

Phonon spectra

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We present a simple way to construct the dispersion relations for lattice vibrations in two- and three- dimensional harmonic lattices.

A simple harmonic chain is often used to illustrate lattice vibrations in a solid. The chain consists of n particles, each of mass m , connected to nearest neighbors on the left and right by identical springs with spring constant K . The two particles at each end of the chain: (a) may be connected by springs to immovable anchors (brick wall boundary conditions); (b) may not be attached to anything (free boundary conditions); or (c) may be attached to each other by a spring (periodic boundary conditions). In the latter two cases the lowest vibration frequency is $\omega = 0$ while in case (a) the lowest frequency is nonzero. For large n the spectrum of eigenfrequencies is otherwise essentially the same in the three cases.

For convenience we adopt periodic boundary conditions [1] and label the particles according to their position in the chain from $j = 0$ to $j = n - 1$, with the n th position identified with the 0th position. The Lagrangian for this chain is $\mathcal{L} = KE - PE$, with $KE = \sum_{j=0}^{n-1} \frac{1}{2} m \dot{x}_j^2$ and $PE = \sum_{j=0}^{n-1} \frac{1}{2} k (x_{j+1} - x_j)^2$. All indices are taken *mod*(n). The Euler Lagrange equations of motion lead to an $n \times n$ cyclic matrix, an example of which is

$$\begin{bmatrix} a & b & c & \cdots & d \\ d & a & b & c & \cdots \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b & c & \cdots & d & a \end{bmatrix} \quad (1)$$

where, for the case at hand $a = 2K - m\omega^2$ and $b = d = -K$.

Cyclic matrices \mathcal{C} have very convenient properties [2]. They are invariant under the permutation operation P whose only nonzero matrix elements are $P_{i+1,i} = P_{0,n-1} = 1$, so that $PCP^{-1} = \mathcal{C}$. Since $P^n = I_n$ the eigenvalues of P are $e^{i\theta}$ where $\theta = 2\pi m/n$, $m = 0, 1, 2, \dots, n-1$. The eigenvectors of a cyclic matrix are $\frac{1}{\sqrt{n}} [e^{i0\theta}, e^{i1\theta}, e^{i2\theta}, \dots, e^{i(n-1)\theta}]^t$. Physically, this means that the motion of mass $i+1$ is phase-shifted by $e^{i\theta}$ from the motion of mass i . The eigenvalues have the form

$$E = a + be^{i\theta} + ce^{i2\theta} + \cdots + de^{-i\theta} = \sum_{j'} \mathcal{C}_{j,j'} e^{i(j'-j)\theta} \quad (2)$$

For the case at hand

$$m\omega^2 = 2K - Ke^{i\theta} - Ke^{-i\theta} = 2K(1 - \cos\theta). \quad (3)$$

If both nearest neighbor (K) and next nearest neighbor (k) interactions are present,

$$m\omega^2 = 2K(1 - \cos\theta) + 2k(1 - \cos 2\theta) \quad (4)$$

Longer range harmonic interactions are treated similarly.

If there are two atoms per unit cell, then the index i labels unit cells. If masses m and M in unit cell i are connected by a spring with spring constant K and M in cell i is connected to m in cell $i+1$ by a spring with spring constant k , then the Euler Lagrange equations for the two atoms in unit cell i are

$$\begin{array}{c|cc|cc|c} & i-1 & & i & & i+1 & \\ \hline & 0 & -k & K+k-m\omega^2 & -K & 0 & 0 \\ & 0 & 0 & -K & K+k-M\omega^2 & -k & 0 \\ \hline & D & & A & & B & \\ \hline \end{array} \quad (5)$$

The matrix elements a, b, c, \dots in Eq. (1) are replaced by 2×2 matrices A, B, C, \dots and the 'eigenvalue' becomes

$$A + Be^{i\theta} + De^{-i\theta} \rightarrow \begin{bmatrix} K+k-m\omega^2 & -K-ke^{-i\theta} \\ -K-ke^{+i\theta} & K+k-M\omega^2 \end{bmatrix} \quad (6)$$

This matrix must be diagonalized to determine the two oscillation frequencies and their corresponding eigenvectors. The two oscillation frequencies occur on the acoustic branch (lower frequency solution) and the optical branch. Now *unit cell* $i+1$ is phase-shifted by $e^{i\theta}$ from the motion of *unit cell* i . The motion of atoms within each unit cell are defined by the two eigenvectors of the matrix in Eq. (6), which are θ -dependent.

In two dimensions the equilibrium positions of atoms are identified by two integer indices (j_1, j_2) . We assume periodicity in both dimensions, so that $0 \leq j_1 < n_1$ where $j_1 = n_1$ is identified with $j_1 = 0$, and similarly for $0 \leq j_2 < n_2$. Figure 1 shows small sections of periodic square and hexagonal lattices. For such lattices with $n_1 \times n_2$ equal mass particles the Lagrangian can be set up in the usual way and the Euler-Lagrange equations lead to a potential energy matrix $\mathcal{K}_{(j_1, j_2), (j'_1, j'_2)}$. This matrix is invariant under cyclic permutation matrices P_1 that act on the first symbols j_1, j'_1 and P_2 that act on the second symbols j_2, j'_2 separately:

$$\begin{aligned} \mathcal{K}_{(j_1, j_2), (j'_1, j'_2)} &\xrightarrow{P_1} \mathcal{K}_{(j_1+1, j_2), (j'_1+1, j'_2)} \\ \mathcal{K}_{(j_1, j_2), (j'_1, j'_2)} &\xrightarrow{P_2} \mathcal{K}_{(j_1, j_2+1), (j'_1, j'_2+1)} \end{aligned} \quad (7)$$

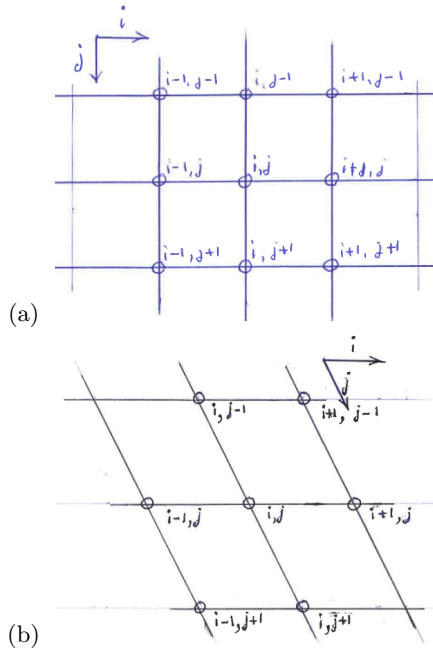


FIG. 1: (a) Part of a two-dimensional square lattice. The four nearest neighbors to atom at site (i, j) are at $(i, j \pm 1)$ and $(i \pm 1, j)$. The four next nearest neighbors are at $(i \pm 1, j \pm 1)$. (b) Part of a two-dimensional hexagonal close packed lattice. In this labeling scheme the six nearest neighbors to (i, j) are at $(i \pm 1, j)$, $(i, j \pm 1)$, $(i \pm 1, j \mp 1)$.

The components of the eigenvectors of $P_1 \otimes P_2$ have the form $e^{ij_1\theta_1} e^{ij_2\theta_2}$, with $\theta_1 = 2\pi m_1/n_1$ and $\theta_2 = 2\pi m_2/n_2$. The eigenvalues of \mathcal{K} are

$$E(m_1, m_2) = \sum_{j'_1, j'_2} \mathcal{K}_{(j_1, j_2), (j'_1, j'_2)} e^{i(j'_1 - j_1)\theta_1} e^{i(j'_2 - j_2)\theta_2} \quad (8)$$

For the square lattice shown in Fig. 1a with nearest neighbor (K) and next nearest neighbor (k) coupling

$$m\omega^2 = 2K(1 - \cos\theta_1) + 2K(1 - \cos\theta_2) + 4k(1 - \cos\theta_1 \cos\theta_2) \quad (9)$$

For the hexagonal lattice shown in Fig. 1b with nearest neighbor coupling K and indexing as shown, and cycling clockwise from the 3 o'clock position, we find

$$\begin{aligned} m\omega^2 &= 6K - K(e^{i\theta_1} + e^{i\theta_2} + e^{i(-\theta_1 + \theta_2)} \\ &\quad + e^{-i\theta_1} + e^{-i\theta_2} + e^{i(\theta_1 - \theta_2)}) \\ &= 6K - 2K(\cos\theta_1 + \cos\theta_2 + \cos(\theta_1 - \theta_2)) \end{aligned} \quad (10)$$

As usual, $\theta_1 = 2\pi m_1/n_1$ and $\theta_2 = 2\pi m_2/n_2$. When there are p atoms in a unit cell, a $p \times p$ matrix must be constructed and diagonalized as described in Eq. (6).

Three dimensional periodic lattices can be treated similarly. For a simple cubic lattice with NN (K) and NNN (k) coupling

$$\begin{aligned} m\omega^2 &= 2K(1 - \cos\theta_1) + 2K(1 - \cos\theta_2) + 2K(1 - \cos\theta_3) \\ &\quad + k \sum_{i < j, \pm, \pm} (1 - \cos(\pm\theta_i \pm \theta_j)) \end{aligned} \quad (11)$$

The three-dimensional HCP lattice is created by adjoining three above-plane sites $(j_1, j_2, j_3 + 1)$, $(j_1, j_2 - 1, j_3 + 1)$, $(j_1 - 1, j_2, j_3 + 1)$ and the corresponding below-plane sites $(j_1, j_2, j_3 - 1)$, $(j_1, j_2 + 1, j_3 - 1)$, $(j_1 + 1, j_2, j_3 - 1)$. If the in-plane spring constants remain K and the out-of-plane spring constants are k , three additional terms must be added to the right hand side of Eq. (10):

$$2k(1 - \cos\theta_3) + 2k(1 - \cos(\theta_3 - \theta_1)) + 2k(1 - \cos(\theta_3 - \theta_2)). \quad (12)$$

We have shown how to compute phonon dispersion spectra for one-, two-, and three-dimensional lattices with periodic boundary conditions using the properties of cyclic, bi-cyclic, and tri-cyclic matrices. The procedure extends easily beyond nearest neighbor interactions and to more than one atom per unit cell.

- [1] J. M. Ziman, *Electrons and Phonons*, Oxford: University Press, 1960.
 [2] B. Kaufman, *Crystal Statistics. II. Partition Function*

Evaluated by Spinor Analysis, *Physical Review* **74**(4), 1232-1243 (1949). See especially Eqs. (44) - (48).