Chapter 4

Lattice Waves and Phonons

(Supplement on Harmonic-Oscillator Model)
4.1.1. Coupled Harmonic Oscillator Model

In the spirit of explaining fundamental aspects of the solid state in a manner accessible to engineers and applied scientists, we embark with a quick review of the mechanical harmonic oscillator model and its simple but sometimes forgotten predictions, many of which carry over to lattice-wave behavior in solids. The model of choice is the mass-spring system of Fig. 4.1(a). The mass corresponds to an atom in the solid, assuming that that atomic location can be quantified by a single point in space. The spring represents the Hooke’s law approximation (i.e., “linearity”) as we have seen previously and that is universally true in solids if the atoms are displaying only small deformation from their relaxed lattice sites. To relate to the infinite lattice analysis that comes later, we embed the mass between two springs, each of spring constant C and each connected to a rigid wall. This creates a mechanically symmetric system that mimics the physical environment of an atom embedded in the solid.

To formulate the dynamics, we suppose the mass is displaced by a small amount $\Delta r$ from its equilibrium position as shown in Fig. 4.1(b), and then released. The force on the mass from the left spring is $F_l = -C\Delta r \mathbf{r}$, and the force from the right spring is $F_r = -C\Delta r \mathbf{r}$, where $\mathbf{r}$ is the unit vector shown in 4.1(b). Thus by linear superposition, the net force equation becomes

$$F = F_r + F_l = -2C\Delta r \mathbf{r} = m \frac{d^2 \Delta r}{dt^2} \mathbf{r}$$

(1)

where the last step follows from Newton’s 2nd law. We anticipate based on experience that the mass will undergo oscillatory motion described by the $\Delta r = \text{Re}\{A\exp(j\omega t)\}$, using phasor

![Fig. 4.1.](image)

(a) Single-mass harmonic oscillator model. (b) Displacement of mass $\Delta r$ from equilibrium position. (c) Two-mass harmonic oscillator model
representation with $A$ as an arbitrary complex constant. Substitution into the equation of motion and exchanging the order of the Re operator with $\frac{d}{dt}$, we get (after cancellations) $2C = m\omega^2$ or

$$\omega = \sqrt{\frac{2C}{m}} \quad (4.2)$$

This result from elementary physics is called the natural oscillation frequency, or simply the resonance frequency. The factor of two arises from the judicious use of two springs in the model.

With the same set of assumptions, we can step forward to a more relevant model, the two-mass coupled-harmonic-oscillator shown in Fig. 4.1(c). Now we have two masses to deal with, each represented by its displacement $\Delta r_1$ and $\Delta r_2$ with respect to their respective equilibrium positions. Both are assumed to be subject to Hooke’s law forces from the neighboring springs such that the net force on mass 1, $F_1$, is given by

$$F_1 = -C\Delta r_1 r + C(\Delta r_2 - \Delta r_1 ) r = m_1 d^2 \Delta r_1/\Delta t^2 r \quad (4.3)$$

and

$$F_2 = -C\Delta r_2 r + C(\Delta r_1 - \Delta r_2 ) r = m_1 d^2 \Delta r_2/\Delta t^2 r \quad (4.4)$$

As before, we seek sinusoidal oscillation frequencies but now must allow for two possible complex phasor amplitudes

$$\Delta r_1 = \text{Re}\{A_1\exp(j\omega t)\} \quad \text{and} \quad \Delta r_2 = \text{Re}\{A_2\exp(j\omega t)\} \quad (4.5)$$

Substitution of these into (4.3) and (4.4) yields

$$-CA_1 + C(A_2 - A_1) = -m\omega^2 A_1 \quad (4.6)$$

$$-CA_2 + C(A_1 - A_2) = -m\omega^2 A_2$$

This is a pair of coupled linear equations, which by inspection can be exactly represented by the matrix form

$$\begin{pmatrix} m\omega^2 - 2C & C \\ C & m\omega^2 - 2C \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = 0 \quad (4.7)$$

This can be solved by some elegant, but often forgotten, mathematical tools.

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**Quick Review of Useful Results from Linear Algebra**

Suppose we have a system of linear equations represented by $M \cdot V = 0$ where $M$ is a matrix
and \( V \) is a column vector. Suppose also that \( M \) and \( V \) represent a real physical system for which we know a real, unique, non-zero solution exists. Then the trivial solution, \( V = 0 \) cannot exist. So the fact that there is a unique solution forces us to discard the trivial solution as a possibility.

Now suppose that the matrix is invertible, i.e., \( M^{-1} \) exists such that \( M^{-1} \cdot M = I \), where \( I \) is the unit matrix (one along diagonal, zeroes elsewhere). If this is true, then we could invert \( M \cdot V = 0 \) by multiplying both sides by \( M^{-1} \) to get \( V = 0 \). To prevent this possibility, we must require that \( M \) not be invertible. And from yet another theorem of linear algebra, the condition that \( M \) not be invertible also means that the determinant of \( M \) vanish, i.e., \( \det \{ M \} = 0 \).

Taking the determinant of the 2x2 matrix in (4.7) we get

\[
m^2 \omega^4 - 4Co\omega^2 + 3C^2 = 0
\]

Although a quartic equation, this is easily soluble by reduction to a quadratic form with the substitution \( v = \omega^2 \), leading to the solution

\[
\omega = \left( \frac{4C / m \pm \sqrt{16C^2 / m^2 - 12C^2 / m^2}}{2} \right)^{1/2}
\]

There are clearly two possible solutions for the natural frequency

\[
\omega_2 = \sqrt{\frac{3C}{m}} \quad \text{and} \quad \omega_1 = \sqrt{\frac{C}{m}} \quad (4.8)
\]

Each of these represents two possible solutions such that each mass oscillates with the same frequency but possibly different phase (through the complex factors \( A_1 \) and \( A_2 \)).

One important aspect of (4.8), present in coupled oscillators of all types, is the splitting in oscillation frequency compared to the single-mass solution of Eqn (4.1).\(^1\) This is displayed through the “fan” diagram in Fig. 4.2(a). One of the solution frequencies in (4.8) is higher, the other is lower, and the number of frequencies equals the number of masses. A second aspect is that the two solutions of (4.5) are linearly independent, as made manifest by their matrix representation in (4.7). Thus any arbitrary motion of the two masses can be represented as the linear superposition of these two functions provided, of course, that the magnitudes of \( A_1 \) and \( A_2 \)

\(^1\) This effect carries over to quantum mechanics as well where the coupling of two energetically-degenerate wavefunctions will be split under the action of a perturbative coupling.
are small enough that Hooke’s law remains valid. This is the basis for their descriptor “normal modes” in the physics literature.

Given the solution frequencies (4.8) we can determine $A_1$ and $A_2$ simply by substitution into (4.6). Substitution of the $\omega_1$ solution yields

$$CA_1 - CA_2 = 0 \quad \text{or} \quad A_1 = A_2. \quad (4.9)$$

Substitution of the $\omega_2$ solution yields

$$CA_1 + CA_2 = 0 \quad \text{or} \quad A_1 = -A_2 \quad (4.10)$$

Clearly, the $\omega_1$ solution corresponds to an in-phase relation (0 relative phase shift) between the two atoms, and the $\omega_2$ solution corresponds to an anti-phase ($\pi$ relative phase shift) relation. A “snapshot” of the relative motion for the two solutions is shown in Fig. 4.2(b), and is consistent with their large splitting in frequency based on the following reasoning. When the two atoms are oscillating in-phase, the spring between them does not contract or expand at any time during the motion. Hence, the net force on each atom is weaker than it is for the single-mass model of Fig. 4.1(a), and the oscillation frequency should be lower. In contrast, when the two atoms are oscillating anti-phase, the maximum expansion and contraction in the spring between them is larger than for the single-mass case, and the oscillation frequency should be higher.

By logical deduction, we can extend the analysis to a very large number of masses $N$ with the following rules: (1) the number of unique oscillatory frequencies will continue to equal the

![Diagram](image)

Fig. 4.2 (a) Fan diagram of natural oscillation frequencies for harmonic oscillator model of Fig. 4.1. (b) Instantaneous motion of two masses for the lower-frequency oscillation $\omega_1$. (c) Instantaneous motion of two masses for the higher-frequency oscillation $\omega_2$. 
number of masses, and (2) the spread in oscillation frequencies will increase but asymptotically so. We expect this intuitively since the lower extent of the extent cannot get any lower than $\omega = 0$ (“dc” in the language of electrical engineering). This is shown by a lower dashed “envelope” in the fan diagram of Fig. 4.2(a). The asymptotic limit for the maximum oscillation frequency $\omega_{\text{max}}$ can be deduced from the relative motion for the $\omega_2$ oscillation displayed in Fig. 4.2(b).

Intuitively, the antiphase relative motion between neighboring masses should continue to yield the highest possible oscillation frequency, independent of $N$, since this will maximize the average force on each mass over the oscillation period. In the limit where a mass is embedded in a long chain so that the walls have negligible effect on its motion, we expect the antiphase behavior of its nearest neighbors to double the average force from neighboring springs compared to the single-mass case, so that $\omega^2 = 4C/m$ instead of $2C/m$. This is represented by the upper envelope in Fig. 4.2(a) and will prove to be the correct result using more rigorous analysis.