1. (ISSP 3.3) Basis of two unalike atoms.

   At $k = \pi/a$, equation (20) becomes

$$\left(2 - \frac{\omega^2 M_1}{C}\right) u = 0 \qquad \left(2 - \frac{\omega^2 M_2}{C}\right) v = 0$$

   Note that the u and v sub-lattices are decoupled at this value of k; u can change without changing v, and vice versa. There are two solutions to the above equations: $u = 0$, $\omega^2 = 2C/M_2$ and v arbitrary; and $v = 0$, $\omega^2 = 2C/M_1$ and u arbitrary.

2. (ISSP 3.4) Kohn anomaly. Equation (16a) gives

$$\begin{aligned}\omega^2 &= \frac{2A}{M} \sum_{p=1}^{\infty} \frac{\sin pk_0 a}{pa}(1 - \cos(pka)) \\ &= \frac{2A}{Ma} \sum_{p=1}^{\infty} \left(\frac{\sin pk_0 a}{p} - \frac{1}{2}\frac{\sin p(k_0 + k)a}{p} - \frac{1}{2}\frac{\sin p(k_0 - k)a}{p} \right)\end{aligned}$$

   Gradshteyn and Ryzhik (*Table of integrals, series and products*)1.441 gives

$$\sum_{p=1}^{\infty} \frac{\sin \alpha p}{p} = \frac{\pi - \alpha}{2} \qquad 0 < \alpha < 2\pi$$

   (you can prove this by writing the sin as the sum of two exponentials, and then using the taylor expansion of $log(1 + x)$.)

   So for $k_0 > k$, we have

$$\begin{aligned}\omega^2 &= \frac{2A}{Ma} \sum_{p=1}^{\infty} \left(\frac{\sin pk_0 a}{p} - \frac{1}{2}\frac{\sin p(k_0 + k)a}{p} - \frac{1}{2}\frac{\sin p(k_0 - k)a}{p} \right) \\ &= \frac{2A}{Ma} \left(\frac{\pi - k_0 a}{2} - \frac{1}{2}\frac{\pi - (k_0 + k)a}{2} - \frac{1}{2}\frac{\pi - (k_0 - k)a}{2} \right) \\ &= 0\end{aligned}$$

   Now consider the case where $k_0 < k$. In order to apply the formula from the tables we need the argument of each sin function to be positive. Then

$$\begin{aligned}\omega^2 &= \frac{2A}{Ma} \sum_{p=1}^{\infty} \left(\frac{\sin pk_0 a}{p} - \frac{1}{2}\frac{\sin p(k_0 + k)a}{p} - \frac{1}{2}\frac{\sin p(k_0 - k)a}{p} \right) \\ &= \frac{2A}{Ma} \sum_{p=1}^{\infty} \left(\frac{\sin pk_0 a}{p} - \frac{1}{2}\frac{\sin p(k_0 + k)a}{p} + \frac{1}{2}\frac{\sin p(k - k_0)a}{p} \right)\end{aligned}$$

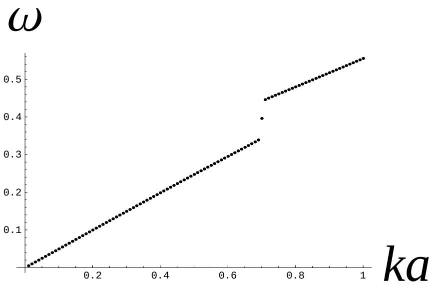

Figure 1: Dispersion for Q2, where I have added a nearest neighbour coupling. For a formula for the $\omega(k)$ that I've plotted, see the text. The units for frequency are arbitrary.

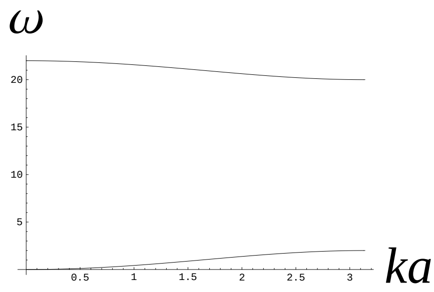

Figure 2: Q3: diatomic chain. Dispersion for the system with springs alternating between 1 and 10. The units for frequency are arbitrary.

Evaluating this gives

$$\begin{aligned}\omega^2 &= \frac{2A}{Ma}\left(\frac{\pi - k_0 a}{2} - \frac{1}{2}\frac{\pi - (k_0+k)a}{2} + \frac{1}{2}\frac{\pi - (k-k_0)a}{2}\right)\\ &= \frac{2A}{Ma}\frac{\pi}{2}\end{aligned}$$

So ω^2 is constant except at $k = k_0$ where it steps up (or down, depending on the sign of A.) Recall that the derivative of a step function is a delta function; therefore

$$\frac{\partial\omega^2}{\partial k} = \frac{2A}{Ma}\frac{\pi}{2}\delta(k-k_0)$$

and so it is indeed infinite at $k = k_0$.

To get a sense of how this kink would show up, we can add a nearest neighbour coupling (which will give a term that goes like $\sin^2(ka/2)$ in ω^2) In figure 1 I plotted (with $A > 0$)

$$\omega = \sqrt{\sin^2(ka/2) + 0.05\sum_{p=1}^{5000}\frac{\sin 0.7p}{p}(1-\cos(pka))}$$

3. (ISSP 3.5) Diatomic chain.

Consider the situation shown in the figure (at the end we will set $C_1 = C$ and $C_2 = 10C$. Then

$$m\frac{d^2u_n}{dt^2} = -(C_2(u_n - v_{n-1}) + C_1(v_n - u_n))$$

$$m\frac{d^2v_n}{dt^2} = -(C_1(v_n - u_n) + C_2(u_{n+1} - v_n))$$

Setting $u_n = ue^{ikna}$, $v_n = ve^{ikna}$, and then dividing both equations by e^{ikna} gives

$$\begin{pmatrix} C_1 + C_2 - m\omega^2 & -(C_1 + C_2 e^{-ika}) \\ -(C_1 + C_2 e^{ika}) & C_1 + C_2 - m\omega^2 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = 0$$

Then

$$(C_1 + C_2 - m\omega^2)^2 + (C_1 + C_2 e^{-ika})(C_1 + C_2 e^{ika}) = 0$$

This can be simplified to

$$(m\omega^2)^2 - 2(C_1 + C_2)m\omega^2 + 4C_1C_2 \sin^2(ka/2) = 0$$

The solution is

$$m\omega^2 = (C_1 + C_2) \pm \sqrt{C_1^2 + C_2^2 + 2C_1C_2 \cos ka}$$

and

$$\frac{v}{u} = \mp \frac{C_1 + C_2 e^{ika}}{|C_1 + C_2 e^{ika}|}$$

Note that the atoms are out of phase in the upper branch and in phase on the lower branch. At $k = 0$ we have

$$\omega = 0 \qquad \text{and} \qquad \omega = \sqrt{\frac{2(C_1 + C_2)}{m}}$$

At $k = \pi/a$, we have

$$m\omega^2 = (C_1 + C_2) \pm \sqrt{(C_1 - C_2)^2} = (C_1 + C_2) \pm (C_1 - C_2)$$

Therefore

$$\omega_1 = \sqrt{\frac{2C_2}{m}} \qquad \omega_2 = \sqrt{\frac{2C_1}{m}}$$

4. (ISSP 3.6) Atomic vibrations in a metal.

   (a) By Gauss's law, the displaced ion feels a force due to the electrons in the sphere of radius r; ie

   $$F = -\frac{3e}{4\pi R^3}\frac{4\pi r^3}{3}\frac{e}{r^2} = -\frac{e^2}{R^3}r$$

   Then

   $$M\omega^2 = \frac{e^2}{R^3} \Rightarrow \omega = \left(\frac{e^2}{MR^3}\right)^{1/2}$$

   (b) For sodium, $e^2/R \simeq (e^2/2a_B)(1/5) = 13.6eV/5 \simeq 2eV \simeq 4 \times 10^{-19}J$.

   $$\omega \simeq \left(\frac{4 \times 10^{-19}}{(30 \times 10^{-27})(25 \times 10^{-20})}\right)^{1/2} \simeq \left(\frac{10^{-19}}{10^{-26}10^{-19}}\right)^{1/2} \simeq 10^{13}s^{-1}$$

(c) In part (a), we found the vibrational frequency of an ion when the others are kept fixed. The spring constant for this motion (I'll denote this K) is given by

$$\omega = \sqrt{\frac{K}{M}} \Rightarrow K = M\omega^2 = \frac{e^2}{R^3}$$

We can use this to find the spring constant that appears in the full hamiltonian. Suppose the full potential is (I'll stick to one-dimensional notation for convenience sake)

$$V = \sum_n \frac{C}{2}(u_n - u_{n+1})^2$$

If all the ions are kept fixed except the zeroth one, then the effective potential is

$$V = z\frac{C}{2}u_0^2$$

where z is the number of nearest neighbours. Since this must be the spring constant that determined the motion in part (a), we can write

$$zC = K \Rightarrow C = K/z$$

Note that the speed of sound in a one-dimensional solid (similar relations are true in higher dimensions) is given by

$$v^2 = \frac{C}{M}a^2 = \frac{1}{z}\frac{K}{M}a^2 = \frac{1}{z}(10^{13})^2(4 \times 10^{-10})^2$$

For a bcc lattice $z = 8$, giving

$$v \simeq \sqrt{2} \times 10^3 \simeq 10^3 m/s$$

According to wikipedia, the speed of sound in sodium is about 3×10^3 m/s.