Lattice vibrations and Phonons

From the study of the atoms vibrations within the solid (lattice vibrations), the objective of this chapter is to deal with the concept of Phonons (quantization of vibrational modes) and the thermal properties of solids. **Sections** within the solid (futtice)

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1D lattice model $\sum_{i=1}^{n}$ is the small amount. Due to force acting on the small tend to r extended position. This results in lattice vibration. The contractions between atoms, various between atoms

For simplicity we consider, first, a 1D crystal lattice and assume that the forces between For a comparison who have a proportional to relative applicements from the equinorium positions (1100KC s law). the atoms in this lattice are proportional to relative displacements from the equilibrium positions (Hooke's law).

This is known as the *harmonic approximation*, which holds well provided that the simple sements are an all II is the displesement of an stem from its confiting negities. displacements are small. U_n is the displacement of an atom from its equilibrium position $F_n^{\prime\prime}$ $C(u_n \quad u_n)$ $C(u_n \quad u_n)$ *xn=na.*

Lattice vibrations atoms move simultaneously, so we have to consider the motion of the entire lattice. **Cone-dimensional lattice**

One might think about the atoms in the lattice as interconnected by elastic springs. Therefore, the force exerted on n-the atom in the lattice is given by: the force exerted on *n*-the atom in the lattice is given by the force exerted on *n*-the atom in the lattice is given by Ine might think about the atoms in the lattice as interconnected by elastic springs. herefore, the force exerted on n-the atom in the lattice is given by:

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 u_n) $F_n = C(u_{n+1} - u_n) + C(u_{n-1} - u_n)$ where C is the interatomic force (elastic) constant. F_n^* $C(u_n^* - u_n)$ $C(u_n^* - u_n)$

For simplicity we consider, first, a one-dimensional crystal lattice and assume that the forces between

the atoms in this lattice are proportional to relative displacements from the equilibrium positions.

 $C(u_{\tilde{M}}^M \underline{d} \hat{u} u) = C\left(\frac{C(u_{\tilde{M}}^M u) - C(u_{\tilde{M}}^M u)}{C(u_{\tilde{M}}^M u + u_{\tilde{M}}^M u)}\right)$ *C*(u_M dt u_n) $F_n = C(2u^{n-1}u^{n-1}u_n) + C(u_{n-1} - u_n) = -C(2u_n - u_{n+1} - u_{n-1})$ Applying Newton's second law to the motion of the n-th atom we obtain: $M_{\frac{d^{2}u}{du}} F_{C} S_{u}^{(u_{1u}u)} F_{u}^{(u_{1u}u)} G_{u}^{(u_{1u}u)} G_{u}^{(u_{1u}u)}$ *dt* u_n F_C $\left(\sum_{u=1}^{\infty} u_u u_u\right)$ $C(u_{-1} u_u)$ $C(2u_{-1} u_{-1} u_u)$ dt^2 is the mass of the mass of the interaction of the interaction of the interaction of the *n*-th atom with 2 $M \frac{d \hat{u} u_n}{dt^2} = F_n = C \left(\frac{2u}{u_{n+1}} - u_n \right) + C \left(u_{n-1} - u_n \right) = -C \left(2u_n - u_{n+1} - u_{n-1} \right)$ $\frac{d\mathbf{u} \cdot \mathbf{v}_{n'}}{dt^2} = F_n^{\mathsf{T}} = \widetilde{C}(u_{n+1} - u_n) + C(u_{n-1} - u_n) = -C(2u_n - u_{n+1} - u_{n-1})$

M is the mass of the atom. We neglect here the interaction of the n-th atom with its nearest neighbors \mathcal{L} is the total showledge should be solved simultaneously (*N* is the total number of the tota all but its nearest nearest nearest neighbors. A similar equation showled be written for each atom in the lattice, resulting α In 1s the mass of the atom. We neglect here the interaction of the n-th atom with all but ats in the lattice in the boundary condition the boundary conditions applied to the end atom in the lattice should be end at the lattic M is the mass of the atom. We neglect here the interaction of the *n*-th atom with all but its nearest neighbors.

This is known as the *harmonic approximation*, which holds well provided that the displacements are we cha with in coupled differential equations, which should be solved simulative.
(N boing the total number of atoms in the lattice). $\frac{1}{\sqrt{2}}$ the cour number on We end with N coupled differential equations, which should be solved simultaneously (N being the total number of atoms in the lattice). (ce) .

 u_n) u_n)Now let us attempt a solution of the form: $u_n = A e^{i(qx_n - \omega t)}$

$$
u_n = Ae^{i(qx_n - \omega t)}
$$

time-dependent factor) we obtain

Now substituting Eq.(5.3) into Eq.(5.2) and canceling the common quantities (the amplitude and the

where *c* is the equilibrium position of the *n* th atom so that $r - \nu a$ n atom so that $x_n=n a$. U_n is a traveling wave, in which all the atoms oscillate with the same frequency ω , wavevector $\overline{}$ where x_n is the equilibrium position of the n-th atom so that $x_n = na$.

same amplitude *A* and same wave-vector *q*.
\n
$$
C(u_{1} - u) - C(2u - u_{1} - u_{1})
$$

where *M* is the mass of the atom. Note that we neglected here by the interaction of the *n*-th atom with

all but its nearest nearest neighbors. A similar equation should be written for each atom in the lattice, result

in *N* coupled differential equations, which should be solved simultaneously (*N* is the total number of

atoms in the lattice). In addition the boundary conditions applied to the end atom in the end atom in the latt

Lattice vibrations For simplicity we consider, first, a one-dimensional crystal lattice and assume that the forces between the atoms in this lattice are proportional to relative displacements from the equilibrium positions. This is known as the *harmonic approximation*, which holds well provided that the displacements are $\left\{ u_n = Ae^{i(qx_n - \omega t)} \right\}$ the force exerted on \overline{a} *n*−1 *n n*+1 *a* u_{n-1} *u_n* u_{n+1} where M is the mass of the mass of the atom. Note that we neglected here by the interaction of the interacti all but its nearest nearest neighbors. A similar equation showledge with the lattice, resulting in the lattice, in *N* coupled differential equations, which should be solved simultaneously (*N* is the total number of \bullet www.components and \bullet $\begin{array}{cccc} n & n & n+1 & q \end{array}$

$$
u_n^j
$$
 $M(-\omega^2)Ae^{iqna}e^{-i\omega t} = -C\{2Ae^{iqna}e^{-i\omega t} - Ae^{iq(n+1)a}e^{-i\omega t} - Ae^{iq(n-1)a}e^{-i\omega t}\}$
\n $M\omega^2 = C\{2 - e^{iqa} - e^{-iqa}\}$
\n $M\omega^2 = 2C\{1 - \cos qa\}$
\n $C(u_n u) - C(2u u_n u_n)$
\nAfter some marks, Newton's second law becomes: $M\omega^2 = 4C\sin\frac{qa}{2}$

 Γ similar equation showld be written for each atom in the lattice, resulting Γ

atoms in the lattice). In addition the boundary conditions applied to the end atom in the lattice should

in *N* coupled differential equations, which should be solved simultaneously (*N* is the total number of ² (1) (1) () 2 *iqna iqna iq ⁿ ^a iq ⁿ ^a M* ^ω *e C e e e* ⁺ [−] [−] ⁼ [−] ! [−] [−] " # \$ (5.4)

 u_n) u_n) Reducing to the first Brillouin zone. $\frac{1}{2}$ this shown in $\frac{1}{2}$ is shown in Fig.

 $\overline{}$

 T *M* \overline{A} / *M* \overline{A} / *M* \overline{A} is seen to the sign change in \overline{A} ch

$$
\frac{qa}{2}
$$

$$
-\frac{\pi}{a} \leq \leq \frac{\pi}{a}
$$

allows us to set the range of independent values of *q* within the first Brillouin zone, i.e.

Lattice vibrations ^π ^π − ≤ ≤ . (5.7)

The frequency is symmetric with respesign change in *q*. $\overline{1}$ frequency is symmetric with respe

 $\left\{\begin{array}{c} \begin{array}{c} \begin{array}{c} \end{array} \end{array} \right\}$ 4*C A* \mathcal{M} and \mathcal{M} and \mathcal{M} is symmetric in q corresponds to $\frac{V}{\sqrt{a^2 + b^2}}$ traveling in the lattice from the left to r π/a be the π/a mode with a negative q corresponds to q traveling from the right to the left.

 $\frac{4C}{M}$

(ii) *Phase and group velocity*. The phase velocity is defined by

Within this range of *q* the ^ω versus *q* is shown in Fig.2.

At the boundaries of the Brillouin zone $q = \pm \pi/a$ the solution represents a star traveling in the lattice of the lattice $q = x/2$ and the system is presented with a negative $q = x/2$ correspondence $q = x/2$ corres wave. $u_n = A(-1)$ e atoms oscinate in the opposite phases dependent n is even or odd. wave: $u_n = A(-1)^n e^{-i\omega t}$ atoms oscillate in the opposite phases depending on wh

4

M

1/2

 $=\frac{w}{q}$ ω

https://www.youtube.com/watch?v=QCiTD_9lE_0

Lattice vibrations are physical. This means that the particular dispersions are physical. This means the particular dispersion relations are physical. This means the particular dispersion relations of the group velocity (i) *Reducing to the first Brillouin zone*. The frequency (5.6) and the displacement of the atoms (5.3) do

 $\frac{1}{2}$ Ca cos $rac{\cos 2}{2}$ *Ca qa* $\frac{9a}{2}$ $\frac{9a}{2}$ $\frac{9a}{2}$

allows us to set the range of independent values of *q* within the first Brillouin zone, i.e.

 $Long wave-length limit: frequency of vibration is$ $\begin{array}{c|c}\n\hline\n\end{array}$ $\begin{array}{c}\n\hline\n\end{array}$ proportional to the wavevector = velocity is independent of frequency. \mathbf{E} wavevector – velocity is
 \mathbf{E} t_{query}

 $rac{\cos 2}{2}$

 $\frac{1}{2}$

2 *Ca qa* cos

velocity for the propagation of energy in the medium.

For the particular dispersion relation (5.6) the group velocity is given by

plane wave, whereas the vg is the velocity of the propagation of the wave packet. The latter is the

 $\frac{9a}{2}$

$$
0.0\begin{array}{c|c}\n & qa & \sqrt{} \\
-\pi/a & 0 & \pi/a \\
\hline\nq & q\n\end{array}\n\qquad\n\begin{array}{c}\n\hline\n\omega = \sqrt{\frac{C}{M}}qa\n\end{array}
$$

 $\frac{4C}{M}$

З $\widehat{\widetilde{A}}$ $\bm{\mathsf{o}}$ / M \frown \gtrsim

 $0.0\frac{1}{-\pi/a}$

0.5

1.0

$$
V_p = \frac{\omega}{q} = \sqrt{\frac{C}{M}}a
$$
 This is the velocity of sound for the one din

qa

M

0

q

 $-\pi/a$ 0 π/a

 $V_p = \frac{\omega}{\omega} = \sqrt{\frac{V}{M}}a$ This is the velocity of sound for the one dimensional lattice \mathbf{S} is independent of frequency. In this independent of \mathbf{S}

 $\overline{\mathbf{a}}$

At the boundaries of the Brillouin zone *q*=±π/*a* the solution represents a standing wave *C a q M* \int_a^b σ and σ on M

Diatomic 1D lattice model Notemia 1D lattice weedel t_{N} that the different features different from the monoctomic case. Fig. 3 shows a monocomic case. Fig. 3 shows a monocomic case. Fig.3 shows a monocomic case. Fig.3 shows a monocomic case. Fig.3 shows a monocomic c

Now we consider a one-dimensional lattice with two non-equivalent atoms in a unit cell. diatomic lattice with the unit cell composed of two atoms of masses *M*¹ and *M*² with the distance Now we consider a one-dimensional lattice with two non-equivalent atoms in a unit cell.

In the present case because we have two different kinds of atoms, we should write two equations of motion: $W_{\rm eff}$ can treat the motion of this lattice in a similar fashion as for monoctomic lattice. However, in this lattice, in this lattice. However, in this lattice, in this lattice. However, in this lattice, in this lattice

(2)
$$
M_1 \frac{d^2 u_n}{dt^2} = -C(2u_n - u_{n+1} - u_{n-1})
$$

\n $C(2u_n - u_n - u_n) M_2 \frac{d^2 u_{n+1}}{dt^2} = -C(2u_{n+1} - u_{n+2} - u_n)$

Diatomic 1D lattice model Notemia 1D lattice weedel t_{N} that the different features different from the monoctomic case. Fig. 3 shows a monocomic case. Fig. 3 shows a monocomic case. Fig.3 shows a monocomic case. Fig.3 shows a monocomic case. Fig.3 shows a monocomic c

Now we consider a one-dimensional lattice with two non-equivalent atoms in a unit cell. diatomic lattice with the unit cell composed of two atoms of masses *M*¹ and *M*² with the distance Now we consider a one-di

Solution in the form of traveling mode for the two atoms: case because we have two different kinds of atoms, we should write two different kinds of motion: we should wri

dt

$$
(2) \qquad \qquad \left[\begin{array}{cc} u_n \\ u_n & u_n \end{array}\right] = \left[\begin{array}{c} A_1 e^{iqna} \\ A_2 e^{iq(n+1)a} \end{array}\right] e^{-i\omega t}
$$

diatomic lattice vibrations and unit cell composed of two atoms of masses \mathbb{R}^n and \mathbb{R}^n with the distance \mathbb{R}^n

$$
M_1 \t M_2
$$
\n
$$
W_1 \t M_2
$$
\n
$$
m_1 \t n_1 + 1 \t n_2
$$
\n
$$
e^{i\omega t}
$$
\n
$$
\left\{\n\begin{aligned}\nM_1 A_1 \omega^2 &= \mathcal{C} \{2A_1 - A_2 e^{iqa} - A_2 e^{-iqa}\} & \text{Sous forme matricielle:} \\
M_2 A_2 \omega^2 &= \mathcal{C} \{2A_2 - A_1 e^{iqa} - A_1 e^{-iqa}\} & \left(2\mathcal{C} - M_1 \omega^2 - 2\mathcal{C} \cos qa\right) \left(\frac{A_1}{A_1}\right) = 0 \\
\vdots \\
M_n \t n_n \text{gen secular determinant to be solved:} & \left| \frac{2\mathcal{C} - M_1 \omega^2}{-2\mathcal{C} \cos qa} \right| = 0 \\
-2\mathcal{C} \cos qa \t 2\mathcal{C} - M_2 \omega^2 & \left| \frac{2\mathcal{C} - M_1 \omega^2}{-2\mathcal{C} \cos qa} \right| = 0 \\
(2 - \omega^2)^2 - \omega^2 & \omega^2 = 0\n\end{aligned}\n\right.
$$

2 different solutions corresponding to **2 different dispersion curves**: $\frac{1}{2}$ the can also solved: which can be readily solved:

$$
\omega^2 = C \left(\frac{1}{M_1} + \frac{1}{M_2} \right) \pm C \sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4 \sin^2 qa}{M_1 M_2}}
$$

 $\cos \theta = 0$ α α $\cos \theta = 0$

diatomic lattice vibrations and unit cell composed of two atoms of masses \mathbb{R}^n and \mathbb{R}^n with the distance \mathbb{R}^n between two neighboring atoms *a*. **Lattice vibrations**

n−1 *n n*+1 *a* M_1 *M₂* ² ² $\frac{2}{\sqrt{1-\frac{1}{2}}}$ ¹ ¹ ¹ ¹ 4sin *qa ^C ^C* $\frac{2}{\sqrt{3}}$ **M** $\frac{1}{\sqrt{3}}$ ' (' (⁼) ⁺ * [±]) ⁺ * [−] $\overline{}$, $\overline{}$ M_1 M_2 $n-1$ in the $n+1$

We can treat the motion of this lattice in a similar fashion as for monoatomic lattice. However, in this The distinction between the acoustic and optical optical branches of lattice vibrations can be seen most clearly by comparing them at $q=0$ (infinite wavelength).

$$
\begin{pmatrix} 2C & -2C \ -2C & 2C \end{pmatrix} \begin{pmatrix} A_1 \\ A_1 \end{pmatrix} = 0
$$

Then
$$
\begin{pmatrix} A_1 = A_2 \end{pmatrix}
$$

have the same amplitude and the phase. The lower curve is called the *acoustic branch*, while the upper curve is called the *optical branch*. The For the acoustic branch $q=0$, $\omega=0$ and $A_1=A_2$. So in this limit the two atoms in the cell

 $\cos \theta = 0$ α α $\cos \theta = 0$

diatomic lattice vibrations and unit cell composed of two atoms of masses \mathbb{R}^n and \mathbb{R}^n with the distance \mathbb{R}^n between two neighboring atoms *a*. **Lattice vibrations**

n−1 *n n*+1 *a* M_1 *M₂* ² ² $\frac{2}{\sqrt{1-\frac{1}{2}}}$ ¹ ¹ ¹ ¹ 4sin *qa ^C ^C* $\frac{2}{\sqrt{3}}$ **M** $\frac{1}{\sqrt{3}}$ ' (' (⁼) ⁺ * [±]) ⁺ * [−] $\overline{}$, $\overline{}$ M_1 M_2 $n-1$ in the $n+1$

 $\sqrt{\frac{2}{\pi}}$ Optical phase. The frequency of these vibrations lies in infrared region which is the reason for referring to this branch as optical.

$$
\begin{pmatrix} 2C(1 - M_1(\frac{1}{M_1} - \frac{1}{M_2})) & -2C \\ -2C & 2C(1 - M_1(\frac{1}{M_1} - \frac{1}{M_2})) \end{pmatrix} \begin{pmatrix} A_1 \\ A_1 \end{pmatrix} = 0
$$

$$
\left(A_2 = -\frac{M_1}{M_2}A_1\right)
$$

To avoid mathematical details we shall present only a qualitative discussion. First, the To avoid mathematical details we shall present only a qualitative discussion. First, the
solution of this equation in three dimensions can be represented in terms of normal modes: each unit cell has a single atom. The equation of motion of motion of \mathbf{r} terms of *normal modes* W turn our attention now to the non-Bravais three-dimensional lattice. Here the unit cell contains the unit cell contains the unit cell contains three-dimensional lattice. Here the unit cell contains the unit cell conta two or more atoms. If there are *s* atoms per cell, then on the basis of our previous experience we

$$
\mathbf{u} = \mathbf{A}e^{i(\mathbf{qr}-\omega t)}
$$

 \checkmark wave vector q = wavelength and direction of propagation that the setties of these roots always vanish at α *and direction of propagation*

 \checkmark vector A = amplitude as well as direction of vibration of the atoms

The wave is defined as longitudinal if **A** is parallel to **q** And transverse when **A** is perpendicular to **q**. perpendicular to **q**).

If there are s atoms per cell, there are 3s dispersion curves = 3 branches are acoustic, and the remaining (3s −3) are optical.

So far we discussed a classical approach to the lattice vibrations, but as we know from quantum mechanics the energy levels of the harmonic oscillator are quantized. *optical* branches can also be classified as longitudinal or transverse when *q* lies along a highbut as we know from quantized. **for a show the unit cell vibrate out of phase relative to phase relative to phase relative to phase r**

Energy levels of lattice vibrations are quantized.
\n
$$
\frac{1}{2} \oint_{\mathcal{D}} \mathbf{P} \cdot \mathbf{
$$

Energy of ill implies and the vibration: $E = (n + \frac{1}{2})\hbar \omega$ and ω n_{nodes} and n_{peak} is given by $\frac{1}{2}$ and $\frac{1}{2}$ is given by $\frac{1}{2}$ is give Eq.(5.20). If the energy of this mode is given by Eq.(5.21) we can say that this mode is occupied by *n* Total energy $=$ sum over all phonons modes entire crystal is specified by giving the occupation numbers for \mathbf{q}) and \mathbf{q} modes. The total of the system of the total of the total order of the \mathbf{q} via energy – sum over an phonons modes $s_{12}\hbar\omega$ individual modes $\mathbf{w} = \text{sum over all phonons modes}$ and the particular modes a particular mode in the energy of t E $3/2\hbar\omega$ \ddot{a} 5 / 2 $\hbar\omega$ ½!^ω $7/2\hbar\omega$ $\hbar\omega$ $\frac{1}{2}$) $\hbar \omega$ mechanics the harmonic oscillator are quantized. Similarly the energy levels of the energy leve lattice vibrations are quantized. The quantum of vibration is called a *phonon* in analogy with the

$$
E = \sum_{\mathbf{q}p} E_{\mathbf{q}p} = \sum_{\mathbf{q}p} (n_{\mathbf{q}p} \; \frac{1}{2} \frac{\lambda}{2} \hbar) \hbar \omega_{\mathbf{q}q}(\mathbf{q}) \qquad \qquad \text{and} \qquad \frac{1}{2} \int_{1/2h}^{3/2h} \omega \; \frac{\hbar \omega}{2}
$$

 $\oint_{\mathcal{P}}$ is the term in the term is the term in the model of the model is the model of the model in the model is the model in the model in the model in the model is the model in the model in the model in the model in t A $1/2$ *hk* photon, which is the electromagnetic wave. Which is the electromagnetic wave. The electromagnetic wave. \mathcal{F}_{max} $\begin{array}{ccc} \hline \end{array}$ the allowed energy levels of the harmonic oscillator are given by \hbar $\vec{F} = (\vec{F}^{1/2})\hbar\omega$ where $\overline{}$ is the $\overline{}$ is given by in a crystal of $\overline{}$ Eq.(5.20). If the energy of this mode is given by Eq.(5.21) we can say that this mode is occupied by *n*

 \overline{A} $\frac{1}{2}$ consider $\frac{1}{2}$ and $\frac{1}{2}$ and $\frac{1}{2}$ and $\frac{1}{2}$ and $\frac{1}{2}$ bration $\frac{1}{2}$ characterized. where n_{qp} is the « occupation number » (number of phonons of energy $\hbar \omega$) of the normal mode of vibration *p* characterized by the wave vector **q**. of the horinal mode of violation ρ enaracterized by the wave vector \mathbf{q} .

 $i(qx \omega t)$ $\iota(qx \ \omega t)$ $u(qx \omega t)$ $u(qx \omega t)$