

Solid State Physics

Homework Set 4

Solutions

1. There are 12 nearest neighbors for Face Central Cubic Crystal (FCC) at positions

$$a/2(\pm\hat{\mathbf{i}} \pm \hat{\mathbf{j}}), a/2(\pm\hat{\mathbf{i}} \pm \hat{\mathbf{k}}), a/2(\pm\hat{\mathbf{j}} \pm \hat{\mathbf{k}})$$

where a is the lattice constant and $d = a/\sqrt{2}$ is the distance between nearest neighbors

$$D_{\mu\nu}(R - R') = \left. \frac{\partial^2 V}{\partial x_\mu(R) \partial x_\nu(R')} \right|_{x(R)=0}$$

where $x_\mu(R)$ is the deviation toward the μ th direction from the equilibrium at position R then $r(R) = R + x(R)$. Assuming that the potential between 2 ions at positions R and R' depends on their separation $|r - r'| = |R + x(R) - R' - x(R')|$. Because of translational invariance we can always choose then $r' = 0$ and write $V(r) = V(|R + x(R) - x(R')|)$ then for nearest neighbors where $R - R' = d$

$$D_{\mu\nu} = \frac{\partial^2 V}{\partial r^2} \frac{R_\mu R_\nu}{d^2} + \frac{\partial V}{\partial r} \frac{1}{d} \left(\delta_{\mu\nu} + \frac{R_\mu R_\nu}{d^2} \right)$$

$$D(k) = \sum_k D(R) e^{-ik \cdot R} = \dots = \sin^2(k_x a/4) \begin{pmatrix} 8A + 4B & & \\ & 8A + 2B & \\ & & 8A + 2B \end{pmatrix}$$

where $A = 2V'/d$ and $B = 2(V'' - V'/d)$. Hence we have a longitudinal mode

$$\omega_L = \sqrt{\frac{8A + 4B}{M}} |\sin(k_x a/4)|$$

in the direction $\hat{\mathbf{i}}$ and 2 transverse mode

$$\omega_T = \sqrt{\frac{8A + 2B}{M}} |\sin(k_x a/4)|$$

in the direction $\hat{\mathbf{j}}$ and $\hat{\mathbf{k}}$

2. The expression for $|s(0)|^2$ is given by

$$s_\alpha = \sum_s \left[\frac{\hbar}{2mN\omega(s)} \right]^{1/2} (e^{ikr} a(s) + e^{-ikr} a^\dagger(s)) e_\alpha(s)$$

$$\Rightarrow \langle s^2 \rangle = \sum_s \frac{\hbar}{2mN\omega(s)} \langle a(s)a^\dagger(s) + a^\dagger(s)a(s) \rangle$$

using the commutation relation

$$[a, a^\dagger] = 1 \Rightarrow \langle s^2 \rangle = \sum_s \frac{\hbar}{2mN\omega(s)} (1 + 2 \langle a^\dagger a \rangle)$$

where

$$\langle a^\dagger a \rangle = n_s = \frac{1}{e^{\beta\hbar\omega(s)} - 1} \Rightarrow \langle s^2 \rangle = \sum_s \frac{\hbar}{2mN\omega(s)} \coth(1/2\beta\hbar\omega(s))$$

From the theory of elasticity we know that in the long wavelength limit where the dominant contribution to $\langle s^2 \rangle$ occurs. We have (Refer to eq. 22.88 from Ashcroft & Mermin)

$$\rho\omega^2\epsilon_\mu = \sum_\tau \left(\sum_{\nu\sigma} C_{\mu\nu\sigma\tau} k_\nu k_\sigma \right) \epsilon_\tau$$

Since A_g forms a FCC system the number of independent elastic constants is 3

$$\begin{cases} C_{11} = C_{xxxx} = C_{yyyy} = C_{zzzz} = 1.24 \times 10^{12} \\ C_{12} = C_{xxyy} = C_{yyzz} = C_{zzxx} = 0.9 \times 10^{12} \\ C_{44} = C_{xyxy} = C_{yzyz} = C_{zxzx} = 0.46 \times 10^{12} \end{cases}$$

In matrix form

$$\rho\omega^2\epsilon = \begin{pmatrix} C_{11}k_x^2 & (C_{12} + C_{44})k_xk_y & (C_{12} + C_{44})k_xk_z \\ (C_{12} + C_{44})k_xk_y & C_{11}k_y^2 & (C_{12} + C_{44})k_yk_z \\ (C_{12} + C_{44})k_xk_z & (C_{12} + C_{44})k_yk_z & C_{11}k_z^2 \end{pmatrix}$$

Thus for k along x

$$\rho\omega^2 = C_{11}k_x^2 \Rightarrow \omega = \sqrt{\frac{C_{11}}{\rho}} k_x = Ck_x$$

Taking an isotropic density of states

$$N = \frac{4\pi/3k^3}{(2\pi/L)^3} = \frac{L^3k^3}{6\pi^2} = \frac{L^3\omega^3}{6\pi^2C^3} \Rightarrow g(\omega) = \frac{dN}{d\omega} = \frac{L^3\omega^2}{2\pi^2C^3}$$

We can estimate $\langle s^2 \rangle$ by converting the sum to integral.

$$\langle s^2 \rangle = \frac{\hbar}{m} \int_0^{\omega_D} d\omega \frac{g(\omega)}{\omega} \left(\frac{1}{e^{\beta\hbar\omega} - 1} + 1/2 \right) = \frac{\hbar L^3}{4m\pi^2C^3} \int_0^{\omega_D} d\omega \omega \left(\frac{2}{e^{\beta\hbar\omega} - 1} + 1 \right)$$

At very low T where $kT \ll \hbar\omega$. Defining $x = \beta\hbar\omega$ where $d\omega = dx/\beta\hbar$. The first integral becomes

$$I_1 = \frac{1}{(\beta\hbar)^2} \int_0^\infty dx \frac{x}{e^x - 1} = \frac{1}{(\beta\hbar)^2} \int_0^\infty dx \sum_{s=1}^\infty e^{-sx} = \frac{1}{(\beta\hbar)^2} \sum_{s=1}^\infty \frac{\Gamma(2)}{s^2} = \frac{\pi^2}{6(\beta\hbar)^2}$$

and the second integral

$$\int_0^{\omega_D} d\omega \omega = \omega_D^2/2 \gg \frac{1}{(\beta\hbar)^2}$$

Thus in this limit the second integral will dominate. Substituting $\omega_d^3 = \frac{6\pi^2C^3N}{L^3}$ we will get

$$\langle s^2 \rangle_{T=0} = \frac{\hbar L^3}{8m\pi^2C^3} \left(\frac{6\pi^2C^3N}{L^3} \right)^{2/3} \propto L^2$$

$$\langle s^2 \rangle_{T=0} = \frac{3}{4} \frac{\hbar}{m\omega_D} = \frac{3}{4} \frac{\hbar^2}{mk\theta_D}$$

where we use $\hbar\omega_D = k\theta_D$. Substituting

$$\begin{cases} MAg = 107.87 \times (1.66053 \times 10^{-24}g) = 1.79 \times 10^{-22}g \\ \theta_D = 215k \text{ for } Ag \end{cases} \Rightarrow \langle s^2 \rangle_{T=0} = 1.57 \times 10^{-19} \text{cm}^2$$

The high T limit where $T = T_M = 1234k$

$$\langle s^2 \rangle = \frac{3\hbar}{2M\omega_D^3} \int_0^{\omega_D} d\omega \omega \left(\frac{2}{e^{\beta\hbar\omega} - 1} + 1 \right)$$

For large T

$$\begin{aligned} e^x &\simeq 1 + x = 1 + \frac{\hbar\omega}{k_B T} \Rightarrow e^{\beta\hbar\omega} - 1 = \frac{\hbar\omega}{k_B T} \\ \Rightarrow \langle s^2 \rangle &\simeq \frac{3\hbar}{2M\omega_D^3} \int_0^{\omega_D} d\omega \omega \left(\frac{2k_B T}{\hbar\omega} + 1 \right) \simeq \frac{3k_B T}{M\omega_D^2} = \frac{3T\hbar^2}{Mk_B\theta_D^2} \propto L^2 \end{aligned}$$

For estimation

$$\langle s^2 \rangle_{T=T_M} \simeq \frac{3(1234k)(1.0545 \times 10^{-27} \text{erg}\cdot\text{s})(7.638 \times 10^{-12})}{(1.79 \times 10^{-22})(215k)^2} \simeq 3.6 \times 10^{-18} \text{cm}^2$$

3. The dispersion relation for a linear chain is derived in Ashcroft and Mermin in chapter 22 page 430-432, where

$$\omega(k) = \sqrt{\frac{2f(1 - \cos(ka))}{M}}$$

for a diatomic linear chain the dispersion relation is (from Iback & Luth eq. 4.15 page 55)

$$\omega^2(k) = f(1/M_1 + 1/M_2) \pm f \left[(1/M_1 + 1/M_2)^2 - 4 \sin^2(kq/2)/(M_1 M_2) \right]^{1/2}$$

let $M_1 = M_2 = M$ and make the substitution $a \rightarrow 2a$, then

$$\omega^2 = \frac{2f}{M} \left(1 \pm \sqrt{1 - \sin^2(ka)} \right) \Rightarrow \omega = \sqrt{\frac{2f(1 - \cos(ka))}{M}}$$

We choose the minus sign because it is the acoustic branch.