

## PHYSICS 231

### Homework 2

Due in class, Friday October 14

#### Rescheduling of two lectures:

There will be no lecture on Monday October 17 and Wednesday October 19. Instead there will be makeup lectures on **Thursday October 20 and October 27, 12:00–1:10 pm. in ISB 231.**

#### 1. Diatomic Linear Chain

Consider a linear chain in which alternate ions have masses  $M_1$  and  $M_2$ , and only nearest neighbors interact.

(a) Show that the dispersion relation for normal modes is

$$\omega^2 = \frac{K}{M_1 M_2} \left( M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 \cos ka} \right), \quad (1)$$

where  $K$  is the spring constant, and  $a$  is the size of the unit cell (so the spacing between atoms is  $a/2$ ).

(b) Discuss the form of the dispersion relation and the nature of the normal modes when  $M_1 \gg M_2$ .

(c) Determine the dispersion relation when  $M_1 - M_2 \rightarrow 0$  and compare with that of the monatomic linear chain discussed in class.

#### 2. Nearest neighbor spring model

Consider a three-dimensional monatomic Bravais lattice in which each ion only interacts with its nearest neighbors. Assume that the interaction between neighboring ions is given by a Hooke's law potential,

$$\phi(\mathbf{r}_i - \mathbf{r}_j) = \frac{1}{2}K(|\mathbf{r}_i - \mathbf{r}_j| - d)^2, \quad (2)$$

where  $d$  is the equilibrium spacing between the atoms, and  $K$  is a spring constant. *n.b.* This model is equivalent to assuming that the atoms are connected by springs.

Show that the frequencies of the three normal modes for each wave vector  $\mathbf{k}$  are given by

$$\omega_s(\mathbf{k}) = \sqrt{\frac{\lambda_s(\mathbf{k})}{M}}, \quad (3)$$

where  $M$  is the mass and the  $\lambda_s(\mathbf{k})$  are eigenvalues of the  $3 \times 3$  matrix:

$$D_{\mu\nu}(\mathbf{k}) = 2K \sum_{R \neq 0} \sin^2\left(\frac{1}{2}\mathbf{k} \cdot \mathbf{R}\right) \hat{R}_\mu \hat{R}_\nu, \quad (4)$$

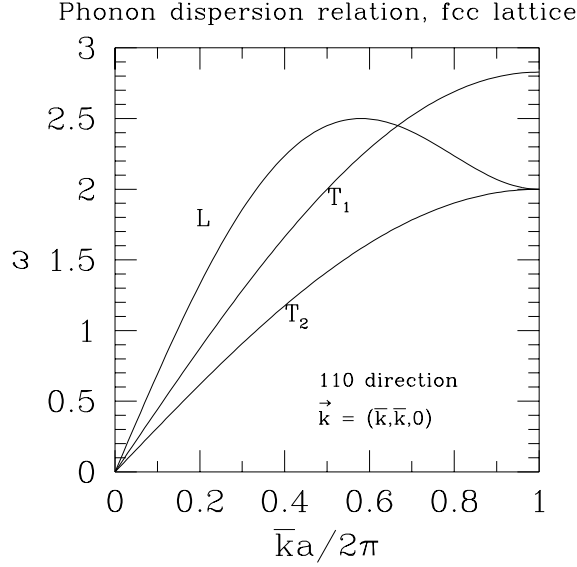
where the sum is over the nearest neighbors of the point  $\mathbf{R} = 0$ , and  $\hat{\mathbf{R}}$  is a unit vector in the direction of  $\mathbf{R}$ .

*n.b.* You may find Eqs. (22.59) and (22.11) of Ashcroft and Mermin are a convenient starting point.

#### 3. Normal modes of a fcc lattice

Consider the spring model for normal modes in the last question and apply it to the fcc lattice where the 12 nearest neighbor vectors are given by

$$\frac{a}{2}(\pm\hat{x} \pm\hat{y}), \quad \frac{a}{2}(\pm\hat{y} \pm\hat{z}), \quad \frac{a}{2}(\pm\hat{z} \pm\hat{x}). \quad (5)$$



- (a) Show that when  $\mathbf{k}$  is in the (100) direction,  $\mathbf{k} = (k, 0, 0)$ , then one normal mode is longitudinal with frequency

$$\omega_L = 2\sqrt{\frac{2K}{M}} \sin \frac{1}{4}ka, \quad (6)$$

and the other two are transverse and degenerate with frequency

$$\omega_T = 2\sqrt{\frac{K}{M}} \sin \frac{1}{4}ka. \quad (7)$$

- (b) Next consider  $\mathbf{k}$  to be in the (111) direction,  $\mathbf{k} = (\bar{k}, \bar{k}, \bar{k})$  so  $k = 3^{1/2}\bar{k}$ . Show that one normal mode is longitudinal with frequency

$$\omega_L = 2\sqrt{\frac{2K}{M}} \sin \frac{1}{2}\bar{k}a, \quad (8)$$

and the other two are transverse and degenerate with frequency

$$\omega_T = \sqrt{\frac{2K}{M}} \sin \frac{1}{2}\bar{k}a. \quad (9)$$

- (c) Consider  $\mathbf{k}$  to be in the (110) direction,  $\mathbf{k} = (\bar{k}, \bar{k}, 0)$  so  $k = 2^{1/2}\bar{k}$ . Show that one normal mode is longitudinal with frequency

$$\omega_L = 2\sqrt{\frac{K}{M} (\sin^2 \frac{1}{4}\bar{k}a + \sin^2 \frac{1}{2}\bar{k}a)}, \quad (10)$$

one is transverse and polarized along the  $z$ -axis with frequency

$$\omega_{T_1} = 2\sqrt{\frac{2K}{M}} \sin \frac{1}{4}\bar{k}a, \quad (11)$$

and the third is transverse and polarized perpendicular to the  $z$ -axis with frequency

$$\omega_{T_2} = 2\sqrt{\frac{K}{M}} \sin \frac{1}{4}\bar{k}a. \quad (12)$$

A sketch of the (110) dispersion relations is shown. Note that it is quite similar to the observed dispersion relation of  $Al$  shown, in Fig. (22.13) of Ashcroft and Mermin.

#### 4. Specific heat of a one-dimensional model

We showed in class that the phonon dispersion relation of a one-dimensional chain of atoms with nearest-neighbor harmonic forces is

$$\omega = \omega_0 \sin(k/2), \quad (13)$$

in units where the lattice spacing,  $a$ , is set to unity, and where  $\omega_0$  is the maximum phonon frequency.

- (a) Compute the group velocity and show that the density of states per atom is given by

$$\rho(\omega) = \frac{2}{\pi} \frac{1}{\sqrt{\omega_0^2 - \omega^2}}, \quad (14)$$

for  $0 < \omega < \omega_0$  and zero otherwise. (*n.b.* You should verify that  $\int \rho(\omega) d\omega = 1$  as required in one-dimension.)

- (b) Explain physically why the density of states *diverges* as  $\omega \rightarrow \omega_0$ . (*n.b.* This is an example of a Van Hove singularity.)

- (c) In the Debye theory one takes an approximate form for the density of states,  $\rho_D(\omega)$ , as follows; the form of  $\rho(\omega)$  obtained at low frequency is assumed to be valid at *all* frequencies up to a cut-off,  $\omega_D$ , determined by the requirement that  $\int \rho(\omega) d\omega$  is correctly given.

One defines  $\hbar\omega_D = k_B\Theta_D$ , where  $\Theta_D$  is the Debye temperature. Determine  $\rho_D(\omega)$  and show that

$$\omega_D = \frac{\pi}{2}\omega_0. \quad (15)$$

- (d) Sketch  $\rho(\omega)$  and  $\rho_D(\omega)$ .

- (e) Show that the Debye specific heat per atom in one dimension is given by

$$\frac{C_D}{k_B} = \frac{T}{\Theta_D} \int_0^{\Theta_D/T} \frac{x^2 e^x}{(e^x - 1)^2} dx. \quad (16)$$

- (f) Consider the limit  $T \rightarrow 0$ , in which case the upper limit in the integral can be sent to  $\infty$ . By expanding the integral in powers of  $\exp(-x)$ , integrating each term, and using the result that

$$\zeta(2) \equiv \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}, \quad (17)$$

show that

$$\frac{C_D}{k_B} = \frac{\pi^2}{3} \frac{T}{\Theta_D} \quad (T \rightarrow 0) \quad . \quad (18)$$

- (g) Consider the limit  $T \rightarrow \infty$ . Show that

$$\frac{C_D}{k_B} = 1 \quad (T \rightarrow \infty) \quad , \quad (19)$$

which is the Dulong-Petit law in one-dimension.

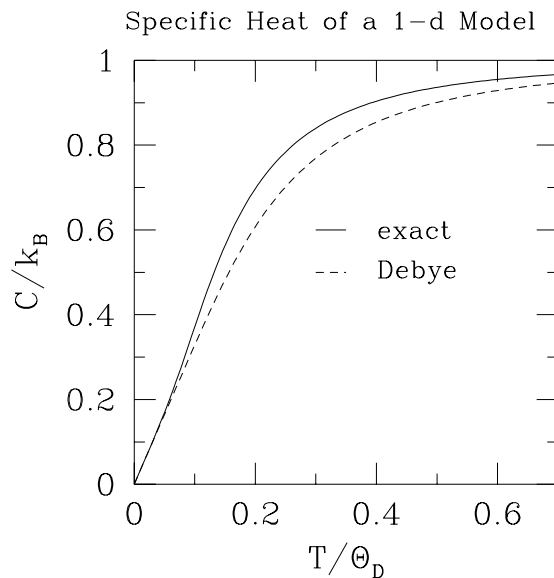
(h) Show that the specific heat obtained using the exact density of states is given by

$$\frac{C}{k_B} = \frac{2}{\pi} \frac{1}{t^2} \int_0^{\pi/2} \frac{e^{\sin \phi/t} \sin^2 \phi}{(e^{\sin \phi/t} - 1)^2} d\phi, \quad (20)$$

where  $t = k_B T / \hbar \omega_0$ .

(i) Evaluate this last expression in the limits  $T \rightarrow 0$  and  $T \rightarrow \infty$  and show that the Debye theory results, Eqs. (18) and (19), are correct in these limits.

*n.b.* This is not a surprise since the Debye theory is cooked up precisely to get these two limits correct. For intermediate temperatures the Debye theory does not agree with the exact calculations, see the figure. However, considering it makes a very crude approximation for the density of states (see your answer to problem (4d) ), the agreement for the specific heat is not too bad. This is because the specific heat is given by a rather crude average over the density of states and is insensitive to its detailed structure.



### 5. Van Hove singularities in two and three dimensions

You showed in the previous question that a *maximum* in the phonon dispersion curve in one dimension gives rise to an inverse square root divergence in the density of states. Show that in two dimensions, a maximum gives a discontinuity in the density of states and that in three dimensions it gives a square root cusp.

*n.b.* Take the dispersion to be of the form

$$\omega = \omega_0 - A|\mathbf{k} - \mathbf{k}_0|^2 \quad (A > 0) \quad (21)$$

near the maximum at  $\mathbf{k} = \mathbf{k}_0, \omega = \omega_0$ .