Lattice vibrations

An atomic chain with one atom per unit cell is shown in Fig. 4.1. From a formal point of view, this is a one dimensional atomic lattice with one atom per unit cell and a lattice vector of length \( a \). This means that the reciprocal lattice is also one-dimensional and the reciprocal lattice vector has a length of \( 2\pi/a \). The atoms at the lattice sites shall be connected with springs of a force constant \( \gamma \). If we take only nearest neighbour interactions into account, the equation of motion for atom \( n \) is

\[
M \frac{d^2 u_n}{dt^2} = -\gamma (u_n - u_{n-1}) + \gamma (u_{n+1} - u_n)
\]

or

\[
M \frac{d^2 u_n}{dt^2} = -\gamma [2u_n - u_{n-1} - u_{n+1}].
\]

where \( u_n \) is the displacement of the \( n \)th atom in the chain. This can be solved by a kind of wave which is only defined on the lattice sites

\[
\omega_n(t) = u e^{i(kn-\omega t)},
\]

(4.8)

where \( k = 2\pi/\lambda \) is the one dimensional wave vector of the wave with the wave length \( \lambda \) and \( u \) is the amplitude of the oscillation. Substituting this into the equation of motion gives

\[
-M \omega^2 e^{i(kn-\omega t)} = -\gamma [2 - e^{-ika} - e^{ika}] e^{i(kn-\omega t)} = -2\gamma (1 - \cos ka) e^{i(kn-\omega t)}.
\]

(4.9)

and this has a solution if we choose the \( \omega = \omega(k) \) such that

\[
\omega(k) = \sqrt{\frac{2\gamma (1 - \cos ka)}{M}} = 2\sqrt{\frac{\gamma}{M}} \sin \frac{ka}{2}.
\]

(4.10)
Lattice vibrations

- The motion of atoms in a linear chain is coupled, giving rise to propagating waves
- The frequency of oscillation depends on the wavelength (i.e. the wave vector) of the propagating wave
- For an infinite chain, the possible frequency of oscillations is a continuous
- For a finite chain of quantum oscillator, only a discrete set of frequencies is possible
- Each propagating wave with a certain frequency and hence a certain group velocity is called a phonon
- The frequency of atomic vibrations in a phonon depends on the phonon wave vector – k: This defines the dispersion relation.
- Phonon wave vectors for a 1D chain of length L are n·2π/L, where n is integer. Number of phonons is
- All phonon wave vectors lie between –π/a and π/a. Therefore the number of phonons in a 1D chain is 2π/a / 2π/L = L/a
- Each phonon can be treated itself as a quantum oscillation. For low temperatures every atom can be approximated by an harmonic oscillator, the energy of the oscillation is

\[ E_l(k) = \left( l + \frac{1}{2} \right) \hbar \omega(k) \]
Lattice vibrations

It is only needed to know the dispersion relation in the range between $-\frac{\pi}{a}$ and $\frac{\pi}{a}$.

Equation (4.10) suggests that the dispersion is periodic in $k$ with a periodicity of $2\pi/a$. This is precisely the reciprocal lattice vector! The reciprocal lattice is not only useful to describe lattice-periodic quantities like the charge density in a Fourier series. It is also fundamental for describing waves in a lattice: In the present case, as in general, the wave is unchanged when we add a reciprocal lattice vector to its wave vector $k$. This is illustrated in Fig. 4.2, which shows the instantaneous displacement of atoms for two waves which differ by a reciprocal lattice vector. The displacement is the same. Another way of viewing this is that the shortest possible wavelength in a lattice of spacing $a$ is $\lambda = 2a$ or $k = \pi/a$ which corresponds to the situation where neighbouring atoms move exactly out of phase. Any wave which is even shorter can be equivalently described by a longer wavelength.

\[ \lambda = 10a \]
\[ k = \frac{2\pi}{10a} \]
\[ \lambda = \frac{10}{11}a \]
\[ k = \frac{2\pi}{10a} + \frac{2\pi}{a} \]

**Figure 4.2:** Instantaneous position of atoms in a chain for two different wavelengths with $\lambda = 10a$ and $\lambda = (10/11)a$. Note that the wave is transversal for illustrative purposes. Otherwise, we have only considered longitudinal waves in one dimensional chains.
Two atoms per unit cell

\[ \begin{align*}
M_1 \frac{d^2 u_n}{dt^2} &= -\gamma [2u_n - v_{n-1} - v_n] \\
M_2 \frac{d^2 v_n}{dt^2} &= -\gamma [2v_n - u_n - u_{n+1}]
\end{align*} \]

ansatz

\[ \begin{align*}
u_n(t) &= u e^{i(kbn - \omega t)} \\
v_n(t) &= v e^{i(kbn - \omega t)}
\end{align*} \]

two linear equations, two unknowns

\[ \begin{align*}
-\omega^2 M_1 u &= \gamma v (1 + e^{-ikb}) - 2\gamma u \\
-\omega^2 M_2 v &= \gamma v (e^{ikb} + 1) - 2\gamma v
\end{align*} \]

(system of homogeneous linear equations)
Two atoms per unit cell

\[-\omega^2 M_1 u = \gamma u (1 + e^{-ikb}) - 2\gamma u \quad -\omega^2 M_2 u = \gamma u (e^{ikb} + 1) - 2\gamma u.\]

this has only a solution when

\[
\begin{vmatrix}
2\gamma - \omega^2 M_1 & -\gamma (e^{ikb} + 1) \\
-\gamma (1 + e^{-ikb}) & 2\gamma - \omega^2 M_2
\end{vmatrix} = 0
\]

two solutions for every value of k

\[
\omega^2 = \gamma \left( \frac{1}{M_1} + \frac{1}{M_2} \right) \pm \gamma \left[ \left( \frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4}{M_1 M_2} \sin^2 \frac{kb}{2} \right]^{1/2}
\]
Two atoms per unit cell

\[ \omega^2 = \gamma \left( \frac{1}{M_1} + \frac{1}{M_2} \right) \pm \gamma \left[ \left( \frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4}{M_1 M_2} \sin^2 \frac{kb}{2} \right]^{1/2} \]
Akustische und optische Gitterschwingungen

M₁ und M₂ schwingen gegenphasig

longitudinal optisch

transversal optisch

longitudinal akustisch

transversal akustisch

first Brillouin zone

\[ k = \frac{2\pi}{\lambda} \]
**Periodic boundary conditions**

Max Born and Theodore von Karman (1912)

chain with \( N \) atoms:

\[
\mathbf{u}_{N+n} = \mathbf{u}_n
\]

longest wavelength for wave solutions

\[
e^{ika} = e^{i(aN+n)}
\]

\[
e^{ikan} = e^{i(aN+n)}
\]

So there are \( N \) possible different vibrations (\( m=0,\ldots,N-1 \))
Finite chain with 10 unit cells and one atom per unit cell

\[ k = \frac{2\pi}{aN} \]

- N atoms give N so-called normal modes of vibration.
- For long but finite chains, the points are very dense.

\[ k = \frac{2\pi}{\lambda} \]
Long atomic chain: quantum model

\[ E_l(k) = \left( l + \frac{1}{2} \right) \hbar \omega(k) \]

- The excitations of these oscillators are called phonons.
- Strong analogy with photons: both bosonic excitations
- Both described by quantum mechanical harmonic oscillators
- Wave-particle duality
Phonons in 3D crystals: Aluminium

- Results from inelastic x-ray scattering / neutron scattering.
Phonons in 3D crystals: diamond

- Results from inelastic x-ray scattering / neutron scattering.
- Acoustic and optical branches present.