CHAPTER 4

1a. The kinetic energy is the sum of the individual kinetic energies each of the form $\frac{1}{2} M u^2$. 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 $\frac{1}{2} M u^2$ is $\frac{1}{4} M \langle \omega^2 \rangle^2$. In the potential energy we have

$$u_{s+1} = u \cos(\omega t - (s+1)K) = u \{\cos(\omega t - sK) \cdot \cos K a + \sin(\omega t - sK) \cdot \sin K a\}.$$ 

Then

$$u_s^* - u_{s+1} = u (\cos(\omega t - sK) \cdot (1 - \cos K a) - \sin(\omega t - sK) \cdot \sin K a).$$

We square and use the mean values over time:

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

Thus the square of $u(\omega)$ above is

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

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

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

$$-\omega^2 M u = -2Cu;$$

$$-\omega^2 M v = -2Cv.$$

Thus the two lattices are decoupled from one another; each moves independently. At $\omega^2 = 2C/M$, the motion is in the lattice described by the displacement $v$; at $\omega^2 = 2C/M$, the $u$ lattice moves.
5. By analogy with Eq. (18),

\[
\begin{align*}
\text{Md}^2 \dot{u}_y / \text{dt}^2 &= C_1 (v_y - u_y) + C_2 (v_{y+1} - u_y); \\
\text{Md}^2 \dot{v}_y / \text{dt}^2 &= C_1 (u_y - v_y) + C_2 (u_{y+1} - v_y),
\end{align*}
\]

whence

\[
\begin{align*}
-\omega^2 \text{Mu} &= C_1 (v - u) + C_2 (v e^{-\text{i}k a} - u); \\
-\omega^2 \text{Mv} &= C_1 (u - v) + C_2 (u e^{\text{i}k a} - v),
\end{align*}
\]

and

\[
\begin{bmatrix}
(C_1 + C_2) - \lambda \omega^2 & -(C_1 + C_2 e^{-\text{i}k a}) \\
-(C_1 + C_2 e^{\text{i}k a}) & (C_1 + C_2) - \lambda \omega^2
\end{bmatrix} = 0
\]

For \( K a = 0 \), \( \omega^2 = 0 \) and \( 2(C_1 + C_2)/M \).

For \( K a = \pi \), \( \omega^2 = 2C_1/M \) and \( 2C_2/M \).

5. (a) The Coulomb force on an ion displaced \( a \).

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(2C/m)^{1/2} \quad \frac{\text{d}^2 C}{\text{d}t^2} \quad K
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(2C/m)^{1/2} \quad \pi
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