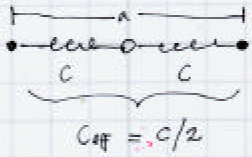
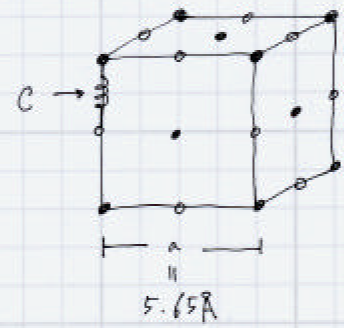
Phy 240B | HW 3 solutions

1. $B = 2.4 \times 10^{11}$ erg / cm^3
$a = 5.65$ Å.
Spring constant : C

(i)





For 2 springs in series, we get an effective spring constant of

$$C_{eff} = \left[\frac{1}{c} + \frac{1}{c}\right]^{-1} = \frac{C}{2}.$$

We need to get the total number of series of springs of a unit cell:

With in unit cell : 3 full series

On the surfaces : 2 series, 6 surfaces

On the edges : 1 each, 12 edges

$$\text{So } N_{series} = 3 + 6 \times \frac{2}{2} + 12 \times \frac{1}{4} = 12$$

So the total energy of the cube, when stretched/compressed to length l, is

$$E = 12 \cdot \frac{C}{2} \cdot \frac{1}{2}(a-l)^2$$

$$= 3C(a - V^{1/3})^2$$

The bulk modulus is

$$B = V\frac{\partial^2 E}{\partial V^2},$$

So

$$B = V\frac{\partial}{\partial V}\left[6C(a - V^{1/3})(-\tfrac{1}{3}V^{-2/3})\right]$$

$$= V\frac{\partial}{\partial V}\left[-2C(aV^{-2/3} - V^{-1/3})\right]$$

$$= 2CV\left(-\frac{1}{3}V^{-4/3} + \frac{2a}{3}V^{-5/3}\right)$$

$$= \frac{2C}{3}\left(2aV^{-2/3} - V^{-1/3}\right)$$

Near equilibrium $(l \simeq a)$,

$$B = \frac{2C}{3}\left(\frac{2}{a} - \frac{1}{a}\right) = \frac{2C}{3a}$$

So

$$C = \frac{3aB}{2} = 1.5(5.65 \times 10^{-8}\,\text{cm})(2.4 \times 10^{11}\,\text{erg/cm}^3)$$

$$\simeq 2.03 \times 10^4\,\text{erg/cm}^2$$

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(ii) Optical phonon mode for 1D system w/ a basis:

$$\omega_{opt}(k) = \sqrt{\frac{2C(M_1+M_2)}{M_1 M_2}}$$

$$= \sqrt{\frac{2(2.03\times10^4\,\mathrm{erg/cm^2})(35.45+22.99)}{35.45\times22.99/(6.023\times10^{23})}}$$

$$\simeq 4.17\times10^3\,s^{-1}$$

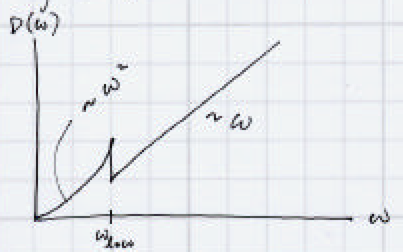
Use ω_{ac} for speed of sound:

$$\omega_{ac}(k) = \sqrt{\frac{C}{2(M_1+M_2)}}\,ka$$

$$C_s = \sqrt{\frac{C}{2(M_1+M_2)}}\,a$$

$$\simeq 5.8\times10^3\,\mathrm{m/s}$$

3. In a quasi-2D system, the spring constant in the $\perp$ direction of the plan is small, so the phonon energies in that direction are low. In the planar directions, the 2D strong bonds are dominant at high ω. So the may look as such:

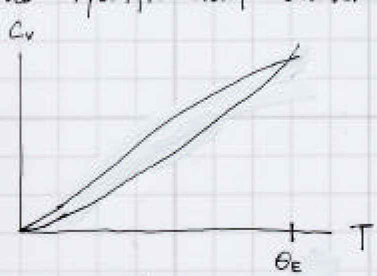


We can write this DOS like

$$D(\omega) \simeq D_{2D}(\omega) + \alpha\,\delta(\omega-\omega_{low})$$

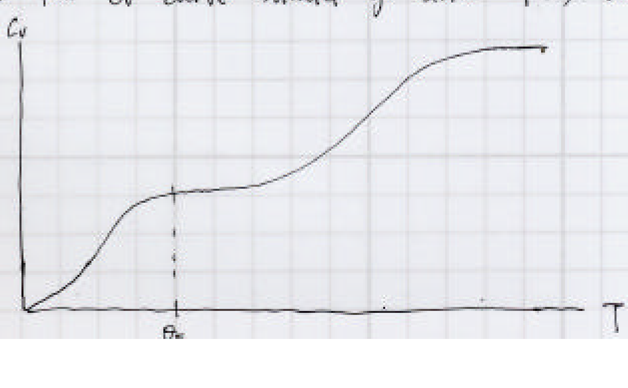
having a 2D Debye component & Einstein component.

The specific heat curves for ~~both me~~ the 2 models look like this (sort of):



$\theta_E \sim \omega_{low}$

So the overall C_v curve should go like T^2, with an Einstein saturation at $T=\theta_E$:



2. (i) Two-dimensional analogy of Eq 13.62 (Marder p. 320):

$$D(\omega) = \int \frac{2\pi k\,dk}{4\pi^2}\,\delta(\omega - ck)$$

$$= \frac{1}{2\pi}\int \frac{ck\,d(ck)}{c^2}\,\delta(\omega - ck)$$

$$= \frac{\omega}{2\pi c^2}$$

So in the Debye model,

$$D(\omega) = \frac{\omega}{2\pi c^2}\,\theta(\omega_D - \omega)$$

$N \equiv$ total # of modes.

Then

$$2N = A\int_0^\infty D(\omega)\,d\omega$$

$$= \frac{1}{2}\omega_D^2\,\frac{1}{2\pi c^2}\,A$$

$$= \frac{k_D^2}{4\pi c^2}\,A$$

$$\therefore k_D = \sqrt{\frac{8\pi N}{A}} = \sqrt{8\pi n}$$

(ii) In 1D,

$$D(\omega) = \int_{-\infty}^{\infty} \frac{d(ck)}{2\pi c}\,\delta(\omega - ck)$$

$$= \frac{1}{\pi c}$$

In 2D,

$$D(\omega) = \frac{\omega}{2\pi c^2}$$

In 3D,

$$D(\omega) = \frac{3\omega^2}{2\pi^2 c^3} \quad \leftarrow \text{Eq (13.67)}$$

(iii)

$$C_A = A\int_0^\infty d\omega\, D(\omega)\,\frac{\partial}{\partial T}\frac{\hbar\omega}{e^{\beta\hbar\omega}-1}$$

$$= A\int_0^\infty \frac{d(\beta\hbar\omega)}{\beta\hbar}\,\frac{\beta\hbar\omega}{2\pi c^2\beta\hbar}\,\frac{\hbar\omega}{(e^{\beta\hbar\omega}-1)^2}\,e^{\beta\hbar\omega}\,\frac{\hbar\omega}{kT^2}$$

$$= A\int_0^\infty \frac{dx\,x^2 e^x}{(e^x-1)^2}\,\frac{k^3T^2}{2\pi c^2\hbar^2} \qquad (x \equiv \beta\hbar\omega)$$

$$\therefore C_A = \frac{Ak^3T^2}{2\pi c^2\hbar^2}\int_0^{x_D}\frac{x^2 e^x}{(e^x-1)^2}\,dx$$

$C_A \sim T^2$, whereas $C_V \sim T^3$ in 3D.

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