Electron and Phonon Dispersion

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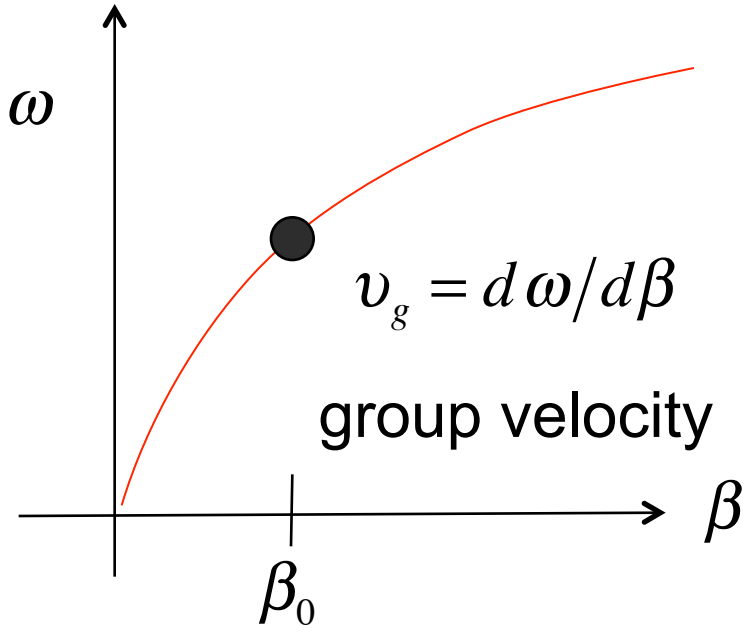
Waves in general

General wave: $u(\vec{r},t) = A(\vec{\beta})e^{i(\vec{\beta}\cdot\vec{r}-\omega t)}$ $\beta = 2\pi/\lambda$



$\upsilon_g = d\omega/d\beta$

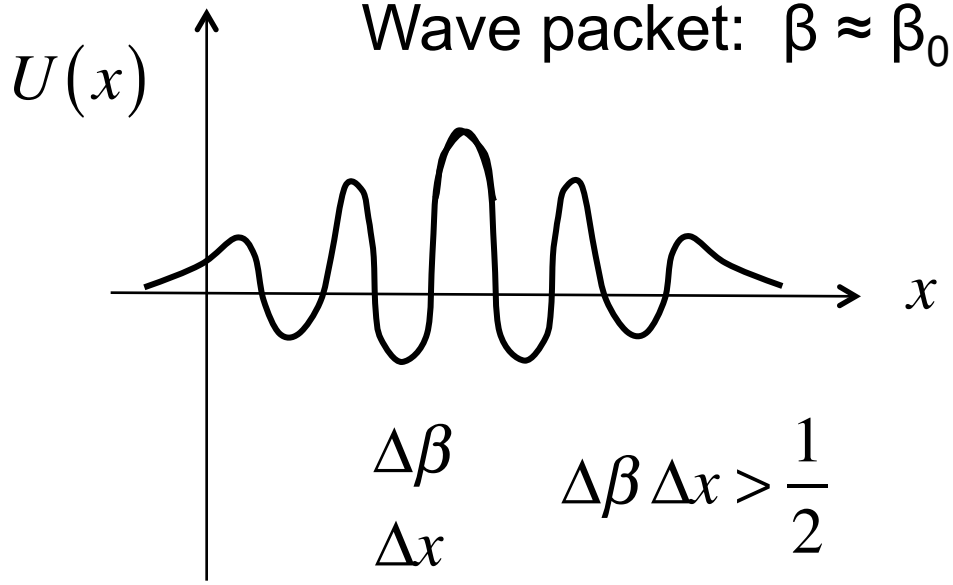
group velocity

$\upsilon_p = \omega/\beta$

phase velocity

$$U(\vec{r},t) = \iiint A(\vec{\beta})e^{i(\vec{\beta}\cdot\vec{r}-\omega(\vec{\beta})t)}d^3\beta$$

Wave packet: $\beta \approx \beta_0$



$\Delta\beta$

Δx

$\Delta\beta\,\Delta x > \frac{1}{2}$

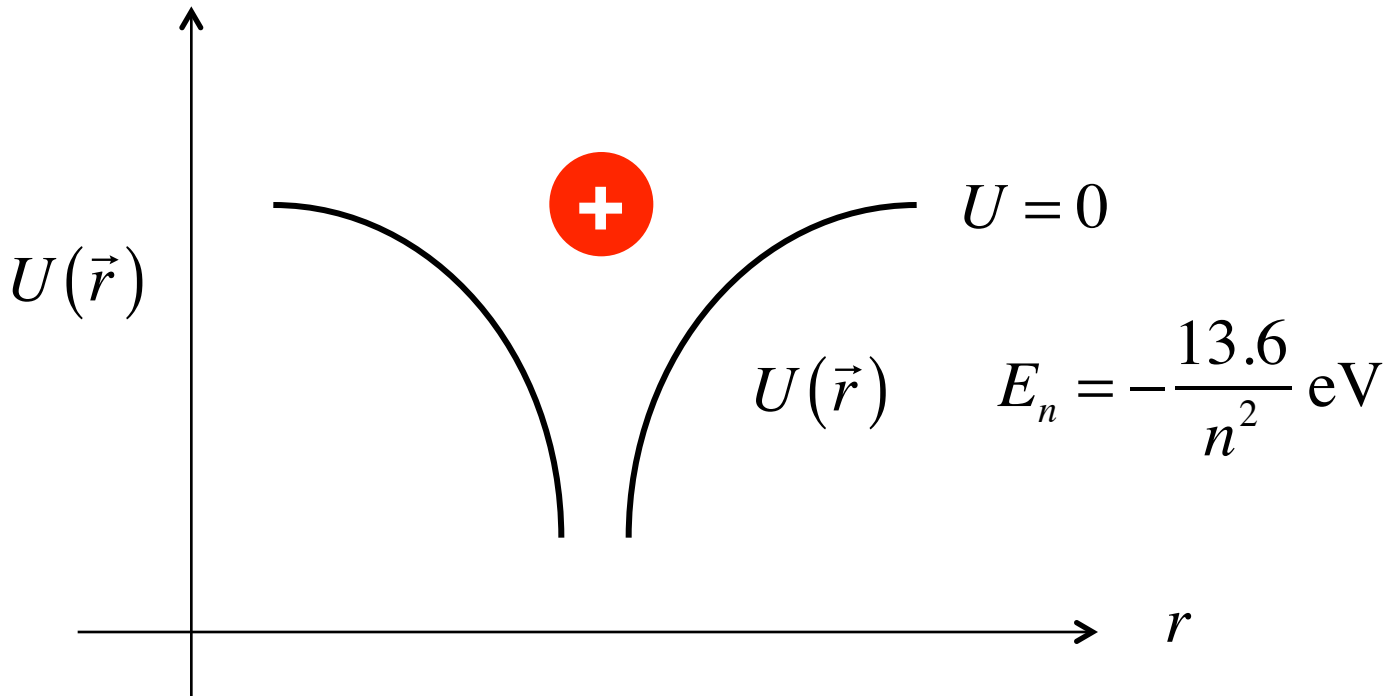
outline

1) **Electron dispersion (band structure)**
2) Simple band structures
3) Phonon dispersion
4) Simple phonon dispersions
5) Electrons vs. phonons

Electrons in atoms

Hydrogen atom:

$$-\frac{\hbar^2}{2m_0}\nabla^2\psi(\vec{r})+U(\vec{r})\psi(\vec{r})=E\psi(\vec{r}) \qquad U(\vec{r})=-\frac{q^2}{4\pi\varepsilon_0 r}$$



Electrons in free space

$$-\frac{\hbar^2}{2m_0}\nabla^2\psi(\vec{r})+U(\vec{r})\psi(\vec{r})=E\psi(\vec{r})$$

$$\Psi(\vec{r},t)=\psi(\vec{r})e^{i\omega t}$$

$$E=\hbar\omega$$

free space, constant potential: $U(\vec{r})=0$

$$-\frac{\hbar^2}{2m_0}\nabla^2\psi(\vec{r})=E\psi(\vec{r})$$

$$\psi(\vec{r})=Ae^{i\vec{k}\bullet\vec{r}}$$

$$\vec{\beta}\rightarrow\vec{k}$$

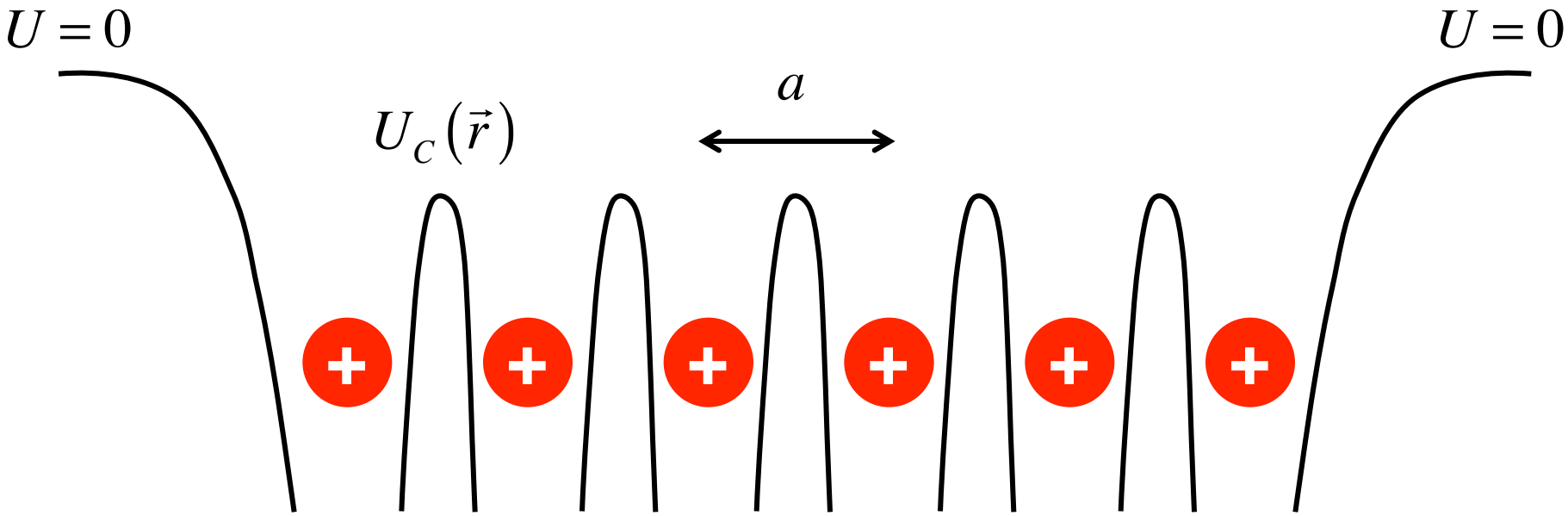
$$k=\sqrt{2m_0E}\,/\hbar$$

momentum: $\vec{p}=\hbar\vec{k}$

$$E(\vec{k})=\frac{\hbar^2k^2}{2m_0}$$

position: $\psi^*(\vec{r})\psi(\vec{r})=|A|^2$

Electrons in crystals



Crystals:

$$-\frac{\hbar^2}{2m_0}\nabla^2\psi(\vec{r})+U_C(\vec{r})\psi(\vec{r})=E\psi(\vec{r}) \qquad U_C(\vec{r}+\vec{a})=U_C(\vec{r})$$

"crystal potential"

Electrons in crystals

$$-\frac{\hbar^2}{2m_0}\nabla^2\psi(\vec{r})+U_C(\vec{r})\psi(\vec{r})=E\psi(\vec{r}) \qquad U_C(\vec{r}+\vec{a})=U_C(\vec{r})$$

$$\psi(\vec{r})=u_{\vec{k}}(\vec{r})e^{i\vec{k}\bullet\vec{r}} \qquad u_{\vec{k}}(\vec{r}+\vec{a})=u_{\vec{k}}(\vec{r})$$

k: Brillouin zone

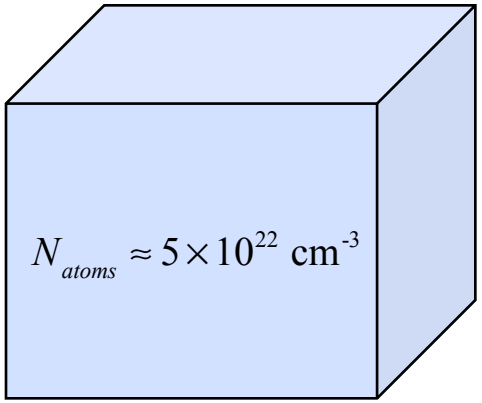
"Bloch wave"

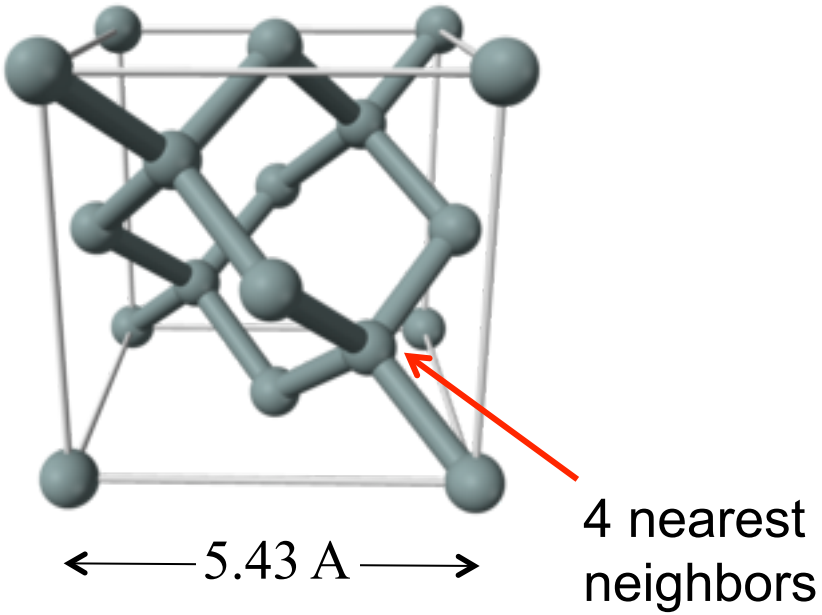
$\vec{p}\neq\hbar\vec{k}$ but…."crystal momentum"

$E(\vec{k})$ bandstructure (dispersion) $E(\vec{k})=\hbar\omega(\vec{k})$

Crystal structure

Silicon

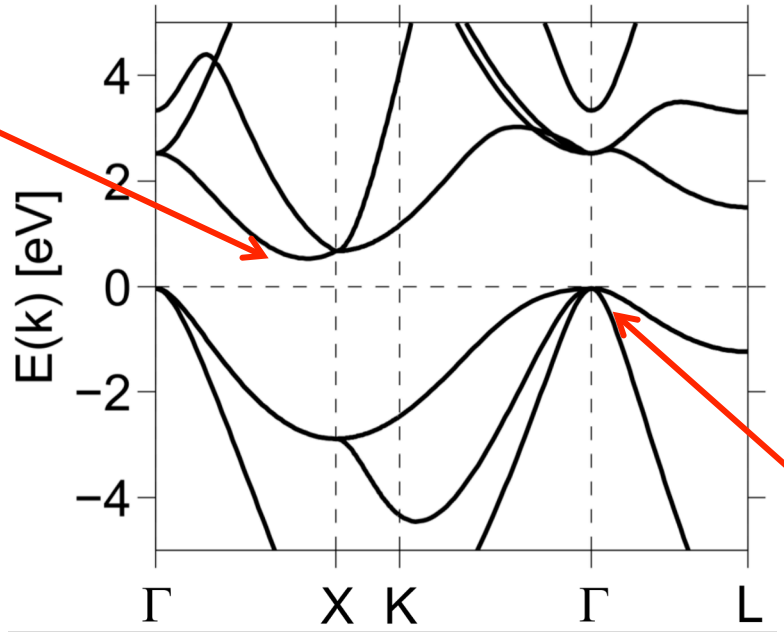




Band structure (electron dispersion)

bottom of conduction band

E(k) for electrons in Si



top of valence band

[100] [111]

DFT calculations by Dr. J. Maassen, Purdue

Constant energy surfaces

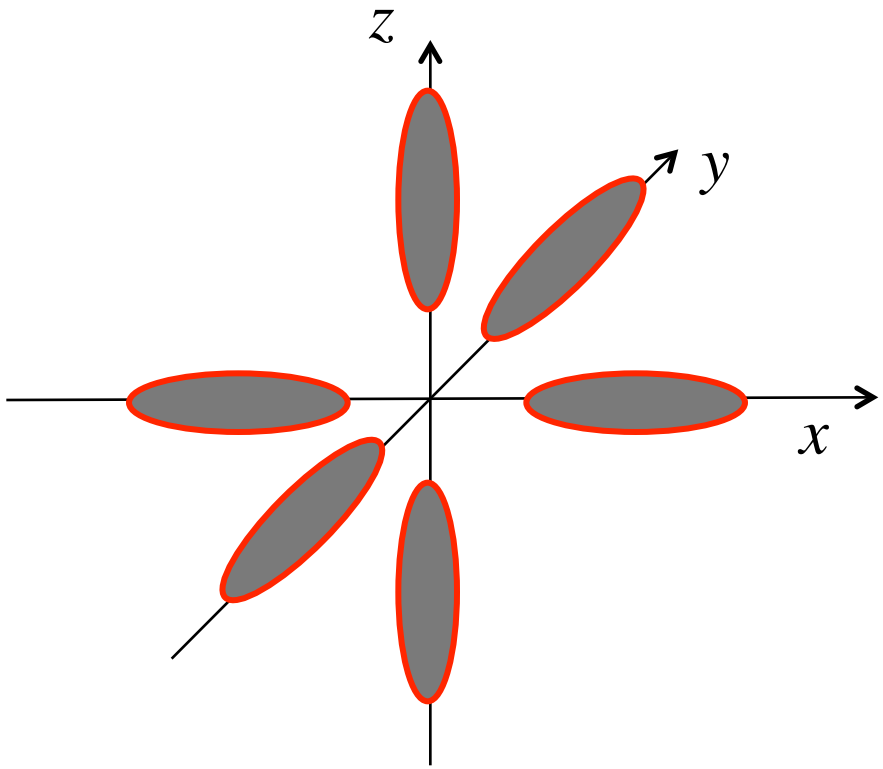
Si conduction band

$$E\left(\vec{k}\right) = \frac{\hbar^2 k_x^2}{2m_{xx}^*} + \frac{\hbar^2 k_y^2}{2m_{yy}^*} + \frac{\hbar^2 k_z^2}{2m_{zz}^*}$$

$$m_\ell^* = 0.9 m_0$$

$$m_t^* = 0.19 m_0$$

"Valley degeneracy" = 6



Valence band is "warped".

outline

1) Electron dispersion (band structure)

2) Simple band structures

3) Phonon dispersion

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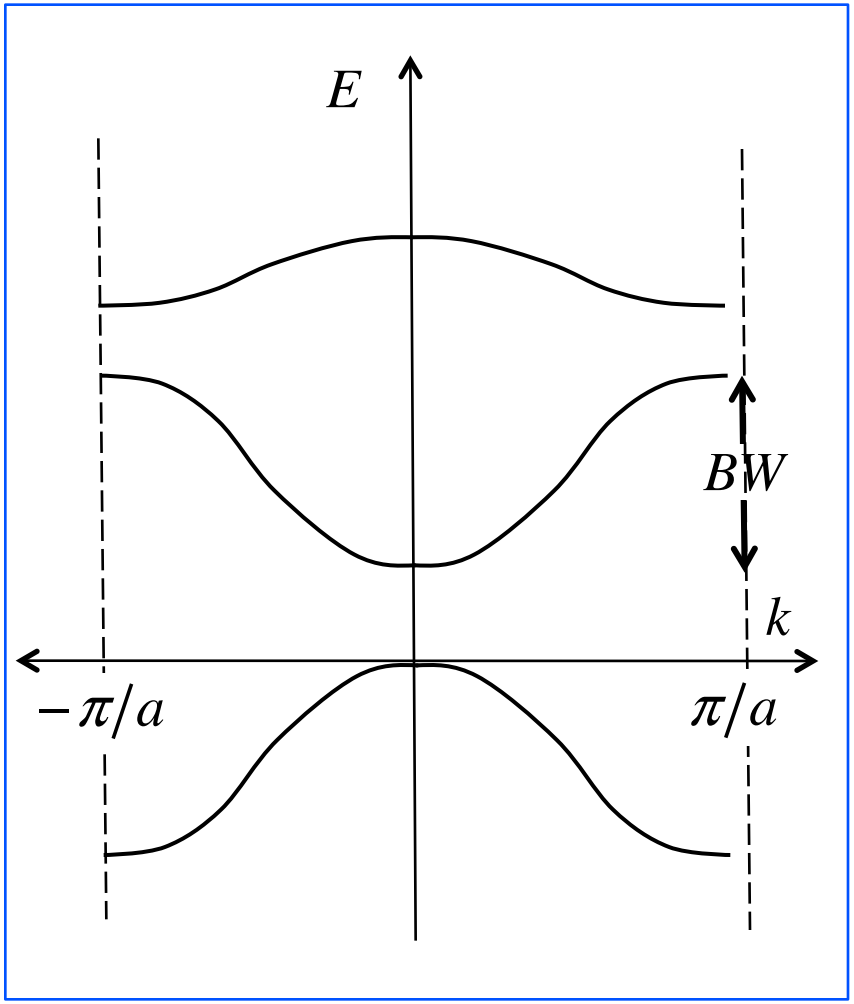
Bandstructure basics

Electrons in a solid behave as both particles (quasi-particles) and as waves.

Electron waves are described by a "dispersion:" $E\left(\vec{k}\right) = \hbar\omega\left(\vec{k}\right)$

Because the crystal is periodic, the dispersion is periodic in *k* (Brillouin zone).

Bandwidth on the order of eV.



12

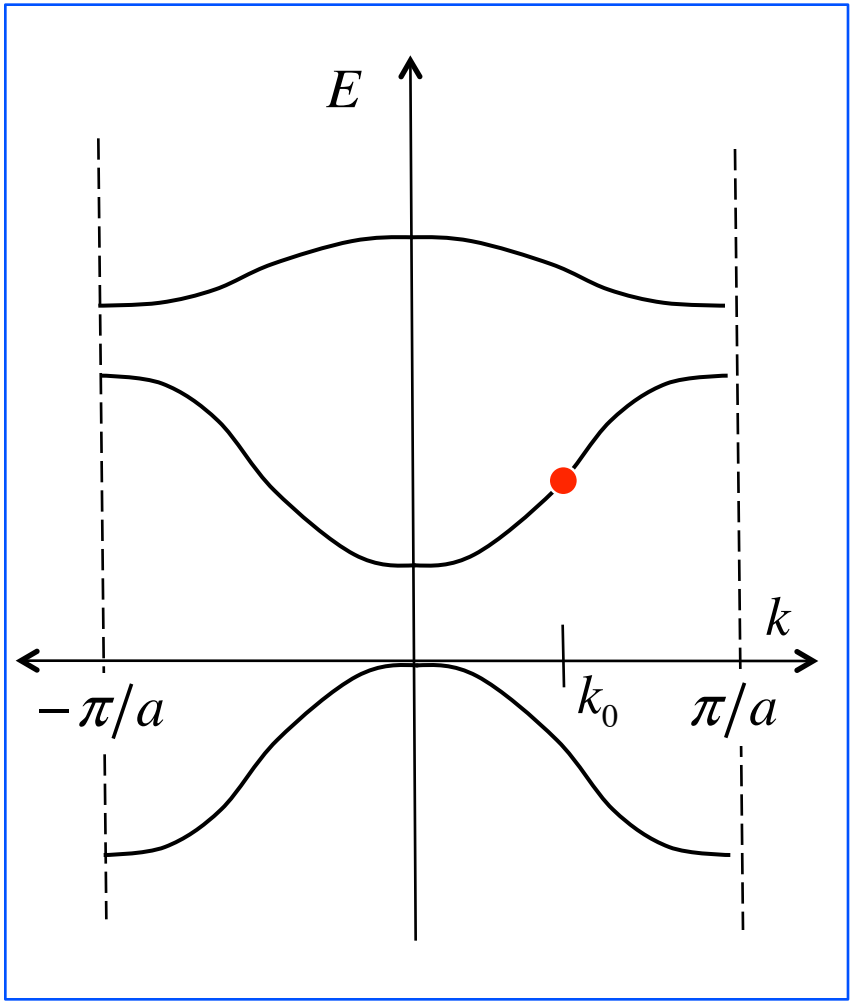
Bandstructure basics

Particles described by a "wavepacket."

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

The "group velocity" of a wavepacket is determined by the dispersion:

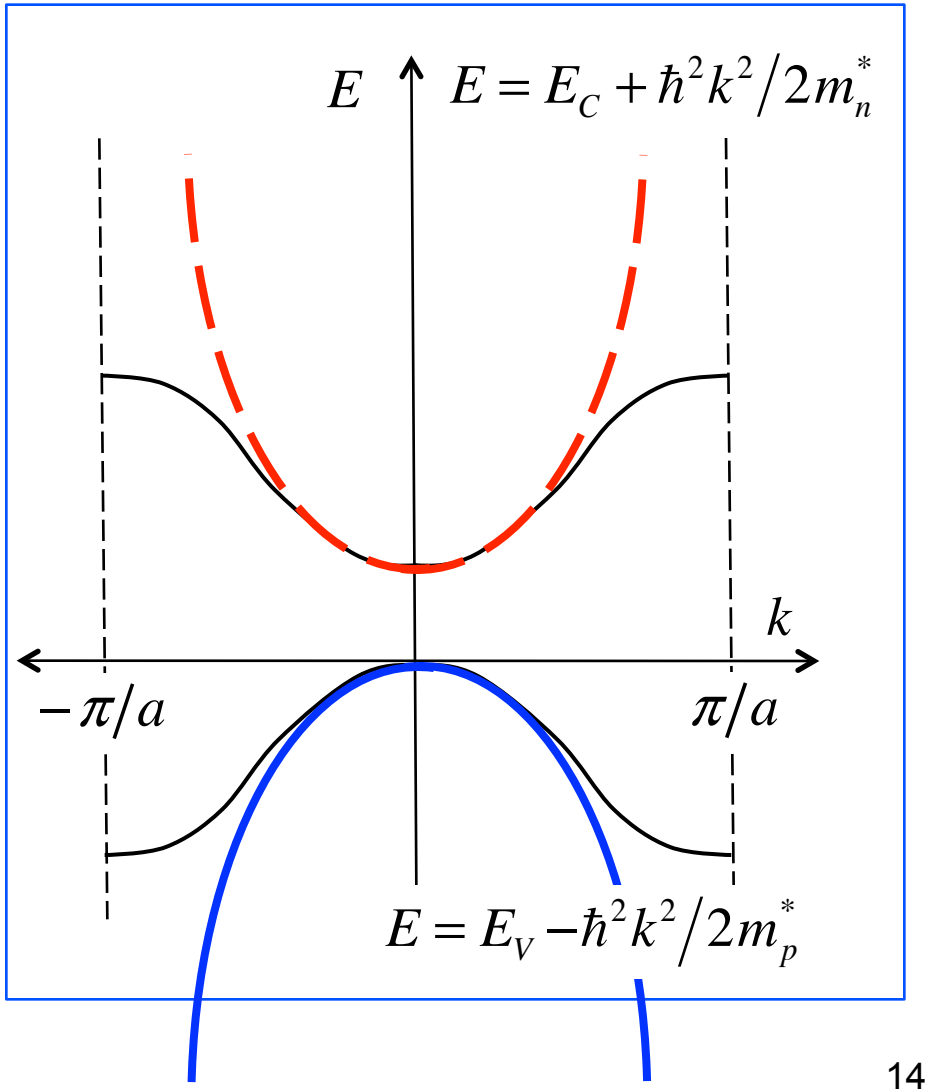
$$\vec{v}_g\left(\vec{k}\right) = \frac{1}{\hbar}\nabla_k E\left(\vec{k}\right)$$



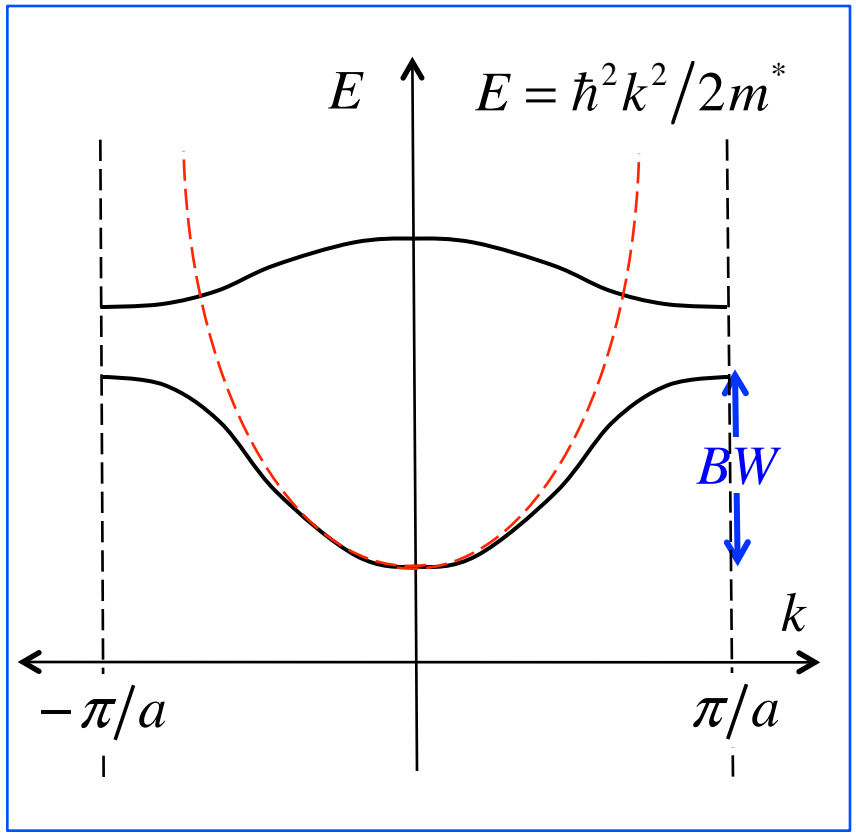
Bandstructure basics

Near a band minimum or maximum, E(k) is a parabola.

The curvature of the parabola is the "effective mass."



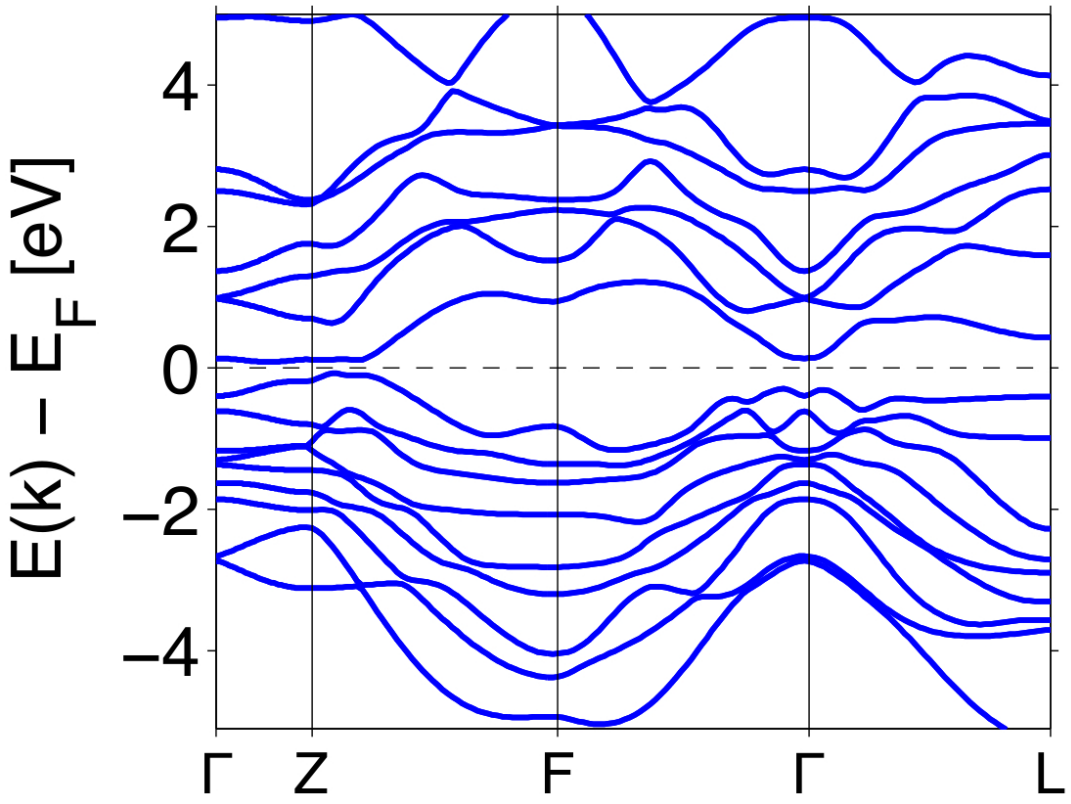
Effective mass model for electrons



As long as the BW >> $k_B T$, the effective mass model often works fine.

Typically, only states near the band edge matter, and these regions can be described by an effective mass approximation.

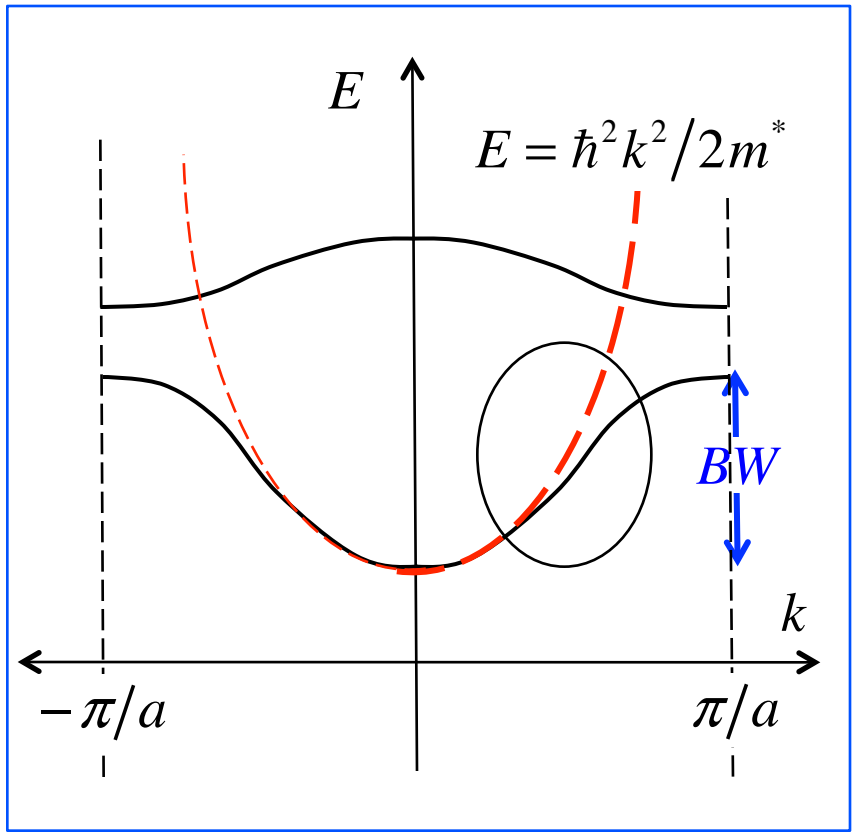
Complex band structures (Bi_2Te_3)



$$E(k) \neq \frac{\hbar^2 k^2}{2m^*}$$

DFT calculations of Bi_2Te_3 by Dr. J. Maassen, Purdue

First order correction for non-parabolicity



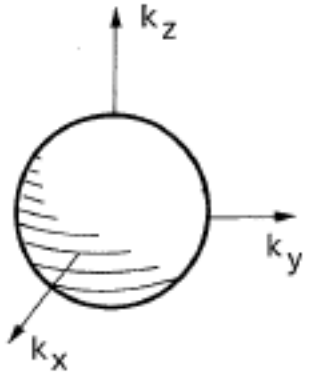
"Kane bands"

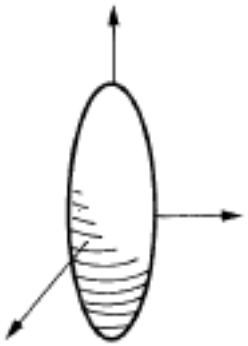
$$E(1+\alpha E) = \frac{\hbar^2 k^2}{2m^*(0)}$$

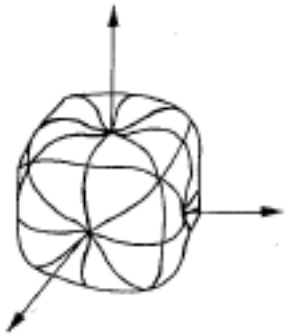
$\alpha = 0.5\ \text{eV}^{-1}$ Si

$\alpha = 0.64\ \text{eV}^{-1}$ Si

Surfaces of constant energy







$$E = \frac{\hbar^2 k^2}{2m^*}$$

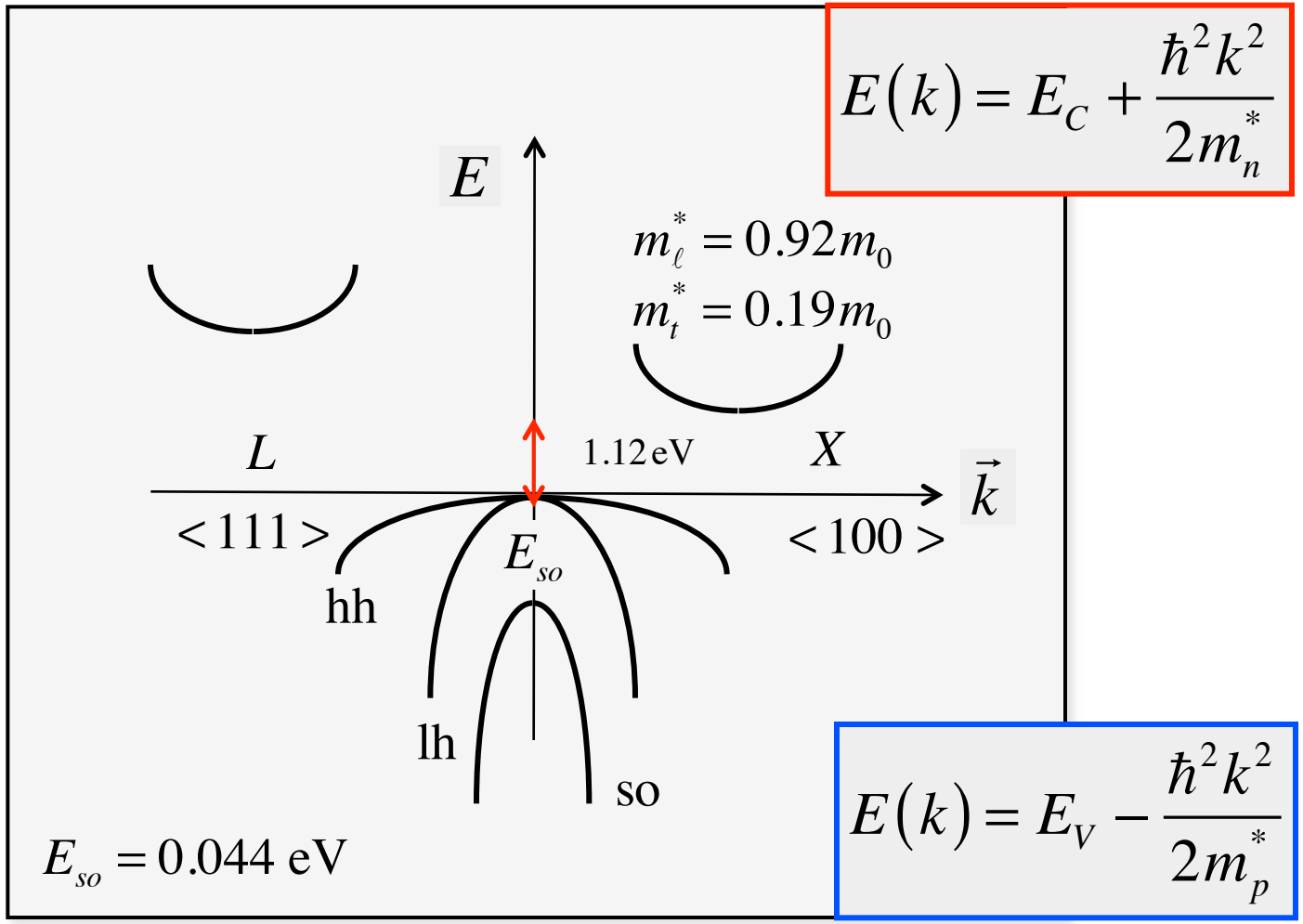
$$E = \frac{\hbar^2 k_x^2}{2m_{xx}^*} + \frac{\hbar^2 k_y^2}{2m_{yy}^*} + \frac{\hbar^2 k_z^2}{2m_{zz}^*}$$

$$E = \frac{\hbar^2 k^2}{2m^*}\left[1 \mp g(\theta,\phi)\right]$$

- \- Heavy hole
- \+ Light hole

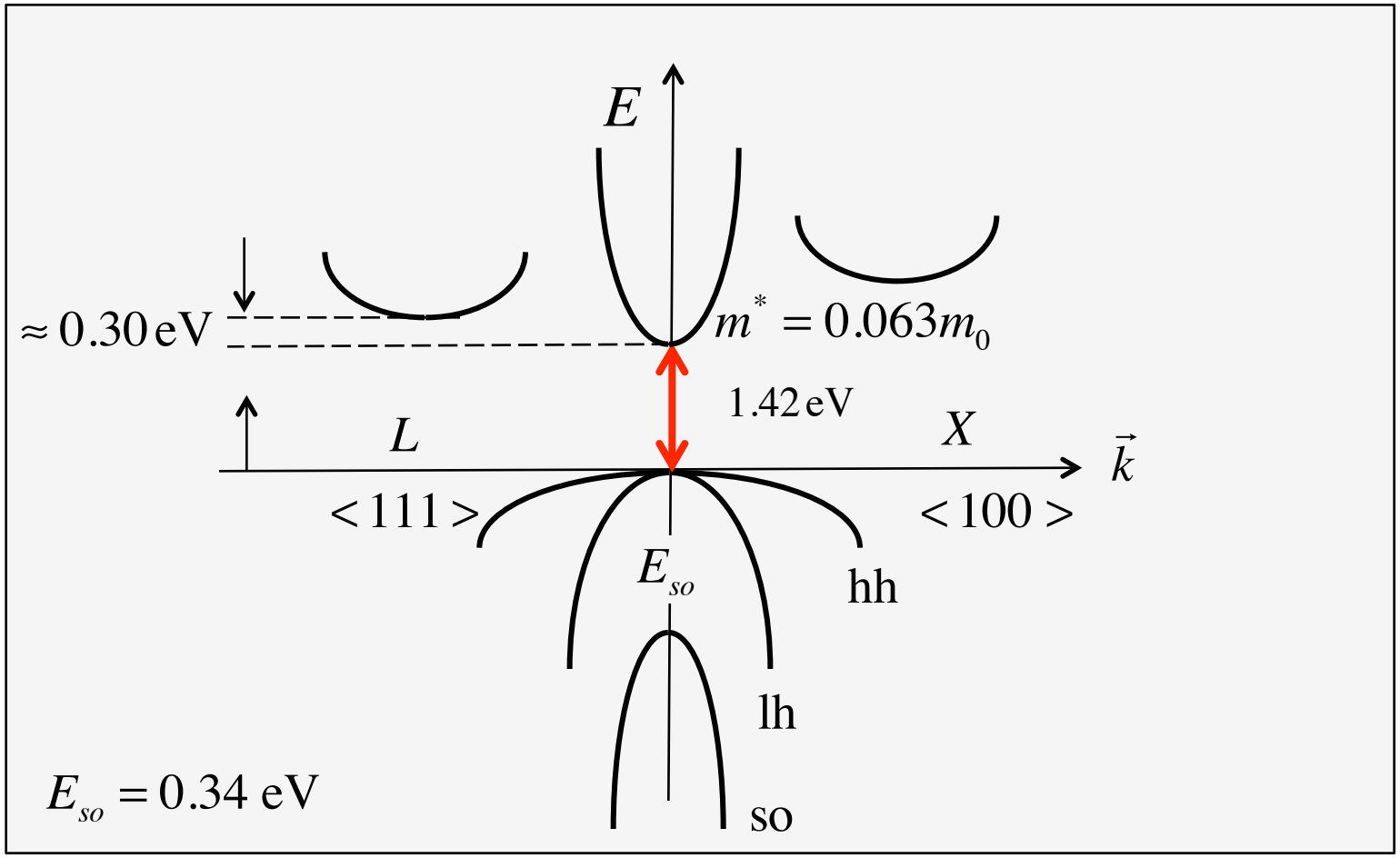
See L. Reggiani, “Chapter 2: General Theory,” pp.7-86, in *Hot Electron Transport in Semiconductors*, Springer-Verlag, New York, 1985

Model bandstructure: Si

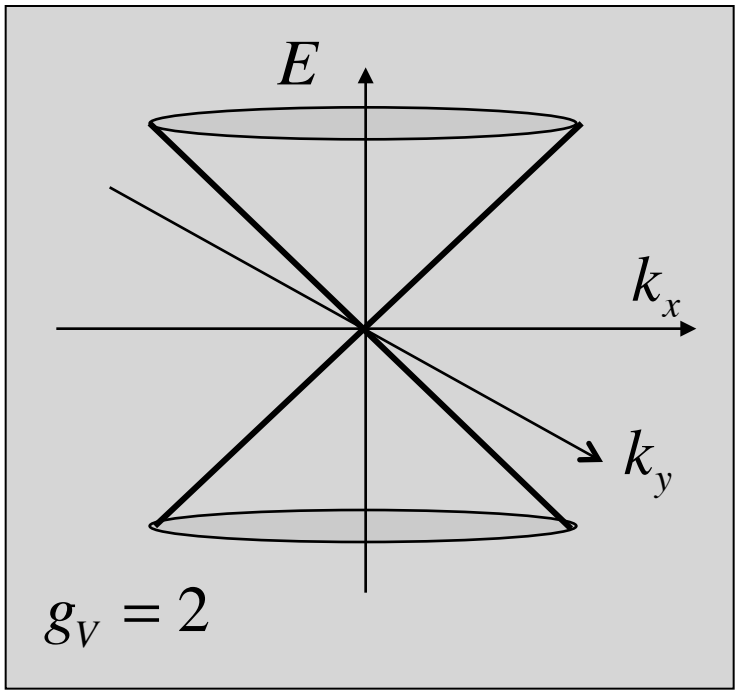


19

Model bandstructure: GaAs



$E(k)$ for graphene



$$E(k) = \pm\hbar\upsilon_F\sqrt{k_x^2 + k_y^2} = \pm\hbar\upsilon_F k$$

Recall:

$$\upsilon_g\left(\vec{k}\right) = \frac{1}{\hbar}\frac{dE(k)}{dk}$$

For graphene:

$$\upsilon_g\left(\vec{k}\right) = \upsilon_F \approx 10^8 \text{ cm/s}$$

Also recall:

$$m^* = \left(\frac{1}{\hbar^2}\frac{d^2E(k)}{dk^2}\right)^{-1}$$

For graphene:

$$m^* = ?$$

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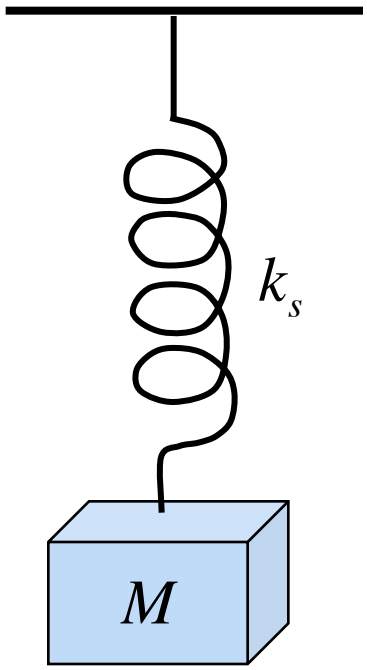
mass and spring



$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega$$

$$U = \frac{1}{2} k_s \left(x - x_0 \right)^2$$

$$F = -\frac{dU}{dx} = -k_s \left(x - x_0 \right)$$

$$M \frac{d^2 x}{dt^2} = -k_s \left(x - x_0 \right)$$

$$x(t) - x_0 = Ae^{i\omega t}$$

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

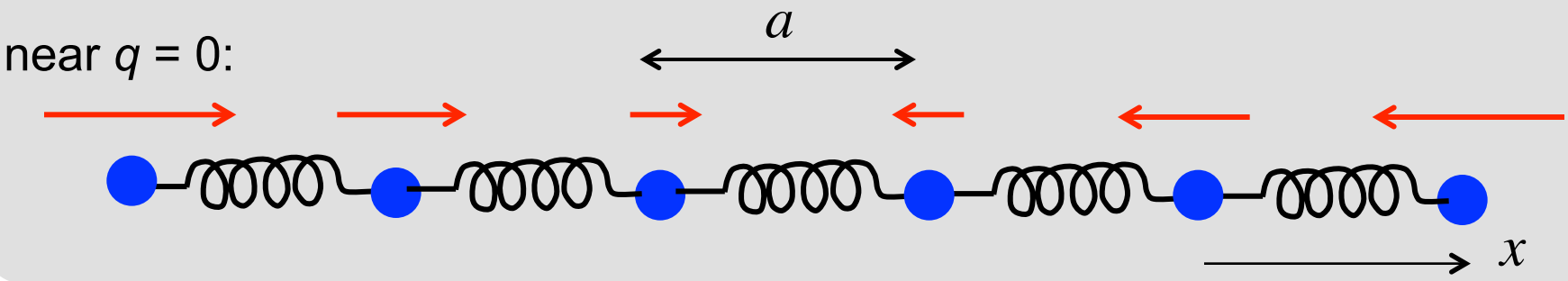
Elastic waves: acoustic modes

$$u(\vec{r}) = A_i \hat{e}_i \; e^{i(\vec{q}\bullet\vec{r}-\omega t)} \qquad \vec{\beta} \rightarrow \vec{q}$$

Longitudinal wave: displacement in the direction of propagation.

Transverse waves: displacement transverse to the direction of propagation.

LA phonons:

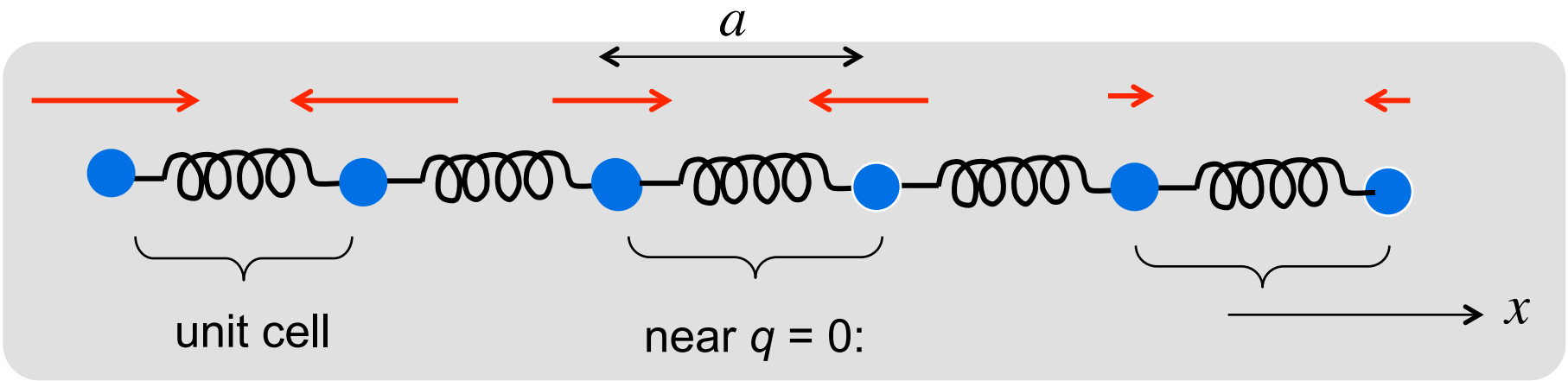


Elastic oaves: optical modes

$$u(\vec{r}) = A_i \hat{e}_i \; e^{i(\vec{q}\bullet\vec{r} - \omega t)}$$

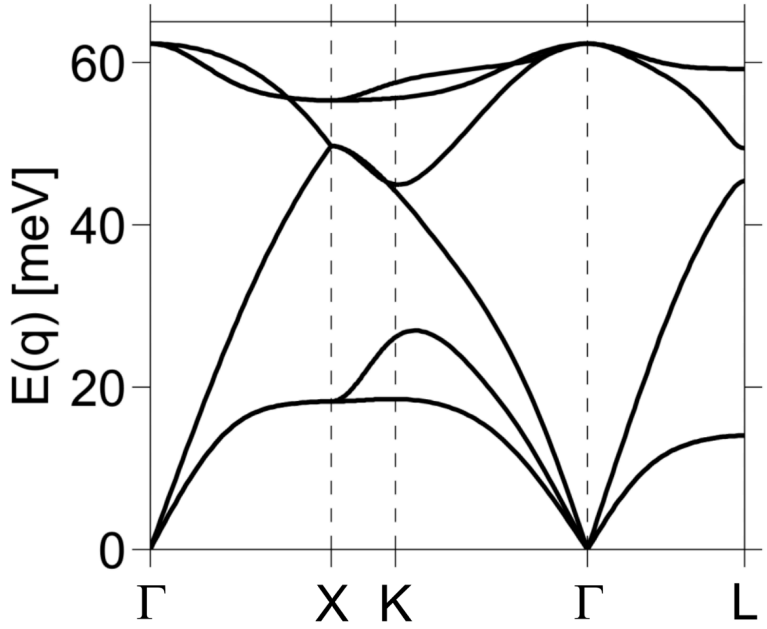
Atoms in the unit cell oscillate against each other.

Longitudinal and **transverse** optical modes.



Lattice (phonon) dispersion

phonons in Si



DFT calculations by Dr. J. Maassen, Purdue

outline

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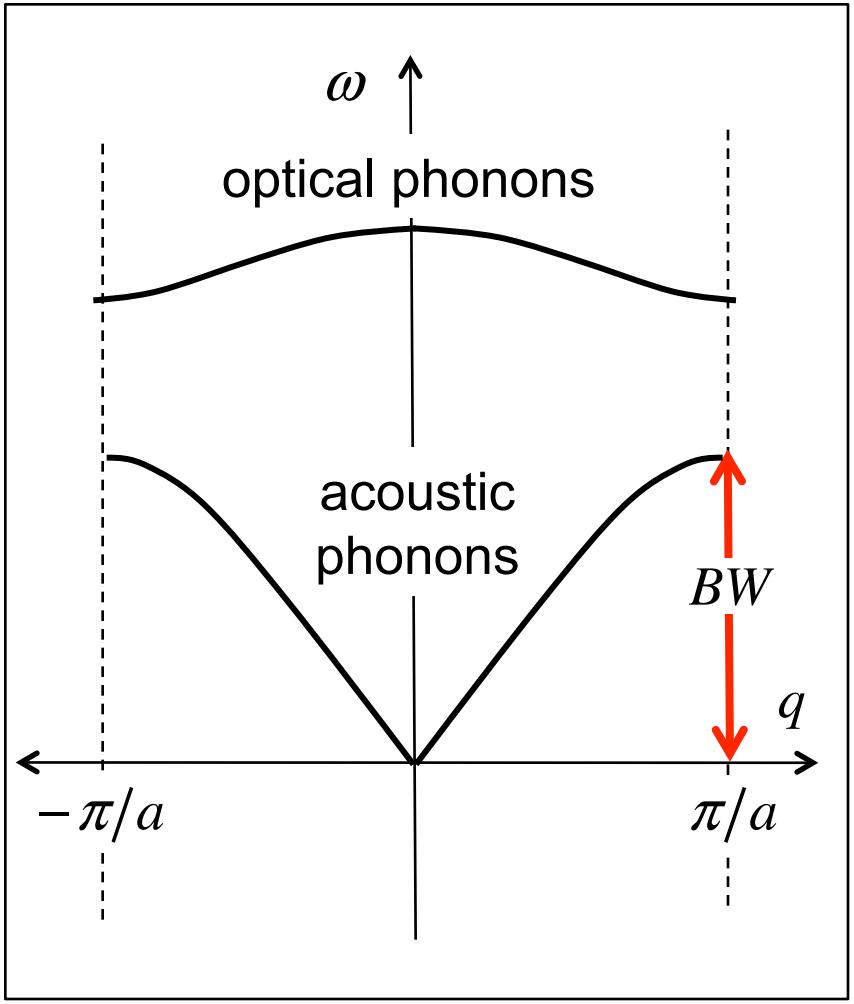
Phonon dispersion basics

Lattice vibrations behave both as particles (quasi-particles) and as waves.

Lattice vibrations are described by a "dispersion:" $\omega(\vec{q}) = E(\vec{q})/\hbar$

Because the crystal is periodic, the dispersion is periodic in *k* (Brillouin zone).

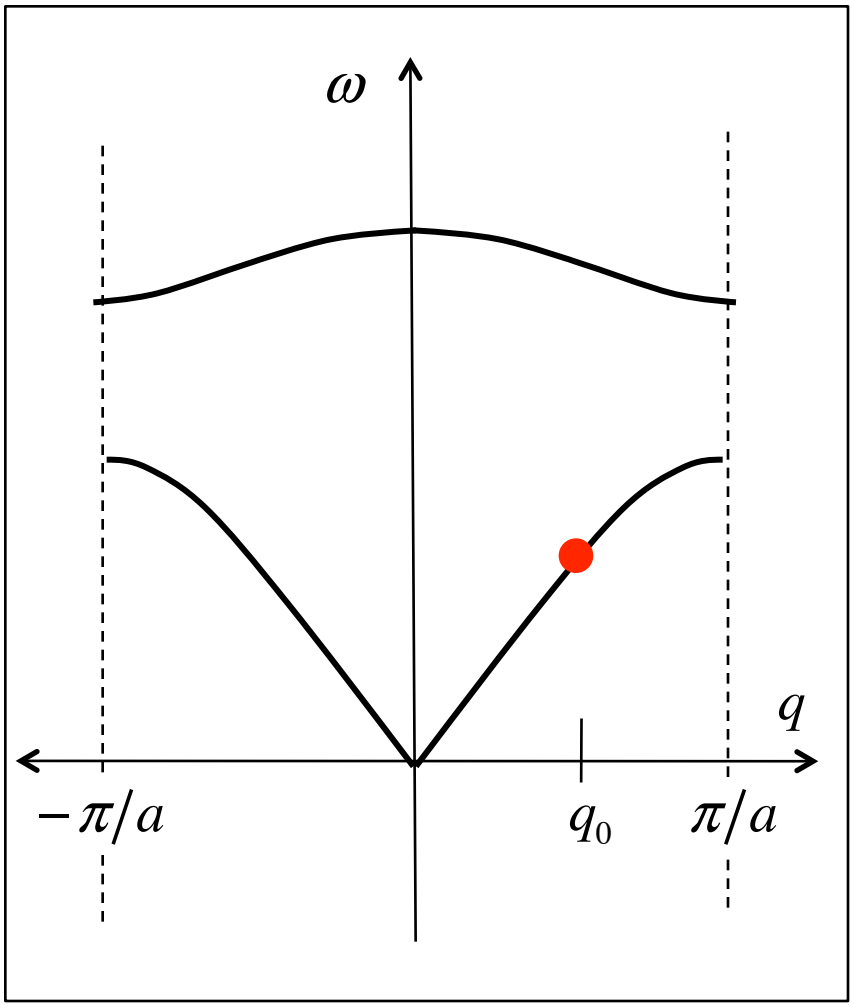


Phonon dispersion basics

Particles described by a "wavepacket" (phonon).

The "group velocity" of a phonon is determined by the dispersion:

$$\vec{v}_g(\vec{q}) = \nabla_q \omega(\vec{q})$$



Phonon dispersion basics

Optical phonons have a flat dispersion (near the zone center).

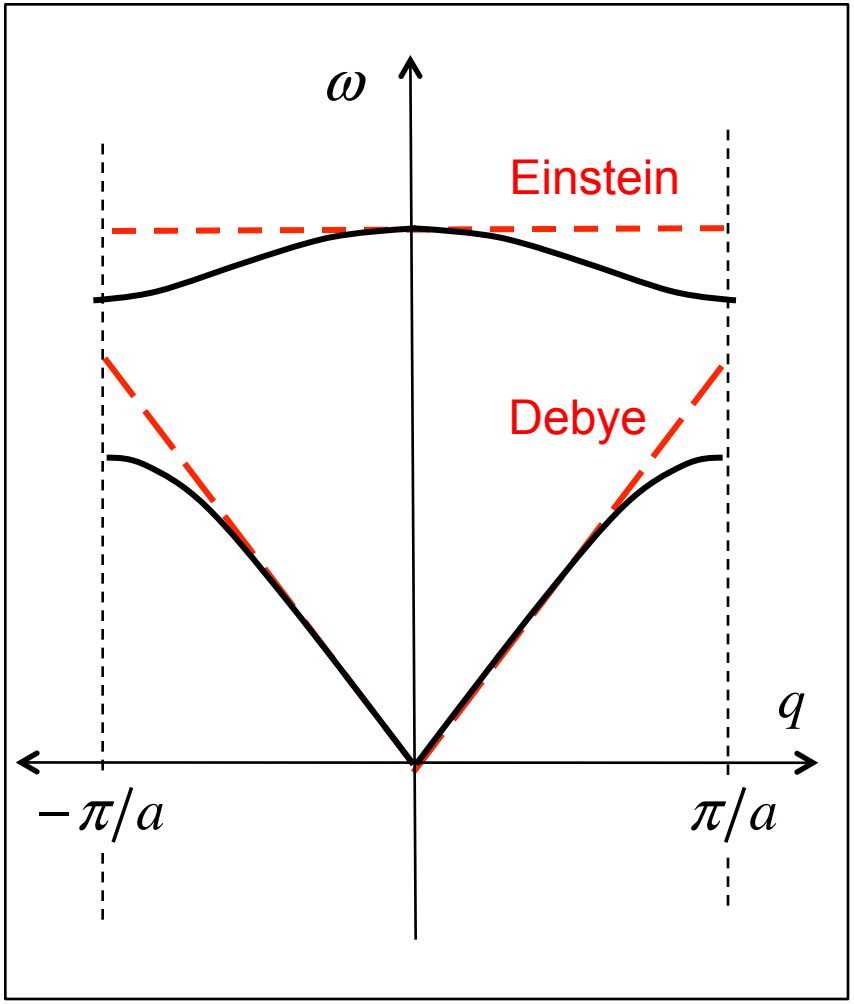
Near zero group velocity.

Einstein approximation

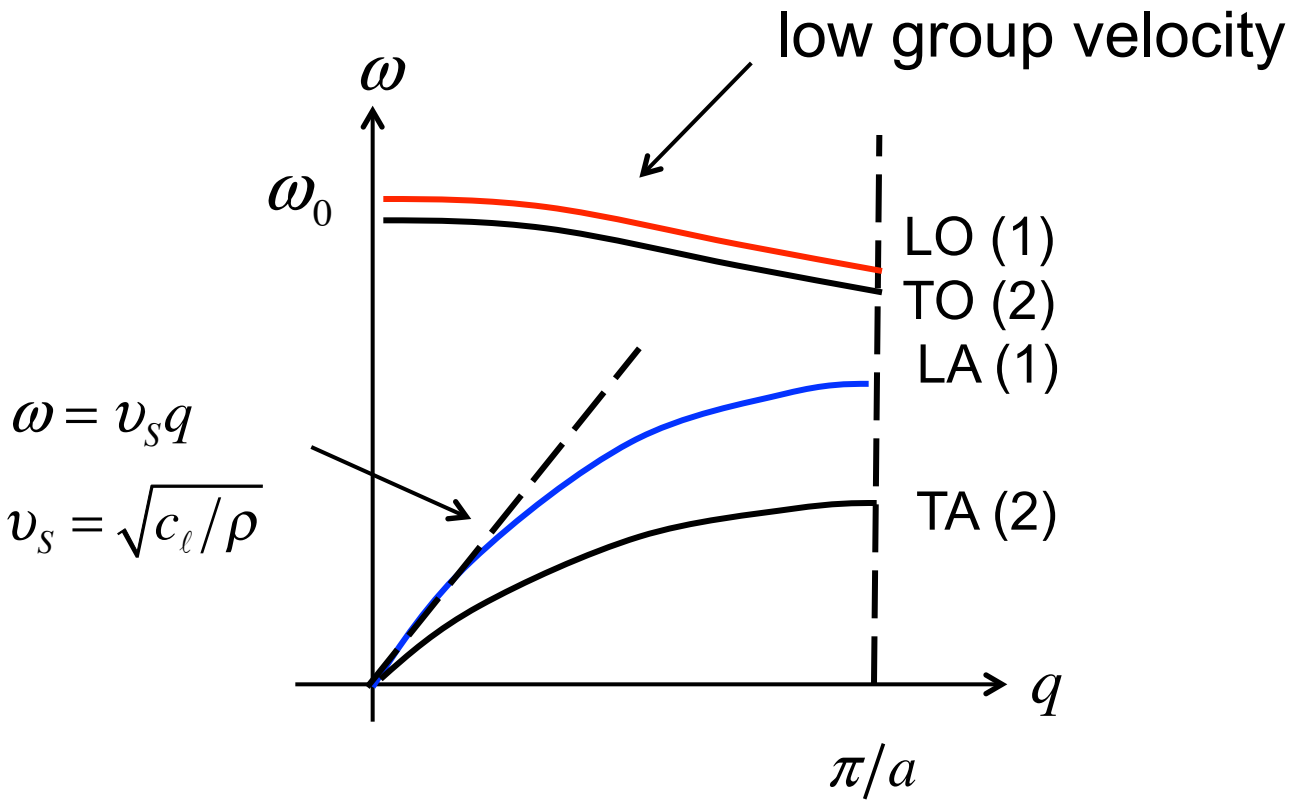
Acoustic modes have a linear dispersion (near the zone center).

Constant sound velocity.

Debye approximation.



General features of phonon dispersion



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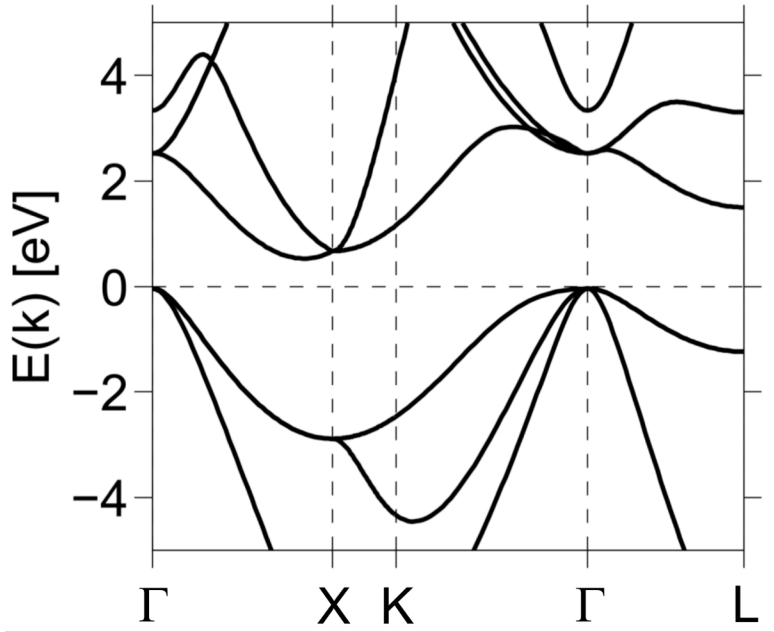
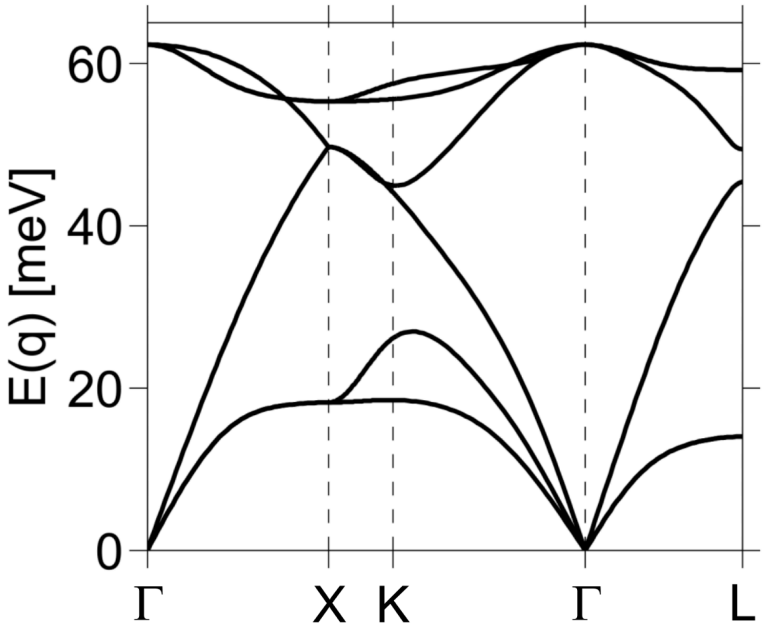
Bandstructure (dispersion)

electrons in Si



phonons in Si

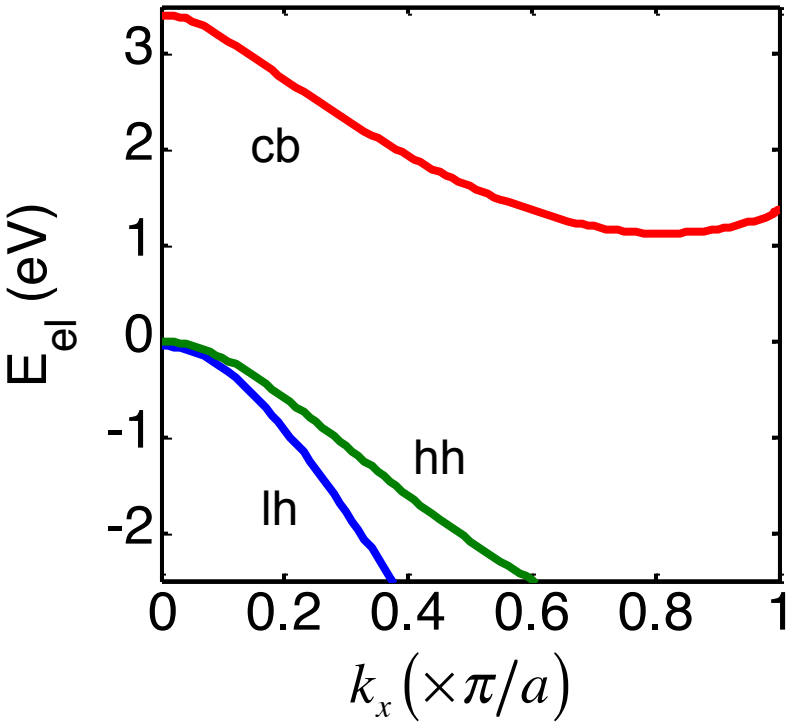


note the different energy scales!

DFT calculations by Dr. J. Maassen, Purdue

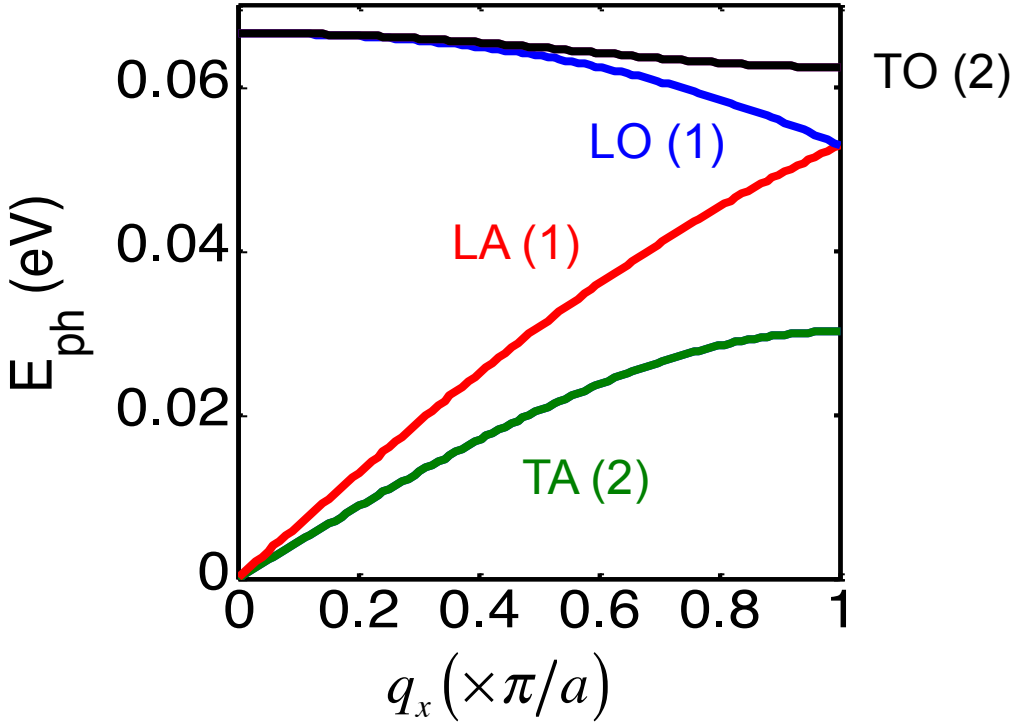
Real dispersions

$BW >> k_B T$



electrons in Si (along [100])

$BW \sim k_B T$



phonons in Si (along [100])

note the different energy scales!

References

For a though treatment of electrons and phonons in crystals, see:

N.W. Ashcroft and N.D. Mermin, *Solid State Physics*, Saunders College, Philadelphia, 1976.

For an introduction to lattice waves and phonons, see:

T.S. Fisher, *Thermal Energy at the Nanoscale*, Chapter 1, World Scientific, 2014.

Summary

1) Electron dispersion (band structure)

2) Simple band structures

3) Phonon dispersion

4) Simple phonon dispersions

5) Electrons vs. phonons