping the atoms together in their most stable state where melting point characterizes the point in which the atoms have so much kinetic energy they collectively change the state of the solid. Cohesive energy is basically the strength resisting an increase in kinetic energy, so as it increases, the baseline kinetic energy for a solid to completely melt into a liquid should also be higher.

I nterestingly enough, it does seem like this relationship breaks down slightly at the nano scale. From reading a little bit about this relationship, there is a lot of literature regarding how this relationship behaves when you get smaller and smaller. A little over my head but nonetheless interesting.

Problem 3

$$U(R_0) = \frac{2Nq^2 \ln 2}{R_0}(1 - \frac{1}{n}) \tag{11}$$

Find our equation for U(R) in terms of parameters

$$\begin{aligned} U(R) &= \frac{A}{R^n} \\ &= \frac{2A}{R^n} - \frac{2q^2}{R}\sum_{m=1}^{\infty}\frac{(-1)^m}{m} \\ &= \frac{2A}{R^n} - \frac{2q^2 \ln 2}{R} \end{aligned} \tag{12}$$

Minimize to find R_0

$$\begin{aligned} \frac{\partial U}{\partial R}[\frac{2A}{R^n} - \frac{2q^2 \ln 2}{R}] &= \frac{\partial U}{\partial R}\frac{2A}{R^n} - \frac{\partial U}{\partial R}\frac{2q^2 \ln 2}{R} \\ &= \frac{-n2A}{R^{n+1}} + \frac{2q^2 \ln 2}{R^2} \\ &= 2[\frac{-nA}{R^{n+1}} + \frac{q^2 \ln 2}{R^2}] \end{aligned}$$

Multiplied by N atoms, set to 0 for minimum

$$\begin{aligned} 0 &= 2N[\frac{-nA}{{R_0}^{n+1}} + \frac{q^2 \ln 2}{{R_0}^2}] \\ \frac{nA}{{R_0}^n R_0} &= \frac{q^2 \ln 2}{{R_0}^2} \\ \frac{A}{{R_0}^n} &= \frac{q^2 \ln 2}{nR_0} \end{aligned} \tag{13}$$

Equivalent to equation in first part