Solid State Physics
Homework Set 4
Solutions

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

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

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 μth 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 $R - R' = d$

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

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

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 ij and $\hat{\mathbf{k}}$

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

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

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

using the commutation relation

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

where

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

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

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

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 $< s^2 >$ by converting the sum to integral.

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

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

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

$$< s^2 >_{T=0} = \frac{3}{4}\frac{\hbar}{m\omega_D} = \frac{3}{4}\frac{\hbar^2}{mk\theta_D}$$

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

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

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

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

For large T

$$e^x \simeq 1 + x = 1 + \frac{\hbar\omega}{k_B T} \Rightarrow e^{\beta\hbar\omega} - 1 = \frac{\hbar\omega}{k_B T}$$

$$\Rightarrow < s^2 > \simeq \frac{3\hbar}{2M\omega_D^3}\int_0^{\omega_D} d\omega\omega\left(\frac{2k_B T}{\hbar\omega}+1\right) \simeq \frac{3k_B T}{M\omega_D^2} = \frac{3T\hbar^2}{Mk_B\theta_D^2} \propto L^2$$

For estimation

$$< s^2 >_{T=T_M} \simeq \frac{3(1234k)(1.0545 \times 10^{-27}erg.s)(7.638 \times 10^{-12})}{(1.79 \times 10^{-22})(215k)^2} \simeq 3.6 \times 10^{-18}cm^2$$

3. The dispersion relation for a linear chain is derived in Aschroft 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)

$$\omega^2(k) = f(1/M_1 + 1/M_2) \pm f\left[(1/M_1 + 1/M_2)^2 - 4\sin^2(kq/2)/(M_1M_2)\right]^{1/2}$$

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.