Solutions homework 3

Phonons

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1) The lattice energy is given by:

$$F = \frac{1}{2} K \sum_j (u_j - u_{j+1})^2 + \frac{1}{2} K' \sum_j (u_j - u_{j+2})^2$$

The force exerting on the j^{th} atom is

$$f_j = -\frac{\partial F}{\partial u_j} = -2(k + k')u_j + k(u_{j+1} + u_{j-1})$$
$$+ k'(u_{j+2} + u_{j-2})$$

The equation of motion for atoms are given by

$$m\ddot{u}_j = -2(k + 6)u_j + k(u_{j+1} + u_{j-1})$$
$$+ k'(u_{j+2} + u_{j-2})$$

The easiest way to solve it is to do a Fourier transformation to u_j w.r.t to both $R_j = j \cdot a$ and time t

$$U_j = \sum_{k\omega} q(k,\omega)\, e^{i(k \cdot R_j - \omega t)}$$

with the periodic boundary condition:

$$K_n = \frac{2\pi n}{N \cdot a} \qquad n = 0, \pm 1, \pm \ \ldots \ N/2$$

Inserting this trial solution into the equation of motion gives:

$$-m\omega^2 q(k,\omega) = [-2(K+K') + 2K\cos(ka) + 2K'\cos(2ka)]\, q(k,\omega)$$

Thus the value of ω is given by

$$\omega = \pm\, \omega_{acoustic}(k)$$

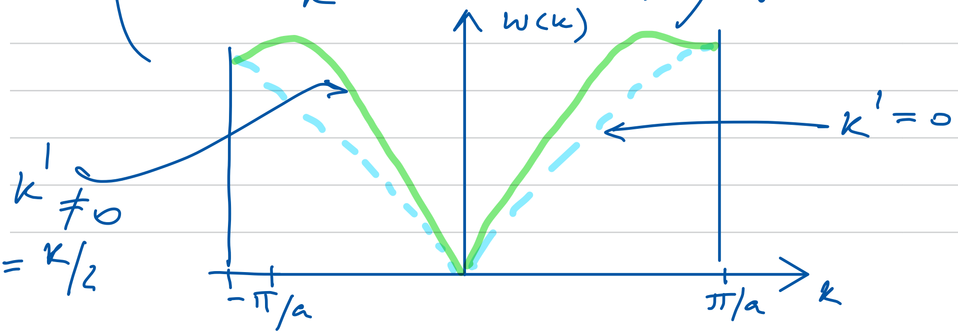
where

$$\omega_{acoustic} = \left(\frac{2K}{m}\right)^{1/2} \left\{1 - \cos(ka) + \left(\frac{K'}{K}\right)\left(1 - 2\cos(2ka)\right]\right.^{1/2} =$$

$$= \left(\frac{4K}{m}\right)^{1/2} \left\{ \sin\left(\frac{ka}{2}\right) \left[1 + \left(\frac{4K'}{K}\right)\cos^2\left(\frac{ka}{2}\right)\right]^{1/2}\right.$$

As you see the presence of n-n-n leads to the new term

$$\left(1 + \frac{4K}{K}\cos^2\left(\frac{ka}{2}\right)\right)^{1/2}.$$



2) To find the contribution of K' to the dispersion we find the extrema of $W^2_{acoustic}$

$$\frac{d\,w_a^2(k)}{d(ka)} = 0 \Rightarrow \sin(ka)\left[1 + \left(\frac{1}{4}\frac{K'}{K}\right)\cdot\cos(ka)\right] = 0 \Rightarrow \begin{cases} \sin(ka) = 0 & * \\ 1 + \dfrac{K'}{4K}\cos(ka) = 0 & ** \end{cases}$$

* - give max only at the zone boundary

** to get a max inside the BZ we require that $\frac{4K'}{K} > 1$

Under this condition the peak position

$$\cos(k_m \cdot a) = -K/4K'$$

$$\boxed{k_m = \frac{1}{a}\arccos\left(-K/4K'\right)}$$

3) The group velocity and phase velocities are given by

$$v_g = \frac{d\omega_{acoustic}(k)}{dk} = \frac{(ka^2/m)^{1/2}\cos(ka/2)}{\left[1+\left(\frac{4k'}{k}\right)\cos^2(ka/2)\right]^{1/2}} *$$

$$* \left[1+\left(\frac{4k'}{k}\right)\cos(ka)\right]$$

$$v_p = \frac{\omega_a(k)}{|k|} = \left(\frac{4K}{m}\right)^{1/2} \frac{\sin\left(\frac{ka}{2}\right)}{k} \Bigg[$$

$$1 + \left(\frac{4K'}{K}\right)\cos^2\left(\frac{ka}{2}\right)\Bigg]^{1/2}$$

Since $\frac{d\omega_a}{dk} = 0$ at k_m, $v_g(k_m) = 0$

This can be seen from the expression for $\omega_a(k)$ and the condition for k_m to peak inside the B.Z.:

$$1 + \frac{4K'}{K}\cos(ka) = 0$$

The phase velocity at k_m:

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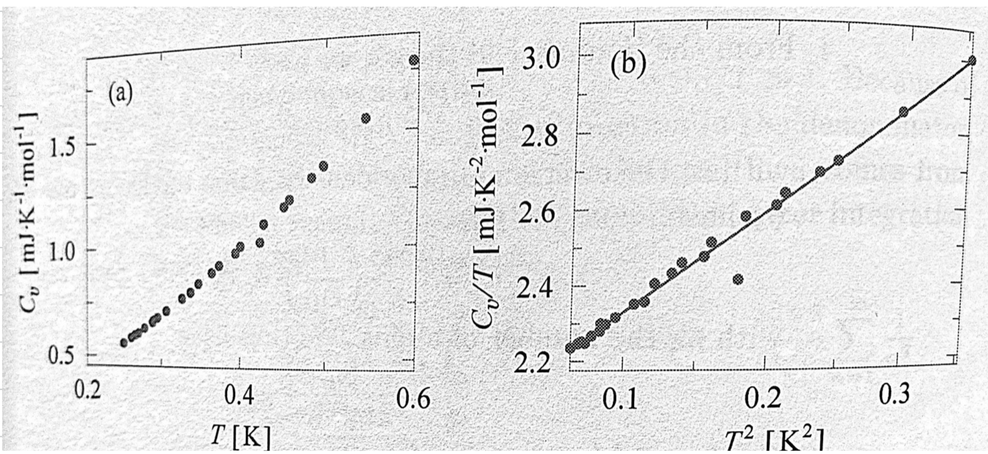
$$v_p(k_m) = \left(\frac{Ka^2}{m}\right)^{1/2} \frac{1 + (K^2 + 16K'^2)/8KK'}{\pi - \tan^{-1}\left[\frac{16K'^2}{K^2} - 1\right]^{1/2}}$$

P2 i The plot of C_v vs. T and C_v/T vs. T^2 is give in the Fig. below



ii The fit to this curve yeilds the following values :

$$\frac{C_v}{T} = \gamma + AT^2$$

fit parameters

$\gamma \approx 2.066 \ \mathrm{mJ \cdot K^{-2}}$, $A \approx 2.650 \ \mathrm{mJ \cdot K^{-4} \cdot mol^{-1}}$

iii In the Debye model for specific heat per mole

$$A = \frac{12\pi^4}{5\theta_D^3} N_A k_B$$

N_A = Avogadro number = $6.022 \cdot 10^{23}$ $mole^{-1}$

and k_B is the Boltzmann constant.

From A from the fit:

$$\frac{12\pi^4}{5\theta_D^3} N_A k_B = 2.650 \cdot 10^{-3} \, J \Rightarrow$$

$$\theta_D = \left(\frac{12\pi^4 N_A k_B}{5 \cdot 2.650 \cdot 10^{-3}} \right)^{1/3} \simeq 90K$$

Which is very much what's reported in the literature for potassium.