CHAPTER 4

1a. The kinetic energy is the sum of the individual kinetic energies each of the form $\frac{1}{2}\,M\dot{u}_S{}^2$. The force between atoms s and s+1 is $-C(u_s - u_{s+1})$; the potential energy associated with the stretching of this bond is $\frac{1}{2}C(u_s - u_{s+1})^2$, and we sum over all bonds to obtain the total potential energy.

b. The time average of $\frac{1}{2}\,M\dot{u}_S{}^2$ is $\frac{1}{4}\,M\omega^2u^2$. In the potential energy we have

$$u_{s+1} = u\cos[\omega t - (s+1)Ka] = u\{\cos(\omega t - sKa)\cdot\cos Ka$$
$$+ \sin(\omega t - sKa)\cdot\sin Ka\}.$$

$$\text{Then}\quad u_s - u_{s+1} = u\,\{\cos(\omega t - sKa)\cdot(1-\cos Ka)$$
$$- \sin(\omega t - sKa)\cdot\sin Ka\}.$$

We square and use the mean values over time:

$$< \cos^2 > \; = \; < \sin^2 > \; = \frac{1}{2}\,; \; < \cos\sin > \; = 0.$$

Thus the square of u{} above is

$$\frac{1}{2}u^2[1 - 2\cos Ka + \cos^2 Ka + \sin^2 Ka] = u^2(1 - \cos\ Ka).$$

The potential energy per bond is $\frac{1}{2}Cu^2(1-\cos\ Ka)$, and by the dispersion relation $\omega^2 = (2C/M)(1 - \cos Ka)$ this is equal to $\frac{1}{4}M\omega^2u^2$. Just as for a simple harmonic oscillator, the time average potential energy is equal to the time-average kinetic energy.

2. We expand in a Taylor series

$$u(s+p) = u(s) + pa\left(\frac{\partial u}{\partial x}\right)_s + \frac{1}{2}p^2a^2\left(\frac{\partial^2 u}{\partial x^2}\right)_s + \cdots\,;$$

On substitution in the equation of motion (16a) we have

$$M\frac{\partial^2 u}{\partial t^2} = (\sum_{p>0} p^2a^2C_p)\frac{\partial^2 u}{\partial x^2}\quad ,$$

which is of the form of the continuum elastic wave equation with

$$v^2 = M^{-1} \sum_{p>0} p^2 a^2 C_p .$$

3. From Eq. (20) evaluated at $K = \pi/a$, the zone boundary, we have

$$-\omega^2 M_1 u = -2Cu \ ;$$
$$-\omega^2 M_2 v = -2Cv \ .$$

Thus the two lattices are decoupled from one another; each moves independently. At $\omega^2 = 2C/M_2$ the motion is in the lattice described by the displacement v; at $\omega^2 = 2C/M_1$ the u lattice moves.

4. $$\omega^2 = \frac{2}{M} A \sum_{p>0} \frac{\sin pk_0 a}{pa} (1 - \cos pKa) \ ;$$

$$\frac{\partial \omega^2}{\partial K} = \frac{2A}{M} \sum_{p>0} \sin\ pk_0 a\ \sin\ pKa$$

$$\frac{1}{2}\ (\cos\,(k_0 - K)\ pa - \cos\ (k_0 + K)\ pa)$$

When $K = k_0$,

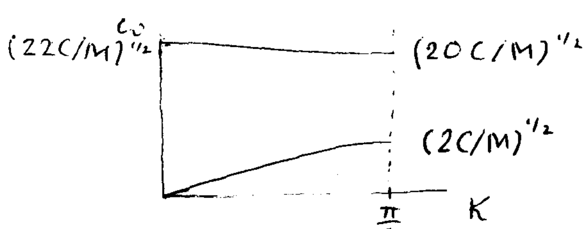
$$\frac{\partial \omega^2}{\partial K} = \frac{A}{M} \sum_{p>0} (1 - \cos\ 2k_0 pa) \ ,$$

which in general will diverge because $\sum_p 1 \to \infty$.

5. By analogy with Eq. (18),

$$Md^2u_s/dt^2 = C_1(v_s - u_s) + C_2(v_{s-1} - u_s);$$
$$Md^2v_s/dt^2 = C_1(u_s - v_s) + C_2(u_{s+1} - v_s), \ \text{whence}$$
$$-\omega^2 Mu = C_1(v - u) + C_2(ve^{-iKa} - u);$$
$$-\omega^2 Mv = C_1(u - v) + C_2(ue^{iKa} - v) \ , \ \text{and}$$

$$\begin{vmatrix} (C_1 + C_2) - M\omega^2 & -(C_1 + C_2 e^{-iKa}) \\ -(C_1 + C_2 e^{iKa}) & (C_1 + C_2) - M\omega^2 \end{vmatrix} = 0$$



For $Ka = 0$, $\omega^2 = 0$ and $2(C_1 + C_2)/M$.
For $Ka = \pi$, $\omega^2 = 2C_1/M$ and $2C_2/M$.

6. (a) The Coulomb force on an ion displaced a distance r from the center of a sphere of static or rigid conduction electron sea is $-e^2\ n(r)/r^2$, where the number of electrons within a sphere of radius r is $(3/4\ \pi R^3)\ (4\pi r^3/3)$. Thus the force is $-e^2 r/R^2$, and the

force constant is e^2/R^3. The oscillation frequency ω_D is (force constant/mass)$^{1/2}$, or $(e^2/MR^3)^{1/2}$. (b) For sodium $M \simeq 4\times10^{-23}$ g and $R \simeq 2\times10^{-8}$ cm; thus $\omega_D \simeq (5\times10^{-10})\ (3\times10^{-46})^{1/2}$ $\simeq 3\times10^{13}\ s^{-1}$ (c) The maximum phonon wavevector is of the order of 10^8 cm^{-1}. If we suppose that ω_0 is associated with this maximum wavevector, the velocity defined by $\omega_0/K_{max} \approx 3\times10^5$ cm s^{-1}, generally a reasonable order of magnitude.

7. The result (a) is the force of a dipole $e_p\ u_p$ on a dipole $e_0\ u_0$ at a distance pa. Eq. (16a) becomes $\omega^2 = (2/M)[\gamma(1-\cos Ka) + \sum_{p>0}(-1)^P(2e^2/p^3a^3)(1-\cos\ pKa)]$.

At the zone boundary $\omega^2 = 0$ if

$$1+\sigma\sum_{p>0}(-1)^P[1-(-1)^P]p^{-3} = 0\ ,$$

or if $\sigma\ \Sigma[1-(-1)^p]p^{-3} = 1$. The summation is $2(1 + 3^{-3} + 5^{-3} + \ldots) = 2.104$ and this, by the properties of the zeta function, is also $7\ \zeta\ (3)/4$. The sign of the square of the speed of sound in the limit $Ka \ll 1$ is given by the sign of $1 = 2\sigma\sum_{p>0}(-1)^p p^{-3}p^2$, which is zero when $1 - 2^{-1} + 3^{-1} - 4^{-1} + \ldots = 1/2\sigma$. The series is just that for log 2, whence the root is $\sigma = 1/(2\log 2) = 0.7213$.