Solutions for Homework Set 3

1. *Kittel Problem 4.4*

Solution

The force constant between the p and $p+s$ planes of atoms is given by

$$C_p = A\left(\frac{\sin(pk_0a)}{pa}\right),$$

and so we generalise the dispersion equation in *Kittel* Equation (4.16a) viz.

$$\omega^2 = \frac{2}{M}\sum_{p>0} C_p\left(1-\cos(pka)\right), \tag{1}$$

to give

$$\omega^2 = \frac{2}{M}\sum_{p>0} A\left(\frac{\sin(pk_0a)}{pa}\right)\left(1-\cos(pka)\right). \tag{2}$$

The derviative is given by differentiating through the sum

$$\frac{\mathrm{d}\omega^2}{\mathrm{d}k} = \frac{2A}{M}\sum_{p>0}\left[\sin(pak)\sin(pak_0)\right]. \tag{3}$$

When $k=k_0$ then the sum becomes

$$\frac{\mathrm{d}\omega^2}{\mathrm{d}k} = \frac{2A}{M}\sum_{p>0}\sin(kpa)^2, \tag{4}$$

which for $ka \neq m\pi$ diverges. For $ka = m\pi$, the sin terms vanish and the sum gives exactly zero.

2. *Kittel Problem 4.5*

Solution

This problem is calculated largely analogously to the two atom lattice example in *Kittel*, Chapter 4. The equations of motion are given by

$$\begin{aligned}
M\frac{\mathrm{d}^2u_s}{dt^2} &= 10C(v_s-u_s)-C(u_s-v_{s-1}),\\
&= C(10v_s+v_{s-1}-11u_s); \qquad (5)\\
M\frac{\mathrm{d}^2v_s}{dt^2} &= 10C(u_s-v_s)-C(v_s-u_{s+1}),\\
&= C(10u_s+u_{s+1}-11v_s). \qquad (6)\\
& \qquad (7)
\end{aligned}$$

We look for plane wave solutions

$$\begin{aligned}
u_s &= u_0e^{-i(\omega t - sKa)},\\
v_s &= v_0e^{-i(\omega t - sKa)}. \qquad (8)
\end{aligned}$$

The equations of motion (5) and (6) become,

$$-M\omega^2u = C\left(10v_0+v_0e^{-iKa}-11u_0\right) \tag{9}$$

$$-M\omega^2v = C\left(10u_0+u_0e^{iKa}-11v_0\right). \tag{10}$$

We can rewrite this as a matrix equation,

$$\begin{pmatrix} -M\omega^2 + 11C & -10C - Ce^{-iKa} \\ -10C - Ce^{iKa} & -M\omega^2 + 11C \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{11}$$

This is a simple eigenvalue equation which we solve in the usual way. That is, we first require that the determinant vanish which will give us the dispersion equation. This gives us

$$M^2\omega^4 - 22M\omega^2 C + 20C^2(1 - \cos Ka) = 0. \tag{12}$$

The dispersion equation is then given by

$$\omega^2 = \frac{11C}{M} \pm \frac{\sqrt{101C^2 + 20C^2 \cos Ka}}{M}. \tag{13}$$

The eigenvectors can be extracted in the usual manner, though this is rather tedious to do and for our purposes not needed. However, we can see by inspection that the two modes given by the $\pm$ above correspond to the acoustic and optical modes respectively. This can be seen by plotting the dispersion equation below.

At $K = 0$, the cutoff frequencies are $\omega = 0$, and $\omega = \sqrt{22C/M}$ for the acoustic and optical modes respectively.

At $K = \pi/a$ the modes reduce to $\omega = \sqrt{20C/M}$, and $\omega = \sqrt{2C/m}$.

The dispersion equation is shown below in Figure 1, which illustrate the acoustic and optical branches.

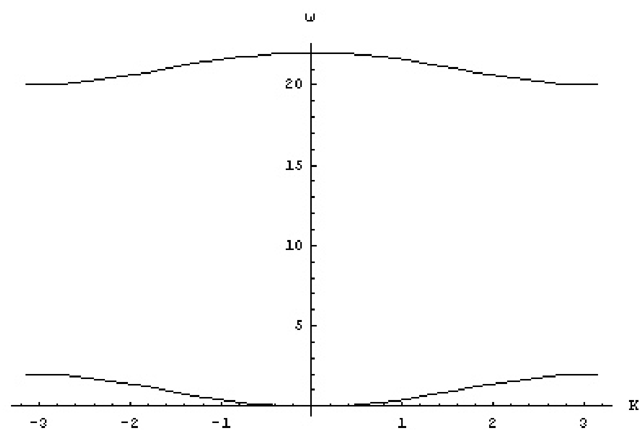

Figure 1: Dispersion equation for Problem 4.5

3. *Kittel Problem 4.6*

(a) This is a problem in electrostatics, but is good to get an idea of lattice vibrations in a rather crude way. We imagine at each lattice point there is an ion and there is a cloud of negative charge surrounding each ion. If the ion moves a distance r from the lattice point, then the force on the ion is due to the electric charge enclosed in a sphere of radius r centred at the lattice point. Hence, if ρ is the density of electric charge then the electric field a distance r from the lattice point is the same as that in a uniformly charged sphere of radius R. A simple calculation using Gauss's law gives the electric field in a uniformly charged sphere is (in SI units):

$$\mathbf{E} = -\frac{er}{4\pi\varepsilon_0 R^3}\hat{\mathbf{r}}.$$

The force on the ion is then

$$\mathbf{F} = \frac{e^2 r}{4\pi\varepsilon_0 R^3}.$$

This is like the force due to that on a spring, with spring constant $k = e^2/(r\pi\varepsilon_0 R^3)$ with natural frequency given by

$$\omega = \sqrt{\frac{e^2}{4\pi\varepsilon_0 m R^3}}.$$

(b) For sodium the mass of a single atom is $m \approx 22.9/6.02 \times 10^{23} \approx 3.8 \times 10^{-23}$g. The lattice radius of a sodium atom $R \approx 3.7 \times 10^{-10}$ (*Ashcroft and Mermin*), and this gives a frequency of

$$\omega \approx 1.1 \times 10^{13}\text{Hz}. \tag{14}$$

(c) A variety of estimates can be used here, so in this context most are equally valid. An example is to take the wavelength of the sound wave to be of the order the length of the ion. Then, $K = \pi/R$ and the velocity of sound becomes

$$v_s = \frac{\omega}{K} \approx 10^3\text{m/s}. \tag{15}$$

4. *Kittel Problem 5.1*

(a) The dispersion equation from Chapter 4 of *Kittel* is given by

$$\omega = \omega_m |\sin Ka/2|, \tag{16}$$

with $\omega_m = (4C/m)^{1/2}$. The group velocity is given by

$$\left|\frac{\mathrm{d}\omega}{\mathrm{d}K}\right| = \frac{\omega_m\, a \cos(Ka/2)}{2}, \tag{17}$$

and so the density of states $\mathcal{D}(\omega)$ is given by

$$\begin{aligned} \mathcal{D}(\omega) &= \frac{L}{2\pi}\frac{1}{|\mathrm{d}\omega/\mathrm{d}K|}, \\ &= \frac{2L}{\omega_m\,\pi\, a}\frac{1}{\sqrt{1-\omega^2/\omega_m^2}}, \\ &= \frac{N}{\pi}\frac{1}{\sqrt{\omega_m^2-\omega^2}}. \end{aligned} \tag{18}$$

(b) The dispersion equation

$$\omega = \omega_0 - AK^2,$$

implies that for all K, we have $\omega \le \omega_0$ and hence there are no states for $\omega > \omega_0$. Therefore, $\mathcal{D}(\omega) = 0$ for $\omega > \omega_0$. For $\omega \le \omega_0$ we have $\mathrm{grad}\,\omega = -2A(k_x, k_y, k_z)$ and hence the density of states becomes

$$\begin{aligned} \mathcal{D}(\omega) &= \frac{VK^2}{2\pi^2}\frac{1}{|\mathrm{grad}\,\omega|}, \\ &= \frac{V}{4\pi^2 A^{3/2}}\sqrt{\omega_0-\omega}. \end{aligned} \tag{19}$$