Chapter 6

LATTICE VIBRATIONS: PHONON SCATTERING

LATTICE VIBRATIONS: PHONONS

In a real crystal atoms are not fixed at rigid sites on a lattice, but are vibrating. In a periodic structure the vibrations have a waveform (just like electronic wavefunctions) with a spatial and temporal part:

$$u(r,t) = u_o \exp(ik \cdot r) \exp(-i\omega t)$$

$k = \dfrac{2\pi}{\lambda}$;$\hbar\omega$ represents a "quantum" of vibration energy.

ω vs. k is the dispersion relation.

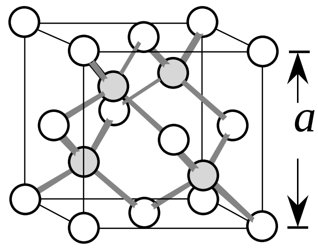
QUESTIONS:

- What controls the ω vs. k relation?

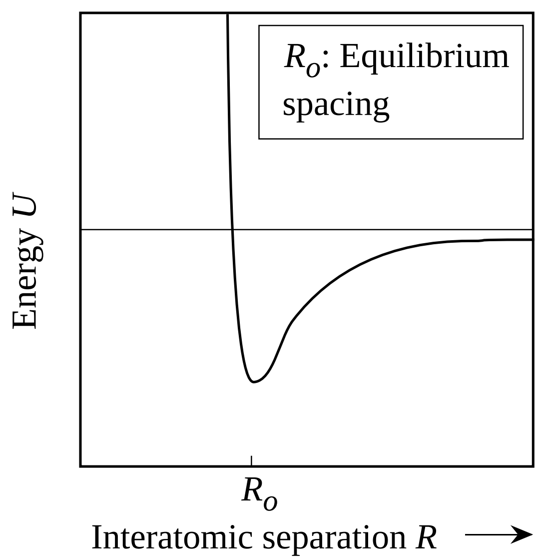
- What is the amplitude of vibrations and how does it depend upon temperature?

- What are the issues involved in second quantization?
What are phonons?

LATTICE VIBRATIONS: RESTORING FORCE



A typical (rigid) lattice



Typical binding energy versus interatomic distance.

RESTORING FORCE

$$U(R) = U(R_o) + \left(\frac{dU}{dR}\right)_{R_o} \Delta R + \frac{1}{2}\left(\frac{d^2U}{dR^2}\right)_{R_o} \Delta R^2 + \ldots$$

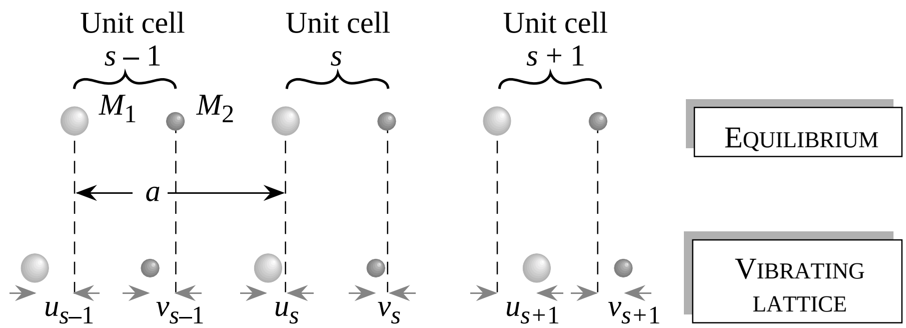
$$= U(R_o) + \frac{1}{2} C(\Delta R)^2$$

$$C = \frac{{}^2U}{R^2} \qquad \text{Force} = -C\Delta R$$

Problem similar to that of coupled harmonic oscillators.

Lattice vibrations: restoring force

Vibrations in a crystal with two atoms per unit cell with masses M_1, M_2 connected by force constant C between adjacent planes.



Equations of motion:

Unit cell s

$$M_1 \frac{d^2 u_s}{dt^2} = C(v_s + v_{s-1} - 2u_s)$$

$$M_2 \frac{d^2 v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s)$$

We look for solutions of the traveling waveform, but with different amplitudes u and v on alternating planes

$$u_s = u \exp(iska)\exp(-i\omega t)$$
$$v_s = v \exp(iska)\exp(-i\omega t)$$

We note that a is the distance between nearest identical planes and not nearest planes, i.e., it is the minimum distance of periodicity in the crystal.

$$-\omega^2 M_1 u = Cv\,[1 + \exp(-ika)] - 2Cu$$
$$-\omega^2 M_2 v = Cu\,[\exp(-ika) + 1] - 2Cv$$

These are coupled eigenvalue equations which can be solved by the matrix method. The equations can be written as the matrix vector product

$$\begin{vmatrix} -\omega^2 M_1 + 2C & -C\,[1 + \exp(-ika)] \\ -C\,[\exp(-ika) + 1] & -\omega^2 M_2 + 2C \end{vmatrix} \begin{vmatrix} u \\ v \end{vmatrix} = 0$$

Equating the determinant to zero, we get

$$\left| 2C - M_1\omega^2 \;\; -C\,[1 + \exp(-ika)] \;\; -C\,[1 + \exp(ika)] \;\; 2C - M_2\omega^2 \right| = 0$$

or

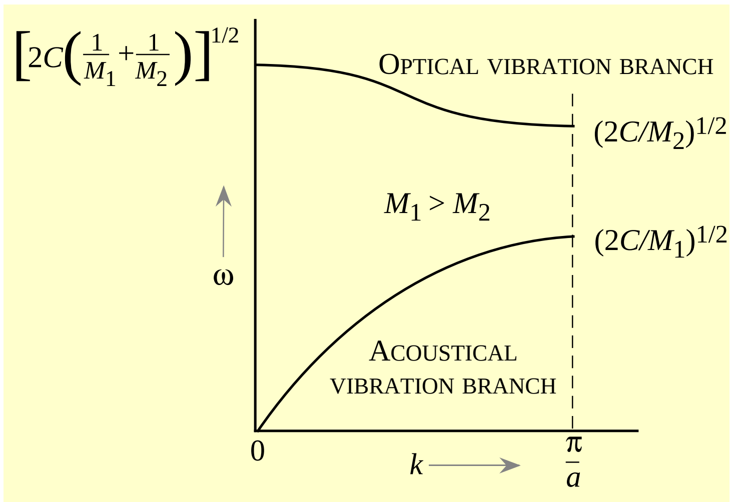
$$M_1 M_2 \omega^4 - 2C(M_1 + M_2)\omega^2 + 2C^2(1 - \cos ka) = 0$$

This gives the solution

$$\omega^2 = \frac{2C(M_1 + M_2) \pm \left[4C^2(M_1 + M_2)^2 - 8C^2(1 - \cos ka)M_1 M_2\right]^{1/2}}{2M_1 M_2}$$

LATTICE VIBRATIONS: ACOUSTIC AND OPTICAL BRANCHES

Solutions for a simple diatomic lattice model



Near $k = 0$

$$\omega^2 \approx 2C\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \qquad \text{Optical branch}$$

$$\omega^2 \approx \frac{C/2}{M_1+M_2} k^2 a^2 \qquad \text{Acoustic branch}$$

Group velocity for acoustic branch (sound velocity)

$$v_s = \frac{d\omega}{dk} = \sqrt{\frac{C}{M_{av}}}\, a$$

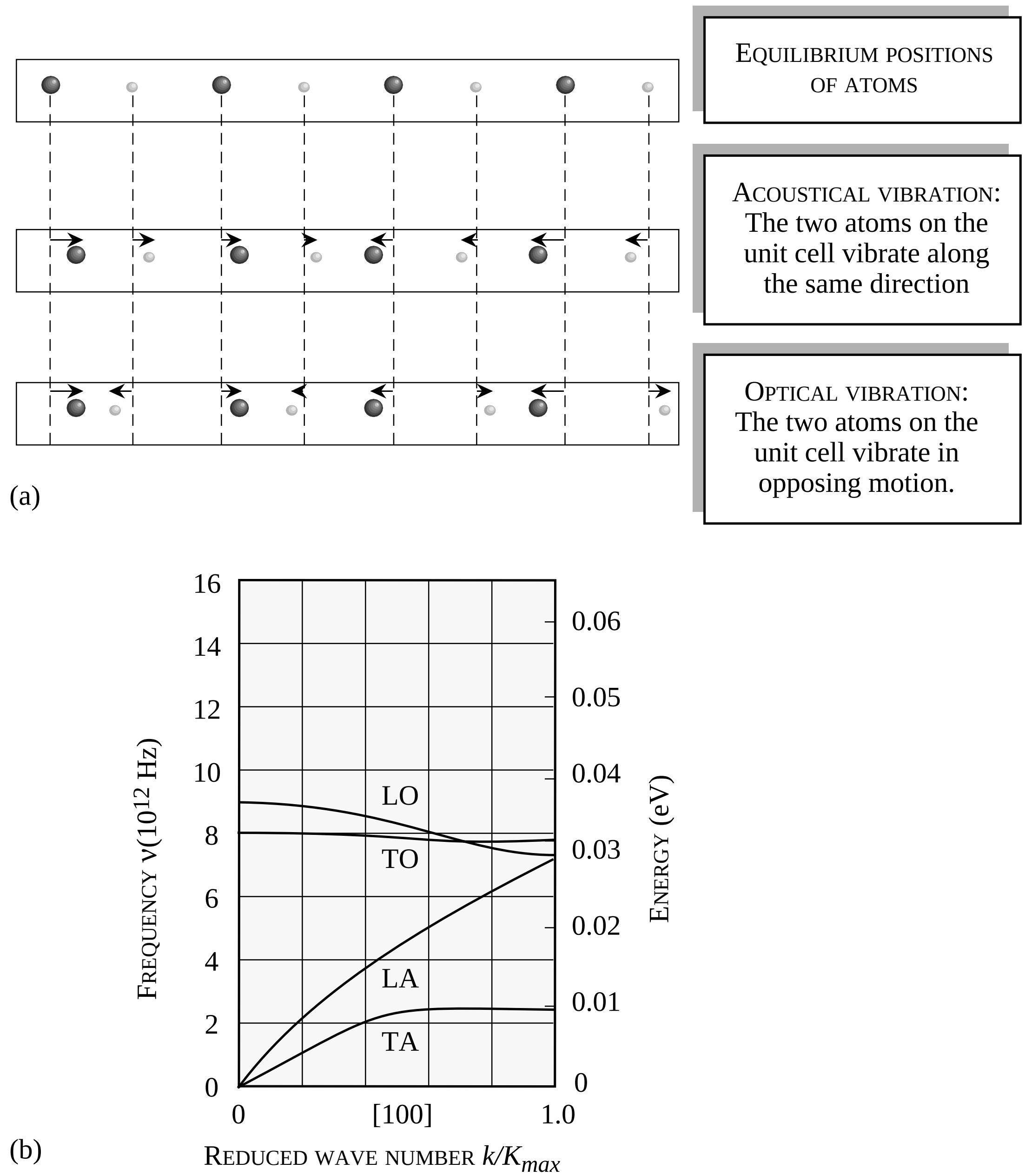
Near $k = 0$ for acoustic branch

$u = v$: vibration in the same direction.

for optical branch

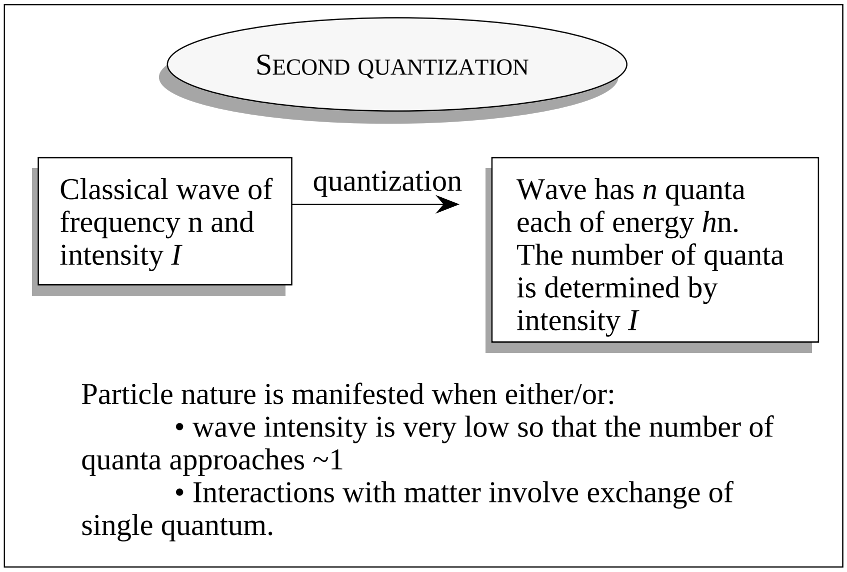
$u = -\frac{M_2}{M_1} v$: two atoms vibrate in opposition.

LATTICE VIBRATIONS: ACOUSTIC AND OPTICAL VIBRATIONS

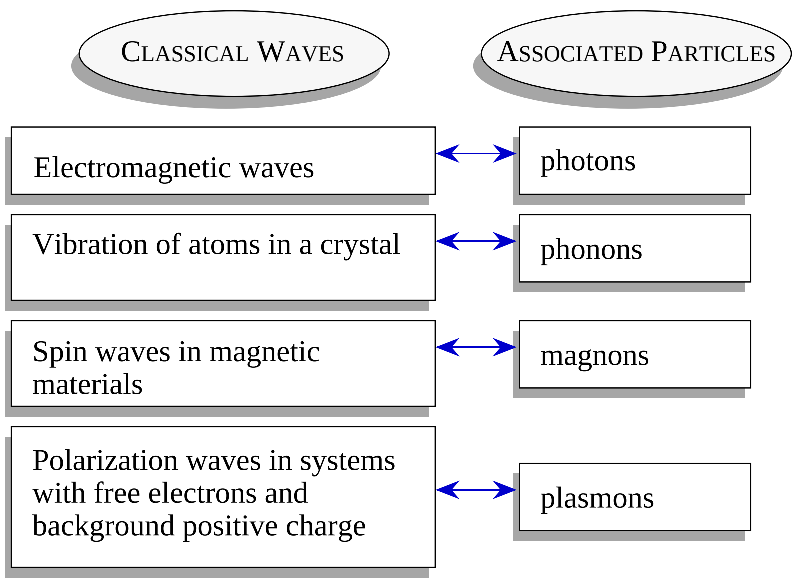


(a) The difference between an acoustical mode and an optical mode is shown. (b) Phonon dispersion relation in GaAs. The longitudinal (LO, LA) and transverse (TO, TA) optical and acoustical modes are shown.

PHONONS: QUANTIZATION OF LATTICE VIBRATIONS



A conceptual picture of second quantization.



Some important classical waves and the particles that result after second quantization.

PHONONS: SECOND QUANTIZATION OF LATTICE VIBRATIONS

Analogy with the harmonic oscillator problem:

Problem: $H = \frac{p^2}{2m} + \frac{1}{2} Cx^2$

Solutions: $\varepsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega$: $\omega = \sqrt{\frac{C}{m}}$

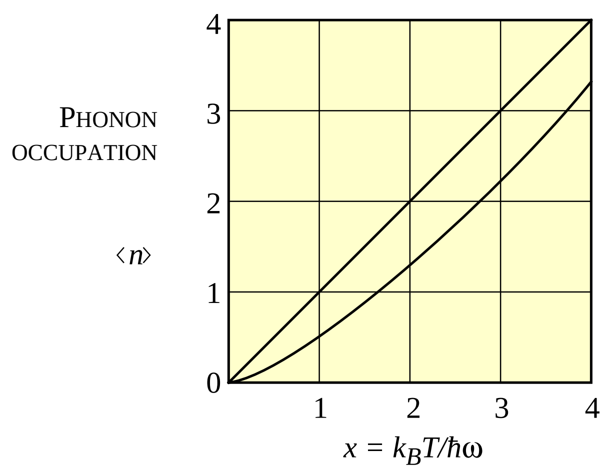
n = number of quanta (0,1,2...)

• In each allowed mode of vibration with frequency ω there are $n(\omega)$ quanta or phonons.

• What is the number of phonons at Temperature T?

Bose Einstein statistics

$$\langle n(\omega)\rangle = \frac{1}{\exp\left(\frac{\hbar\omega}{k_BT}\right) - 1}$$



$\hbar\omega \ll k_BT$

$\langle n\rangle \sim \frac{k_BT}{\hbar\omega}$

PHONON NUMBER:
ACOUSTIC AND OPTICAL PHONONS

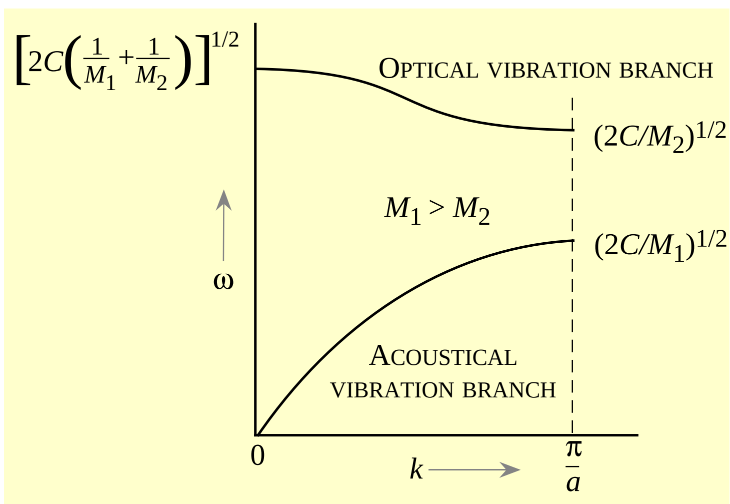
Phonons are an important source of scattering in charge transport. Electrons scatter from phonons by creating or destroying a phonon. These processes are strongly dependent on phonon occupation.

ACOUSTIC PHONONS: Near $k = 0$, acoustic phonon energies are small

$$n(\omega) \sim \frac{k_B T}{\hbar\omega}$$

$\Longrightarrow$ Even at low temperatures acoustic phonons are important.

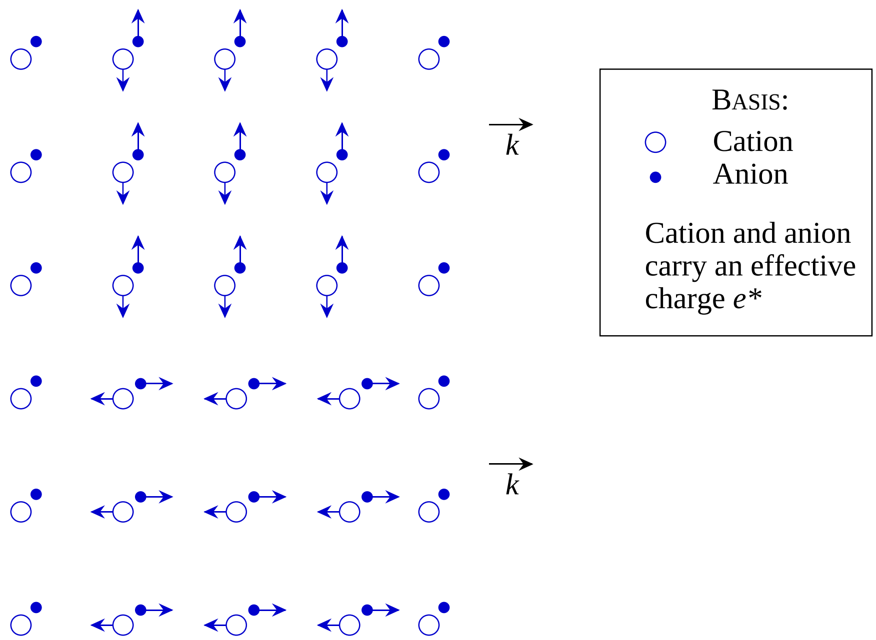
OPTICAL PHONONS: Near $k = 0$, optical phonon energies are quite large (~30-60 meV). At low temperatures, phonon number is negligible.



OPTICAL VIBRATIONS IN POLAR MATERIALS: POLAR OPTICAL PHONONS

In optical vibrations the two atoms in the unit cell vibrate against each other. This can produce polarization effects.

Optical modes of vibration of an ionic crystal. During transverse modes, (a), the vibrations do not produce any polarization effects, while long range electric fields due to polarization are produced in longitudinal modes, (b).



(a)

(b)

For longitudinal optical vibrations there is an <u>additional</u> restoring force due to the polarization field generated by the vibration.

$$P = ne^* u_r \quad ; n \text{ is the unit cell density}$$
$$u_r \text{ is the relative displacement}$$

Electric field

$$F = -4\pi P = -4\pi ne^* u_r \quad \text{(in cgs units)}$$

$$= -\frac{P}{\varepsilon_o} \qquad \text{(MKS)}$$

OPTICAL VIBRATIONS: LONGITUDINAL AND TRANSVERSE

TRANSVERSE MODES: u_r = relative vector for the two atoms on the unit cell

$$M\ddot{\boldsymbol{u}}_r + M\omega_t^2 \boldsymbol{u}_r = 0 : M \text{ reduced mass}$$

LONGITUDINAL MODES: Additional restoring force

$$-\omega_l^2 M\boldsymbol{u}_r = -\omega_t^2 M\boldsymbol{u}_r + \boldsymbol{F}_i e^*$$

$$= -\omega_t^2 - \frac{4\pi n e^{*2}}{M}$$

$$\omega_l^2 = \omega_t^2 + \frac{4\pi n e^{*2}}{M} \quad \text{(cgs)}$$

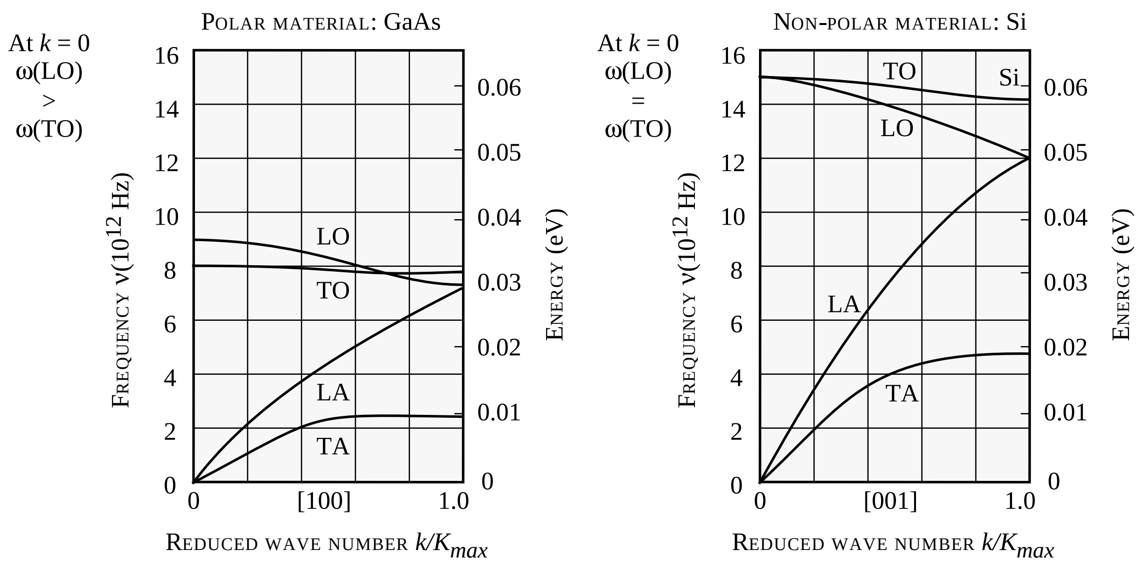
$$\omega_l^2 = \omega_t^2 + \frac{n e^{*2}}{\varepsilon_o M} \quad \text{(Mks)}$$

It can also be shown that:

$$\omega_l^2 = \frac{\varepsilon_o}{\varepsilon_{oo}} \omega_t^2$$

ε_o: static dielectric constant (eg., 13.18 for GaAs)

ε_{oo}: high frequency dielectric constant (11.0 for GaAs)



ELECTRON-PHONON SCATTERING: SOME CONSIDERATIONS

Phonons have to be treated within second quantization

$\Rightarrow$ Energy states: $\left(n + \frac{1}{2}\right)\hbar\omega = \left(a^{+}a + \frac{1}{2}\right)\hbar\omega$

Displacement: Written in terms of creation and destruction operators

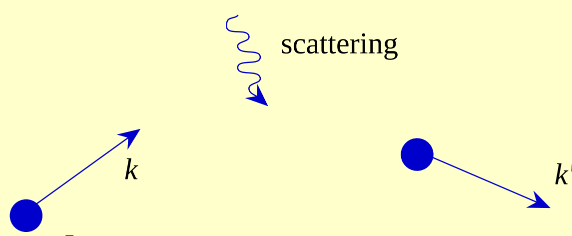
Creation operator: (a^{+}) $\quad a^{+}|n\rangle = (n+1)^{1/2}\,|n+1\rangle$

Destruction operator: (a) $\quad a|n\rangle = n^{1/2}\,|n-1\rangle$

θ_{qb}: displacement of normal coordinates

$$\theta_{qb} = \sqrt{\frac{\hbar}{2m\omega_{qb}}}\,(a^{+}_{-q} + a_{q})$$

SCATTERING PROBLEM



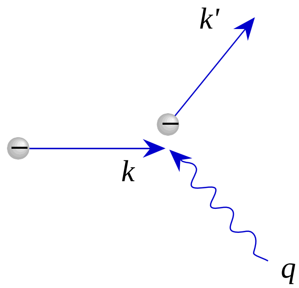
INITIAL STATE:
electron: k
phonons: $|n_{qb}\rangle$

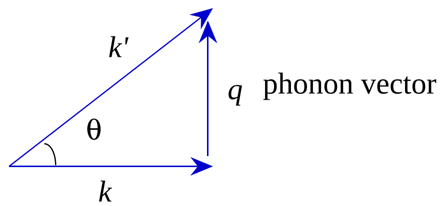
FINAL STATE:
electron: k'
phonons: $|n'_{qb}\rangle$

ABSORPTION OF PHONON: $n' = n - 1$

EMISSION OF PHONONS: $n' = n + 1$

ELECTRON-PHONON SCATTERING: SOME IMPORTANT ISSUES





Energy has to be conserved:

$$E(k') = E(k) \pm \hbar\omega(q)$$

Momentum has to be conserved (within a reciprocal lattice vector):

$$k' = k \pm q \Rightarrow k'^2 = k^2 + q^2 \pm 2kq\cos\theta$$

Assuming parabolic bands:

$$\begin{aligned}
\frac{\hbar^2 k'^2}{2m^*} &= \frac{\hbar^2 k^2}{2m^*} \pm \hbar\omega \\
&= \frac{\hbar^2 k^2}{2m^*} + \frac{\hbar^2 q^2}{2m^*} \pm \frac{\hbar^2 kq\cos\theta}{m^*} \\
\frac{\hbar^2 q^2}{2m^*} &= \mp \frac{\hbar^2 kq\cos\theta}{m^*} \pm \hbar\omega \\
\hbar q &= \hbar k\left[\mp 2\cos\theta \pm \frac{2\omega m^*}{\hbar kq}\right] \\
&= \hbar k\left[\mp 2\cos\theta \pm \frac{2\omega}{v(\mathbf{k})q}\right] \quad v(k)\,\frac{\hbar k}{m^*}\text{, electron velocity}
\end{aligned}$$

Electron-phonon scattering: Phonon energies and vectors

Intravalley acoustic phonon scattering

Sound velocity: $v_s = \dfrac{\omega}{q}$

Phonon vector: $\hbar q = 2\hbar k\left[\mp \cos\theta \pm \dfrac{v_s}{v(\boldsymbol{k})}\right]$

Maximum phonon vector: $\hbar q_{max} = 2\hbar k\left[1 \pm \dfrac{v_s}{v(\boldsymbol{k})}\right]$

Maximum phonon energy: $\Delta E_{max} = \hbar k_{max}$
$\sim 2\hbar k\, v_s$

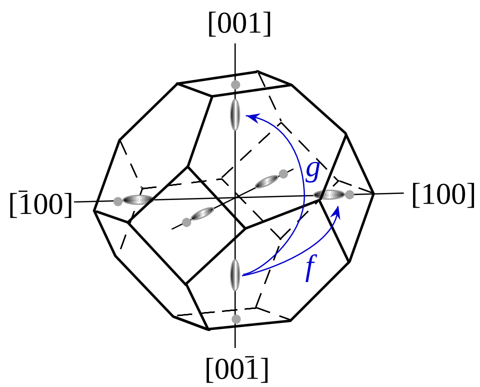
Intravalley optical phonon scattering

Phonon vector: $\hbar q = \hbar k\left[-\cos\theta + \sqrt{\cos^2\theta \pm \dfrac{\hbar\omega_0}{E(\boldsymbol{k})}}\right]$

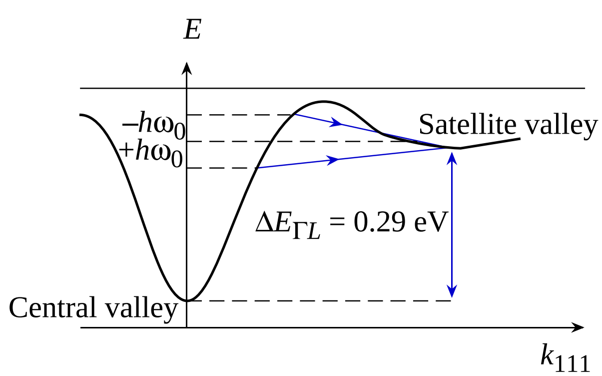
Maximum vector: ($\cos\theta = -1$)

$$\hbar q_{max} = \hbar k\left[1 + \sqrt{1 \pm \frac{\hbar\omega_0}{E(\boldsymbol{k})}}\right]$$

Intravalley phonon scattering



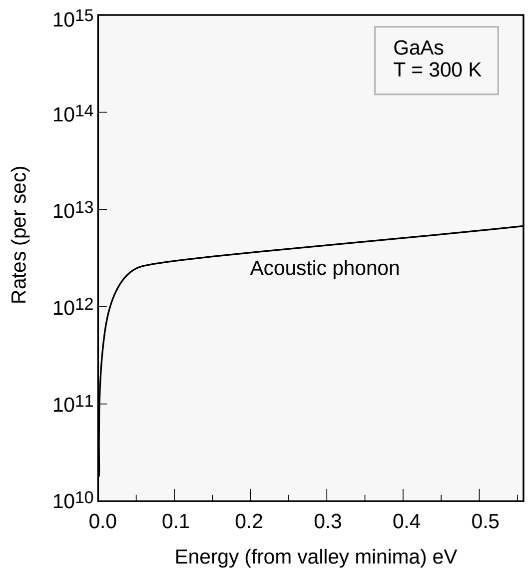
Si: g scattering:
$\Delta q = 0.3 \cdot 2\pi/a\ (1,0,0)$



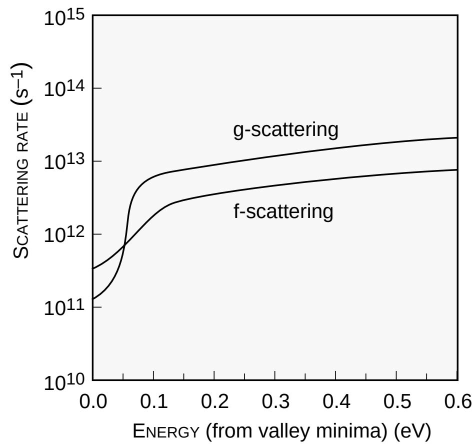
GaAs:
$\Gamma - L$ scattering

PHONON SCATTERING RATES

Silicon:

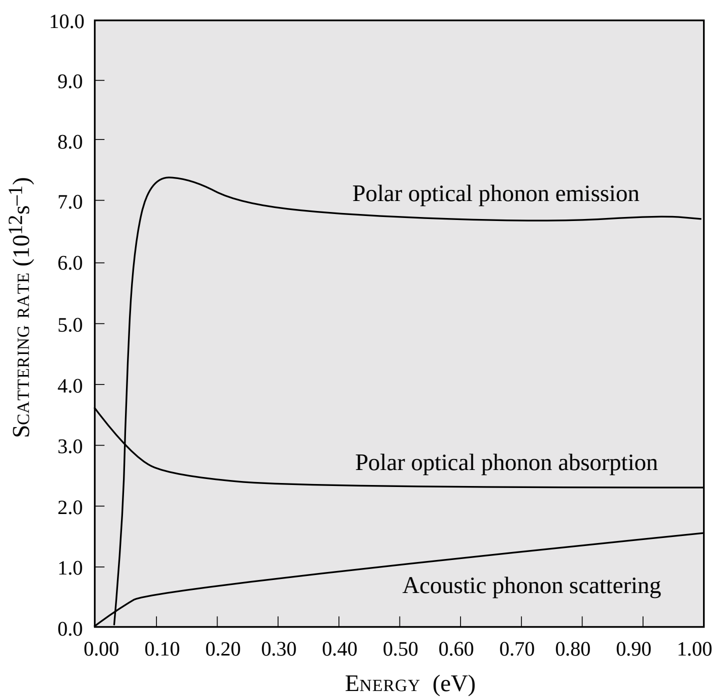


Acoustic phonon scattering rates in silicon as a function of energy.



The g and f intervalley scattering rates in Si at 300 K.

GaAs:



A comparison of the polar optical phonon scattering and acoustic phonon scattering in GaAs at room temperature.