Quantum Transport:
Atom to Transistor

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Lecture 37: Phonons, emission & Absorption

Ref. Chapter 10.2 & 10.4

Network for Computational Nanotechnology

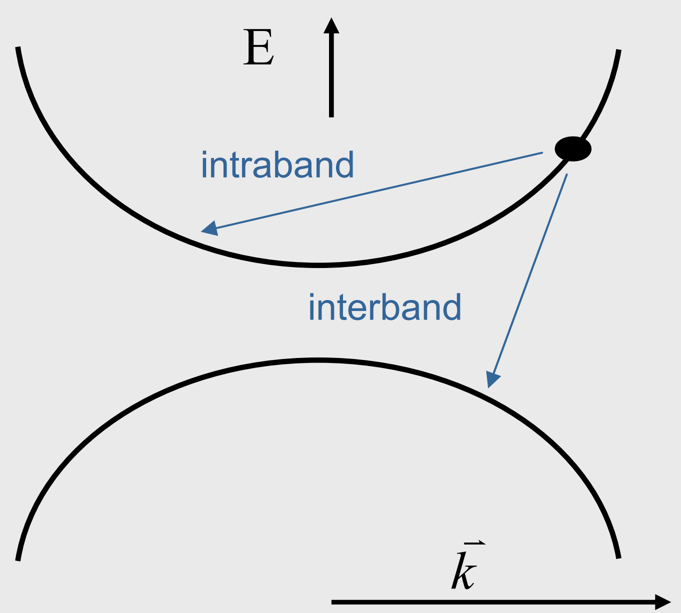
NCN nanoHUB online simulations and more

Introduction

00:00

• In the first part of this lecture we discuss intraband transitions. Up till now we have covered only interband transitions

Transitions



• Interband transitions are a lot like atomic transitions

• Intraband transitions, otherwise known as Cerenkov radiation, can occur with both phonons and photons

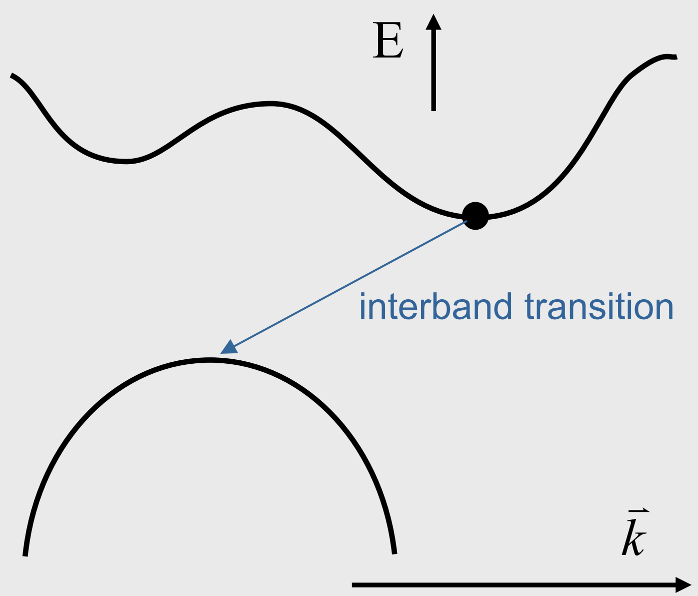
• Intraband transitions could take picoseconds whereas interband transitions usually take nanoseconds

Silicon Interband Transitions

00:50

• However, silicon interband transitions take as long as a millisecond

Interband Silicon Transitions



• From the diagram on the left one can see that for emission,

$$\vec{k}_f = \vec{k} - \vec{\beta}$$

and absorption

$$\vec{k}_f = \vec{k} + \vec{\beta}$$

where the photon wave vector $\vec{\beta}$ required is very large. Since $\vec{\beta}$ is often very small for light the coupling between non-vertical transitions is weak and hence τ is large

• Note: vertical transitions are not permitted in silicon because there is not any empty state available in the valence band if the electron is to drop vertically.

Intraband Formalism

05:30

- Just as with interband transitions, intraband transition lifetimes are defined as:

→ Emission

$$\Gamma = \hbar/\tau = \sum_{\vec{\beta}} \left[\left(N_{\vec{\beta}} + 1\right) 2\pi |K|^2 \delta\left(\varepsilon(\vec{k}) - \varepsilon(\vec{k} - \vec{\beta}) - \hbar\omega(\vec{\beta})\right)\right]$$

→ Absorption

$$\Gamma = \hbar/\tau = \sum_{\vec{\beta}} \left[\left(N_{\vec{\beta}}\right) 2\pi |K|^2 \delta\left(\varepsilon(\vec{k}) - \varepsilon(\vec{k} + \vec{\beta}) + \hbar\omega(\vec{\beta})\right)\right]$$

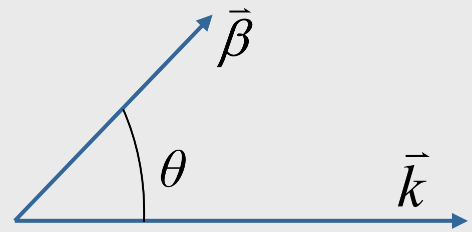
- Importantly, for intraband transitions the final state retains the initial state wave function. Therefore, $\vec{k}_f = \vec{k} \pm \vec{\beta}$ and for emission we require $\varepsilon(\vec{k}) - \varepsilon(\vec{k} - \vec{\beta}) - \hbar w(\vec{\beta}) = 0$ likewise for absorption $\varepsilon(\vec{k}) - \varepsilon(\vec{k} + \vec{\beta}) - \hbar w(\vec{\beta}) = 0$

$$\varepsilon(\vec{k}) - \varepsilon(\vec{k} - \vec{\beta}) - \hbar w(\vec{\beta}) = 0 \Rightarrow \frac{\hbar^2}{2m}k^2 - \frac{\hbar^2}{2m}\underbrace{\left(k^2 + \beta^2 - 2k\beta\cos\theta\right)}_{(\vec{k}-\vec{\beta})\cdot(\vec{k}-\vec{\beta})} - \hbar\bar{c}\beta = 0$$

$$\therefore \cos\theta = \frac{\hbar\bar{c}\beta + \hbar\beta^2/2m}{\hbar^2 k\beta/m} = \bar{c}/(\hbar k/m) + \beta/2k$$

Coupling

- So, we need to have a phonon or photon with direction $\vec{\beta}$ and an electron with direction $\vec{k}$



- Inspecting the equality

$$\cos\theta = \frac{\bar{c}}{\hbar k/m} + \frac{\beta}{2k}$$

we see that since cos θ ≤ 1 emission is only possible if the electron velocity, ħk/m, exceeds the photon/phonon velocity $\bar{c}$

- Note: for phonons c_s is usually used in place of $\bar{c}$ (Velocity of sound instead of velocity of light)

- The term cos θ gives the Cerenkov cone for phonons /photons, this effect is exactly the same as the sonic boom produced by jets

- We can work out the same result for absorption, only a sign change results

Phonons

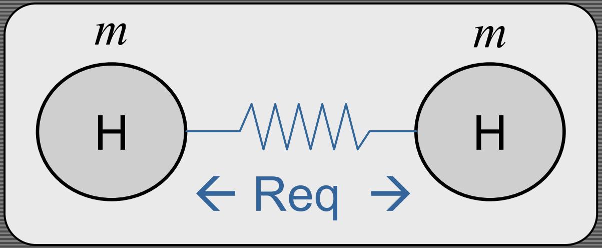
20:52

• *Next*: An introduction to phonons and their dispersion curves

• *Basic Definition*: phonons are the lattice vibrations (sound) which propagate through a solid or molecule

• For example, hydrogen molecules vibrate about an equilibrium bond distance, R_{eq}, with an intensity proportional to temperature much like a spring mass system

H2 Harmonic Oscillator



• Similar to a classical harmonic osscilator this mass-spring system has a resonant frequency defined by

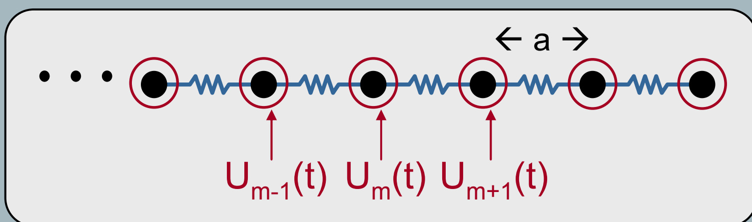
$$\omega = \sqrt{K/M}$$

with discrete energies. We define phonons as the quantized energy exchanged between vibrating masses

1-Dimensional Lattice

23:00

- We can make a similar extension to the infinite 1-D lattice producing a mass-spring structure of the form



where m is the mass of each atom and $U_m(t)$ is the displacement of the m^{th} atom from equilibrium its equilibrium position.

- Thus, according to Newton's law the force exerted on the m^{th} atom is

$$m\frac{d^2U_m}{dt^2} = K\left(U_{m+1} - U_m\right) - K\left(U_m - U_{m-1}\right)$$

- Now, assuming sine or cosine solutions to the equation we can write

$$\frac{d^2U_m(t)}{dt^2} = -\omega^2 U_m$$

or

$$-\omega^2 U_m = K/m\left(U_{m+1} - 2U_m + U_{m-1}\right)$$

- The above translates easily into matrix form:

$$\omega^2 \begin{Bmatrix} U_1 \\ U_2 \\ U_3 \\ \vdots \end{Bmatrix} = \frac{K}{m} \begin{bmatrix} 2 & -1 & & -1 \\ -1 & 2 & -1 & \\ & -1 & \ddots & \ddots \\ -1 & & \ddots & \end{bmatrix} \begin{Bmatrix} U_1 \\ U_2 \\ U_3 \\ \vdots \end{Bmatrix}$$

1-D Dispersion Relation

28:37

- Likewise, taking advantage of matrix periodicity, for phonon $\vec{\beta}$ we may use the ansatz

$$U_m = U_0 e^{\pm i\beta a}$$

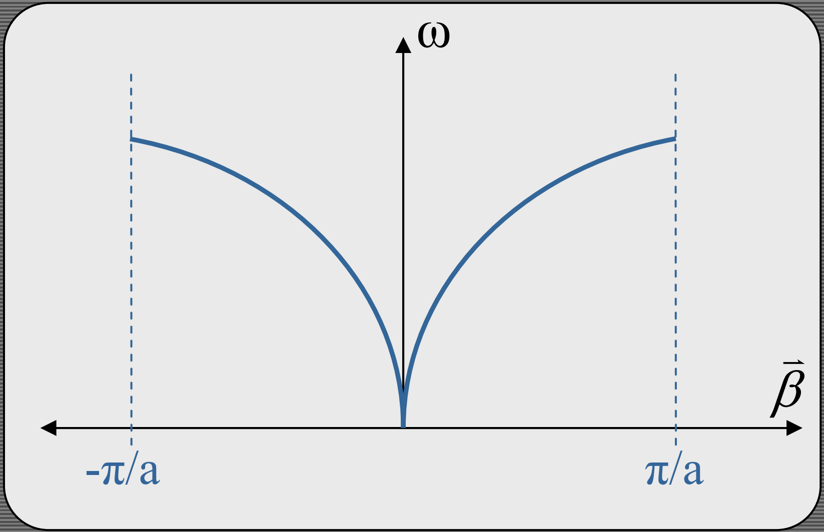
such that

$$\omega^2 = {}^{2k}\!/\!_m (1 - \cos\beta a)$$

$$= 2\left({}^{2k}\!/\!_m\right)\sin^2\left({}^{\beta a}\!/\!_2\right)$$

$$\therefore \omega = 2\sqrt{k/m}\,\sin\left({}^{\beta a}\!/\!_2\right)$$

- This gives rise to a dispersion relation which looks like…



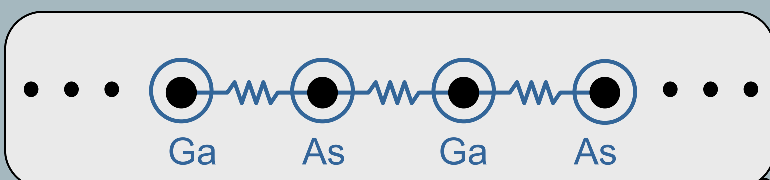
… and around the origin the curve is often approximated linearly by the relation

$$\omega = \sqrt{\frac{k}{m}}a\beta$$

Optical Phonons

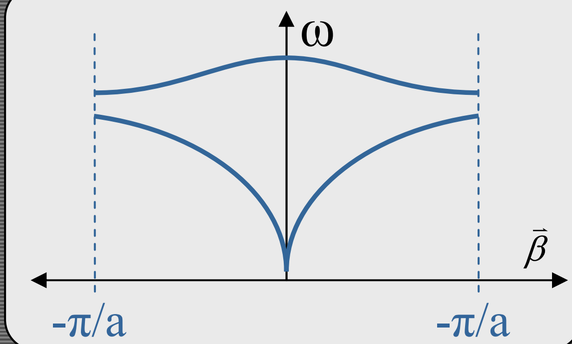
32:40

- In semiconductors another phonon ω vs. β branch often occurs, otherwise known as optical phonons. This results when two types of atoms, and hence two different masses, exist in a unit cell. For example, GaAs:



- In the dispersion relation we denote the upper branch "optical branch" (has nothing to do with light) and the lower branch "acoustic branch". The reason we call the upper one optical is because if you shine light on the solid you can excite this branch.

Acoustic and Optical Branches



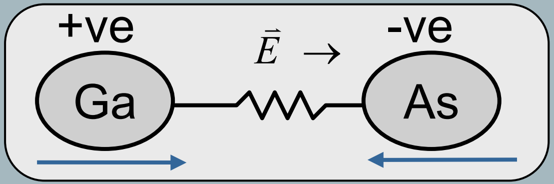
- Acoustic phonons propagate in one direction

- Optical phonons "squeeze" or "push" two atoms together

Closing Comments

38:00

The electric field, $\vec{E}$, of a photon is uniform on an atomic scale and induces opposite force on the +ve and -ve bonding pair



Physical intuition on the flatness of the upper branch & strong dependence of lower branch on β

Let's ask ourselves why does the frequency generally go up with β? Frequency goes up as the spring gets stiffer is a certain deformation is caused. β is like the wavelength. When you have a 1-D series of atoms and you excite the first one, if the wavelength is relatively large, the first atom moves a lot, the second moves by almost the same amount, the third moves almost the same and so on. So the spring itself is not distorted a lot. However**,** for shorter wavelengths the displacement in the atom 1 and atom 2 is considerably different such that the spring feels a lot stiffer and so for short wavelengths the frequency goes up. This does not happen for the optical branch. It doesn't matter if the wavelength is lone or short. Within a unit cell, the two atoms move opposite to each other and that's what determines the stiffness (they are moving against each other, it's very stiff anyway). For short or long wavelength the spring is distorted. So ω-β curve for the optical branch tends to be relatively flat.

The final coupling constant for any phonon as found in Γ is a product of the phonon strain and the induced deformation potential. The deformation potential is the actual shift in the conduction band of a solid due to the passage of a phonon. It is derived experimentally