Solutions to Homework set II

Kittel chap 4: 4) Kohn Anomaly $\qquad C_p = A \dfrac{\sin pk_0a}{pa}$

Eq (16 a) $\qquad \omega_K^2 = \dfrac{2}{M} \sum\limits_{p>0} C_p (1-\cos pKa)$

$$= \frac{2A}{M} \sum_{p>0} \frac{\sin pk_0a}{pa} (1-\cos pKa).$$

So we need to find sums of the type $\sum\limits_{p=1}^{\infty} \dfrac{\sin px \cos py}{p}$

which can be transformed to $\sum\limits_{p=1}^{\infty} \dfrac{1}{2p} \left[\sin p(x+y) + \sin p(x-y) \right]$

Let $f(x) = \sum\limits_{p=1}^{\infty} \dfrac{\sin px}{p} = \mathrm{Im} \sum\limits_{1}^{\infty} \dfrac{e^{ipx}}{p}$ (is an odd function of X)

$f'(x) = \mathrm{Im} \sum\limits_{1}^{\infty} ip \dfrac{e^{ipx}}{p} = \sum\limits_{1}^{\infty} \cos px = \mathrm{Re} \sum\limits_{1}^{\infty} e^{ipx} = \mathrm{Re}\left[e^{ix} (1 + e^{ix} + e^{2ix} + \cdots) \right]$

$= \mathrm{Re}\left[\dfrac{e^{ix}}{1-e^{ix}} \right]$ (for $x \neq 0$) ; $\quad f(0) = 0 \quad \Rightarrow f(x) = \int_0^x f'(t)\,dt$

$f(x) = \mathrm{Re} \int_0^x \dfrac{e^{it}}{1-e^{it}}\,dt = \mathrm{Re}\, i \int_0^x d \ln (1-e^{it}) = \mathrm{Re}\, \dfrac{i}{2} \int_{-x}^{x} d \ln (1-e^{it})$

finally : $f(x) = -\dfrac{i}{2} \ln \left(\dfrac{1-e^{-ix}}{1-e^{ix}} \right)$

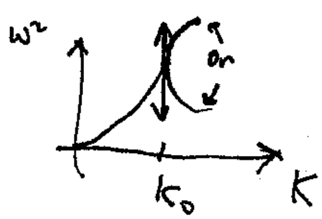
$$\omega_K^2 = \frac{2A}{Ma} \cdot \frac{1}{2} \left[-f(k_0a + Ka) - f(k_0a - Ka) + 2f(k_0a) \right]$$

$K=0$ contribution in $(1-\cos Ka)$

$$\frac{\partial \omega_K^2}{\partial K} = \frac{-A}{M} \left[f'[(k_0+K)a] + f'[(k_0-K)a] \right]$$

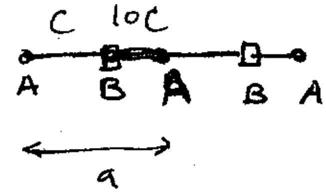
since $f'(0) = \infty$ $\left(= \sum\limits_p \cos 0p \right)$ the second term in $\dfrac{\partial \omega^2}{\partial K}$ diverges.

$$\left. \frac{\partial \omega^2}{\partial K} \right|_{K=k_0} = \infty$$



Solution to Homework set II

Pb 2 : Kittel chap 4 - 5) Diatomic chain



From the equation of motion, we have :

$$-M\omega^2 u_A^n = -10C\left(u_A^n - u_B^{n-1}\right) - C\left(u_A^n - u_B^n\right)$$
$$-M\omega^2 u_B^n = -10C\left(u_B^n - u_A^{n+1}\right) - C\left(u_B^n - u_A^n\right)$$

where the integer n refers to the n^{th} unit cell.

using $\quad u_\alpha^n = e^{ikna}\, v_\alpha \quad (\alpha = A \text{ or } B)$, we get

$$-M\omega^2 v_A = -10C\left(v_A - v_B e^{-ika}\right) - C\left(v_A - v_B\right)$$
$$-M\omega^2 v_B = -10C\left(v_B - v_A e^{+ika}\right) - C\left(v_B - v_A\right)$$

$$\begin{bmatrix} -M\omega^2 + 10C + C & -10C e^{-ika} - C \\ -10C e^{+ika} - C & -M\omega^2 + 10C + C \end{bmatrix}\begin{bmatrix} v_A \\ v_B \end{bmatrix} = 0$$

for $K = 0$ $\quad \begin{bmatrix} -M\omega^2 + 11C & -11C \\ -11C & -M\omega^2 + 11C \end{bmatrix}\begin{bmatrix} v_A \\ v_B \end{bmatrix} = 0 \Rightarrow \mathrm{Det}[\;\;] = 0$

$$\Rightarrow -M\omega^2 + 11C = \pm 11C \Rightarrow \begin{cases} \omega^2 = 0 \\ \omega^2 = \dfrac{22C}{M} \end{cases}$$

for $K = \frac{\pi}{a}$ $\quad \mathrm{Det}\begin{bmatrix} -M\omega^2 + 11C & 9C \\ 9C & -M\omega^2 + 11C \end{bmatrix} = 0 \Rightarrow -M\omega^2 + 11C = \pm 9C$

$$\Rightarrow \begin{cases} \omega^2 = \dfrac{20C}{M} \\ \omega^2 = \dfrac{2C}{M} \end{cases}$$