

Primer on Semiconductors

## Unit 2: Quantum Mechanics

# **Lecture 2.4: Electron waves in crystals**

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# Wave equation in a constant potential

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - U_0]\psi(x) = 0$$

$$E > U_0 \quad k^2 = \frac{2m_0}{\hbar^2}[E - U_0] \quad \frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$$

Solution:  $\psi(x) = Ae^{\pm ikx}$

This is a wave solution

$$\Psi(x, t) = \psi(x)\phi(t)$$

$$E(k) = U_0 + \frac{\hbar^2 k^2}{2m}$$

$$\Psi(x, t) = Ae^{\pm i(kx - \omega t)}$$

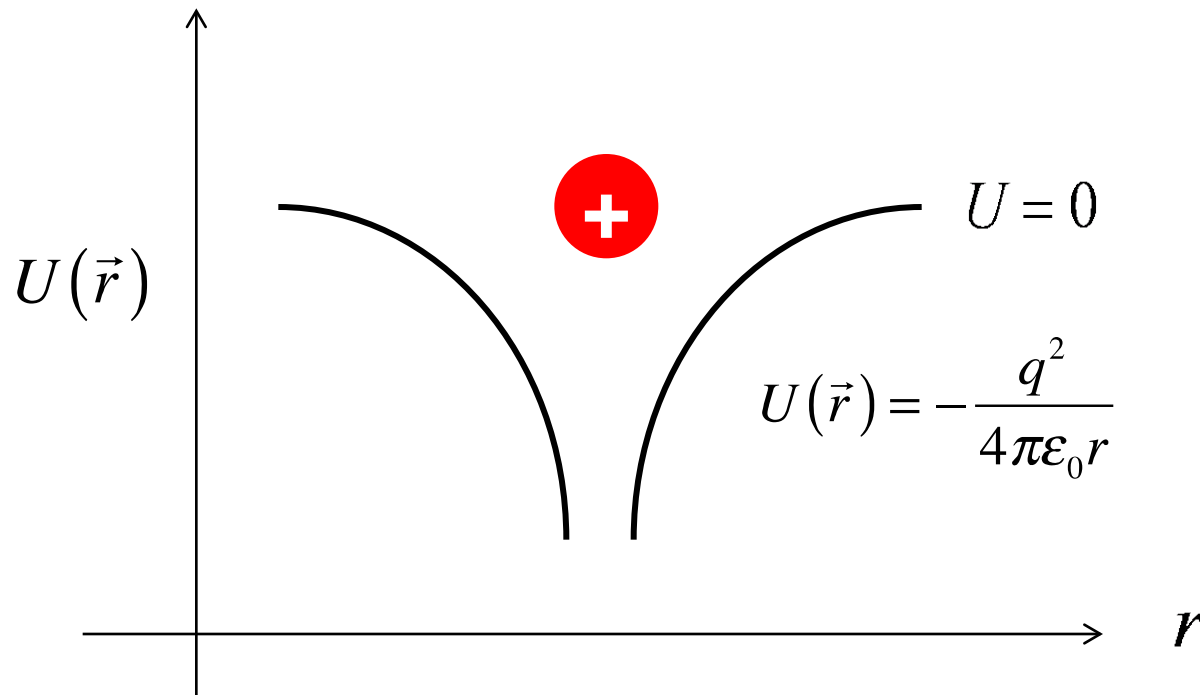
$$p = \hbar k \quad v_g = \hbar k / m$$

# Electrons in atoms

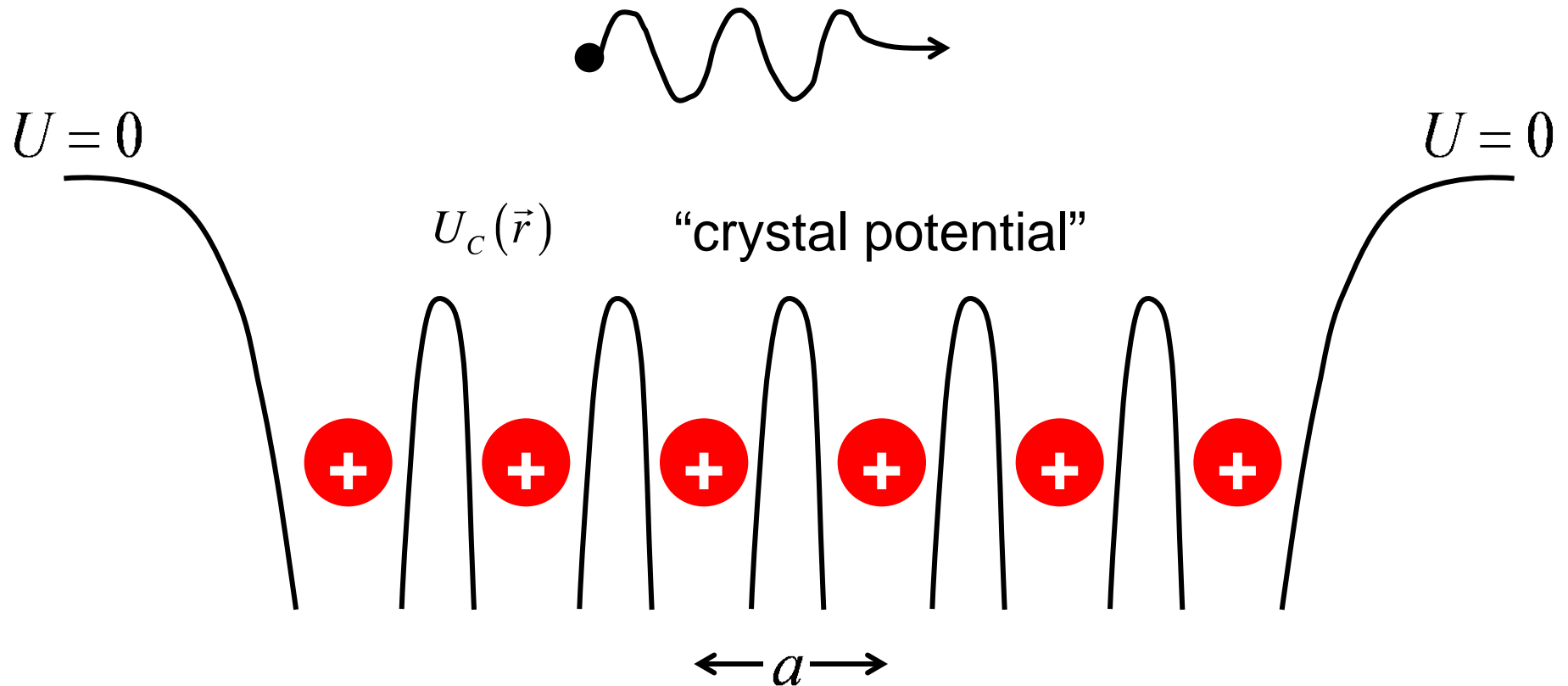
Hydrogen atom:

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

$$E_n = -\frac{13.6}{n^2} \text{ eV}$$



# Mobile electrons in crystals



# Electrons in crystals

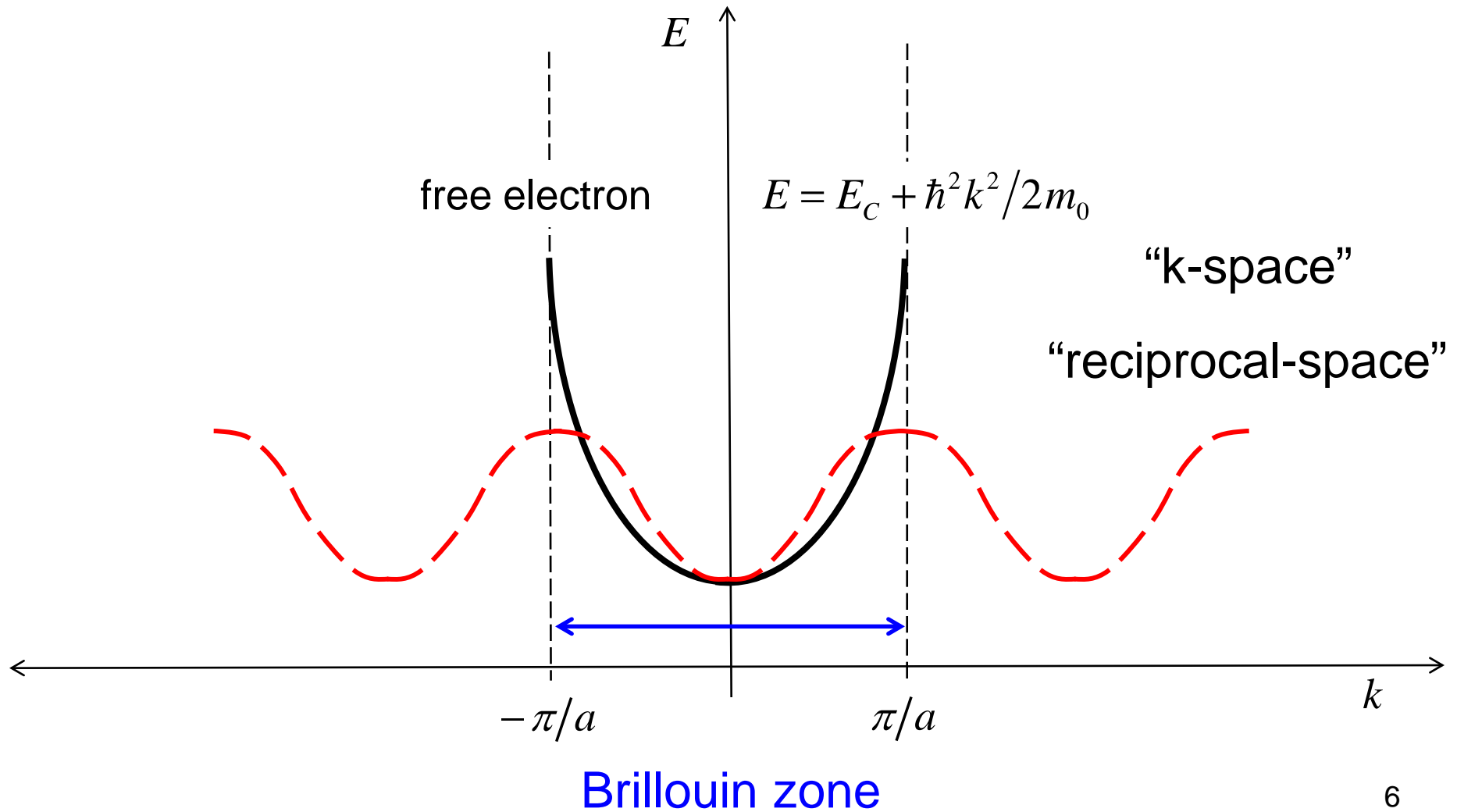
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$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + U_C(x)\psi(x) = E\psi(x) \qquad U_C(\vec{r} + \vec{a}) = U_C(\vec{r})$$

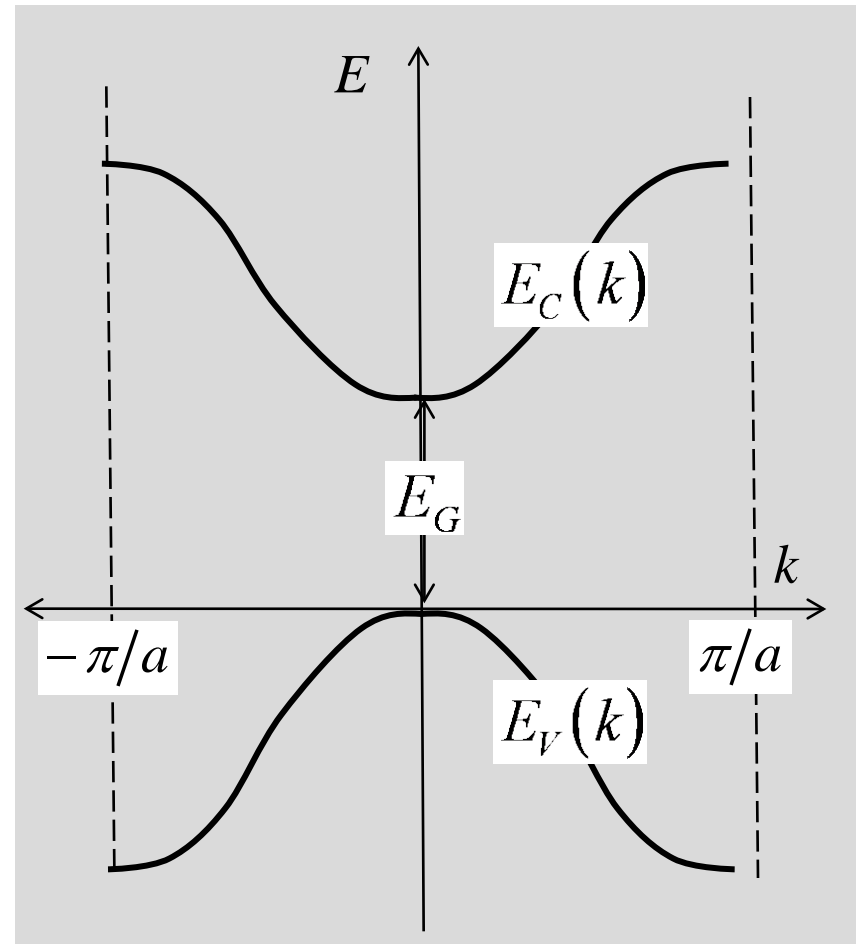
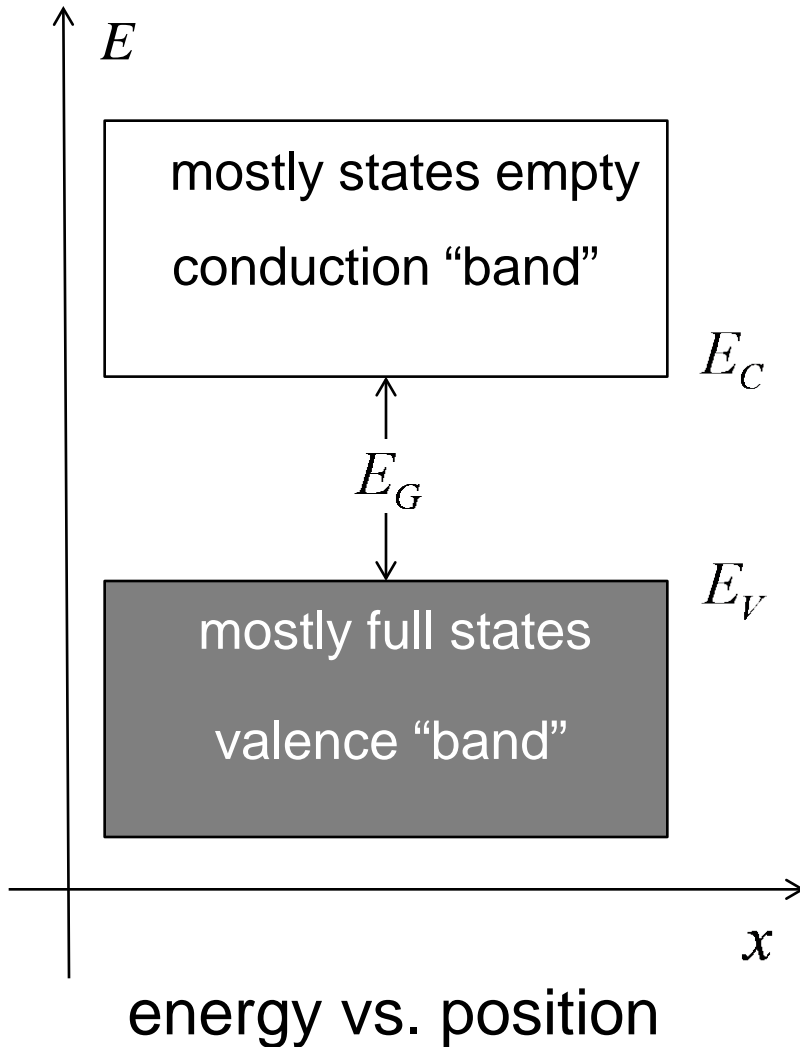
$$\psi(\vec{r}) = u_{\vec{k}}(\vec{r}) e^{i\vec{k} \cdot \vec{r}} \qquad u_{\vec{k}}(\vec{r} + \vec{a}) = u_{\vec{k}}(\vec{r}) \qquad \text{“Bloch wave”}$$

The wave functions are periodic in space. They are also periodic in k-space.

# Energy vs. momentum ( $k$ )



# Conduction and valence bands



energy vs.  $k$

# Crystal momentum

$$-\frac{\hbar^2}{2m_0} \frac{d^2\psi(x)}{dx^2} + U_C(x)\psi(x) = E\psi(x)$$

$$U_C(\vec{r} + \vec{a}) = U_C(\vec{r})$$

$$\psi(\vec{r}) = u_{\vec{k}}(\vec{r}) e^{i\vec{k} \cdot \vec{r}}$$

$$u_{\vec{k}}(\vec{r} + \vec{a}) = u_{\vec{k}}(\vec{r})$$

$\vec{k}$ : Brillouin zone

*“Bloch wave”*

$\vec{p} \neq \hbar\vec{k}$  but....“crystal momentum”

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



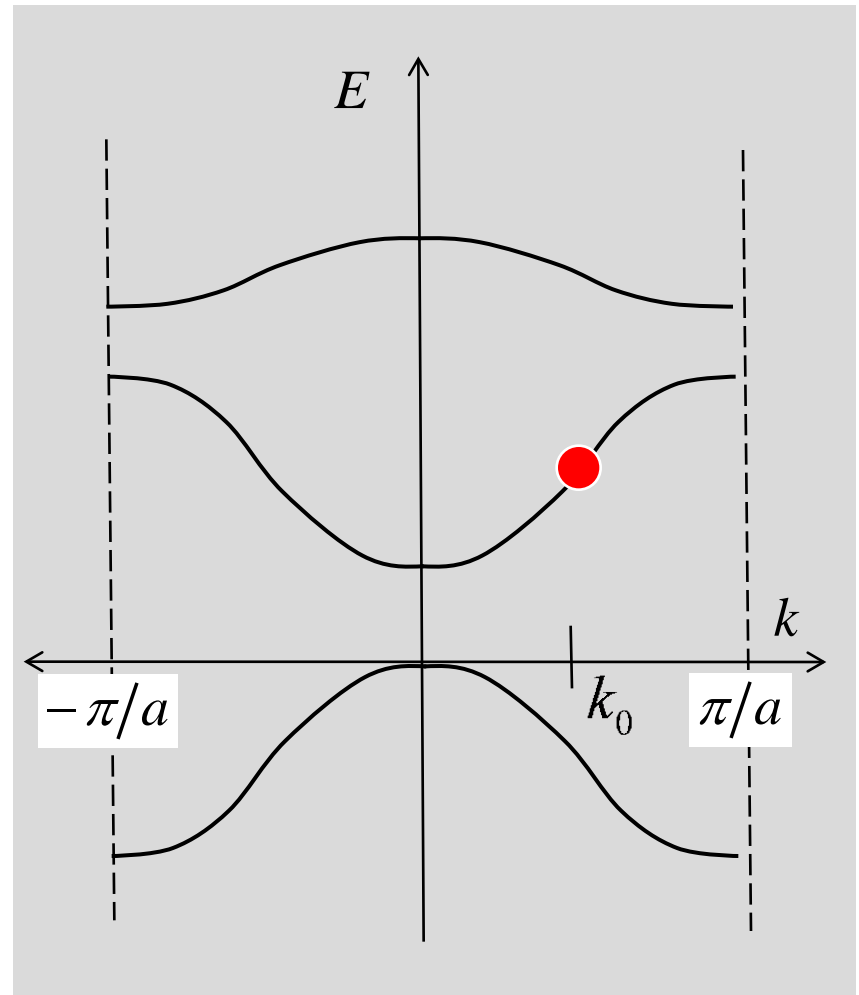
# Bandstructure basics

Particles described by a “wavepacket.”

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

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

$$\vec{v}_g(\vec{k}) = \frac{1}{\hbar} \frac{dE}{dk}$$



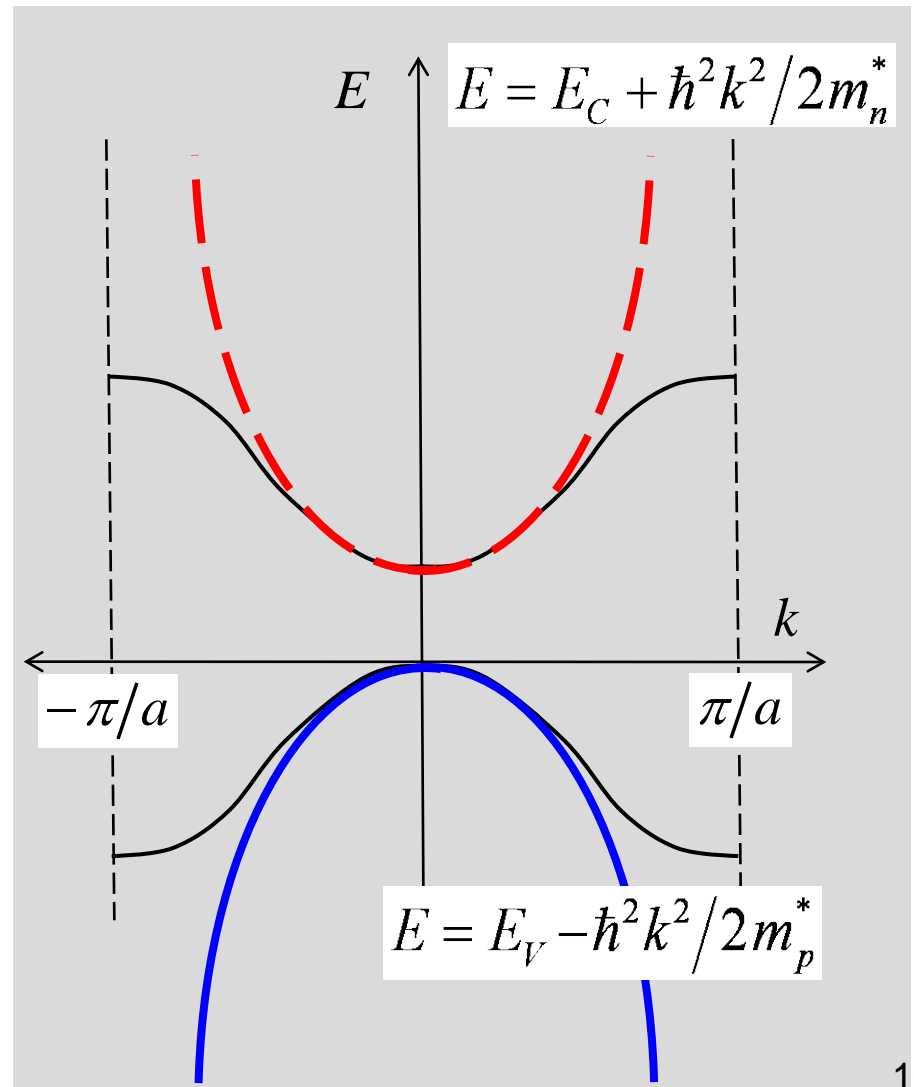
# Parabolic bands

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

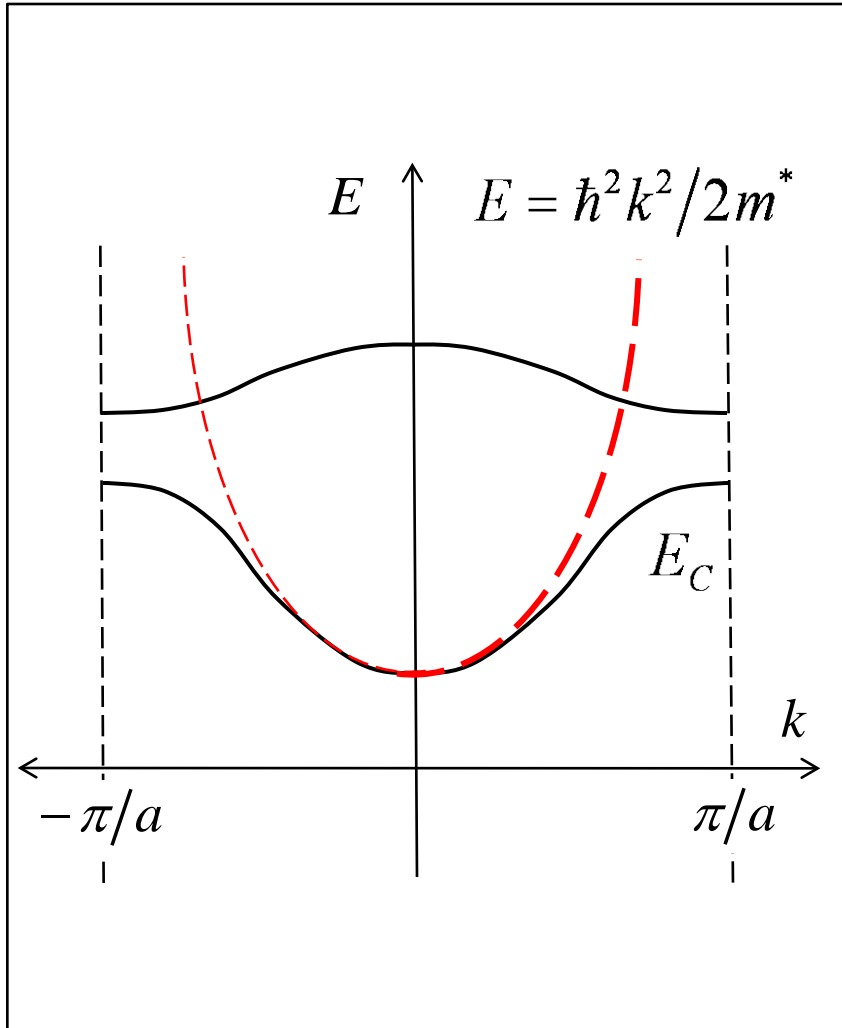
$$E \approx E_C + \hbar^2 k^2 / 2m_n^*$$

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

$$v_g(k) = \frac{1}{\hbar} \frac{dE(k)}{dk} = \frac{\hbar k}{m^*}$$

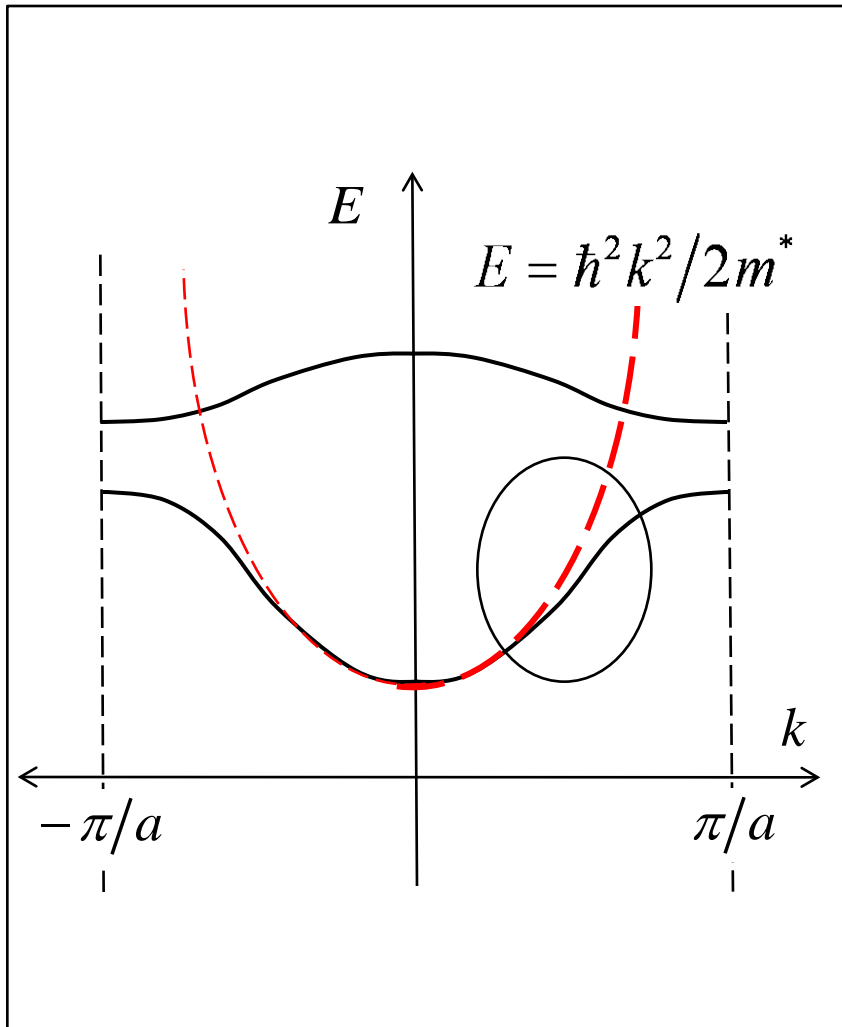


# Effective mass model for electrons



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

# First order correction for non-parabolicity



“Kane bands”

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

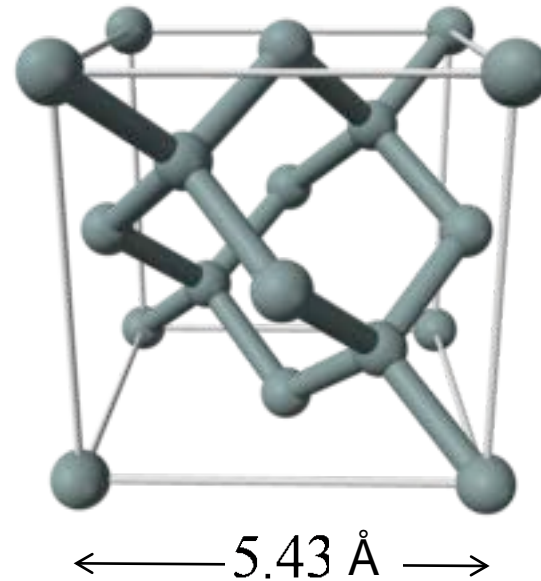
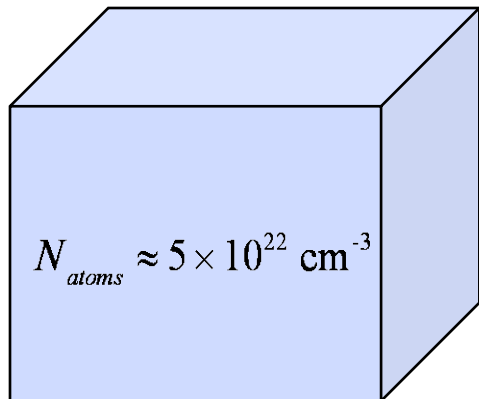
$$\alpha = 0.5 \text{ eV}^{-1} \quad \text{Si}$$

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

# 3D crystals

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## Silicon

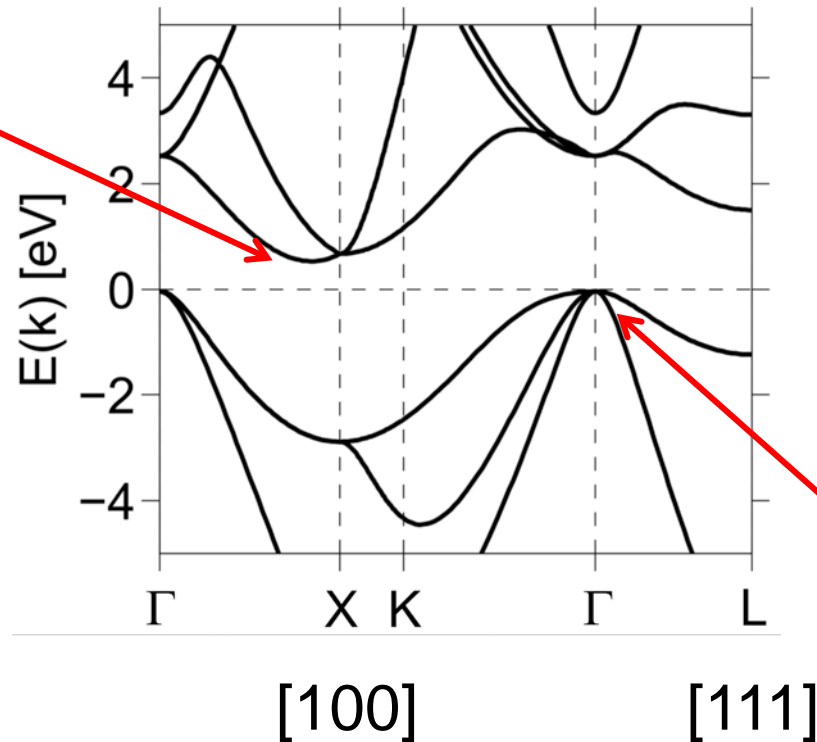


real space structure

# Band structure (electron dispersion)

bottom of  
conduction band

$E(k)$  for electrons in Si



top of valence  
band

# Constant energy surfaces

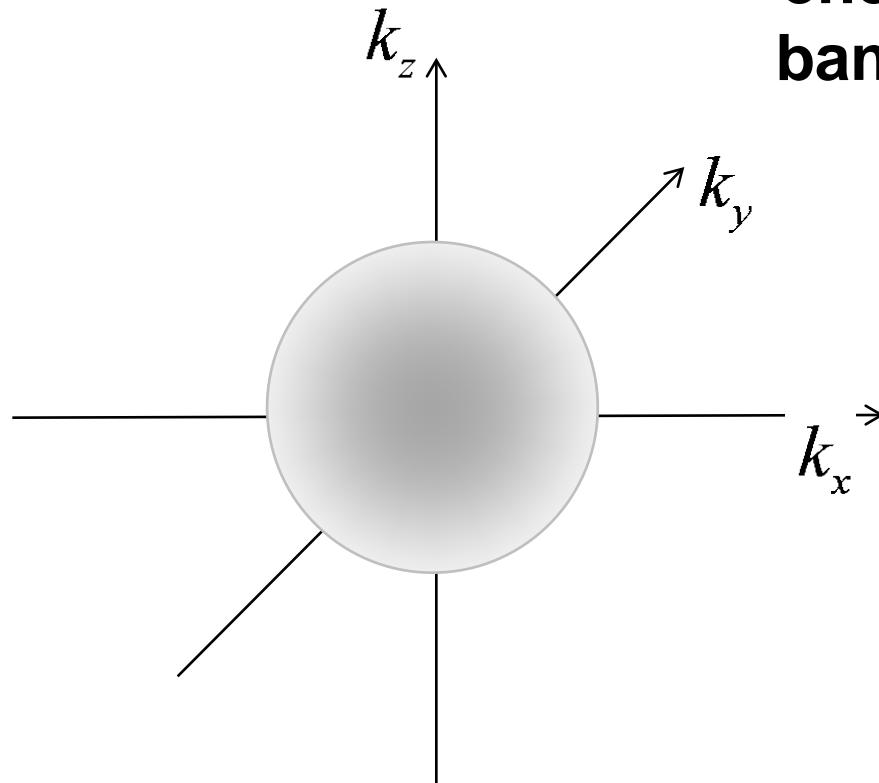
GaAs conduction band

**“spherical  
energy  
bands”**

$$E(\vec{k}) = \frac{\hbar^2 k_x^2}{2m_n^*} + \frac{\hbar^2 k_y^2}{2m_n^*} + \frac{\hbar^2 k_z^2}{2m_n^*}$$

equation of a sphere

$$m_n^* = 0.063m_0$$



# Constant energy surfaces

Si conduction band

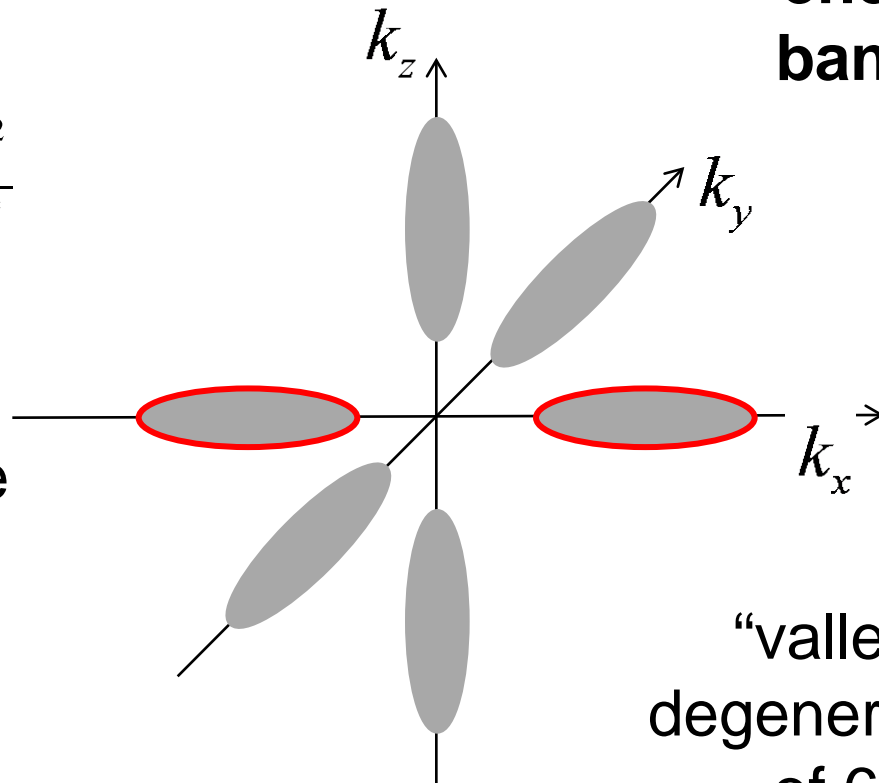
**“ellipsoidal  
energy  
bands”**

$$E(\vec{k}) = \frac{\hbar^2 k_x^2}{2m_\ell^*} + \frac{\hbar^2 k_y^2}{2m_t^*} + \frac{\hbar^2 k_z^2}{2m_t^*}$$

equation of an ellipse

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

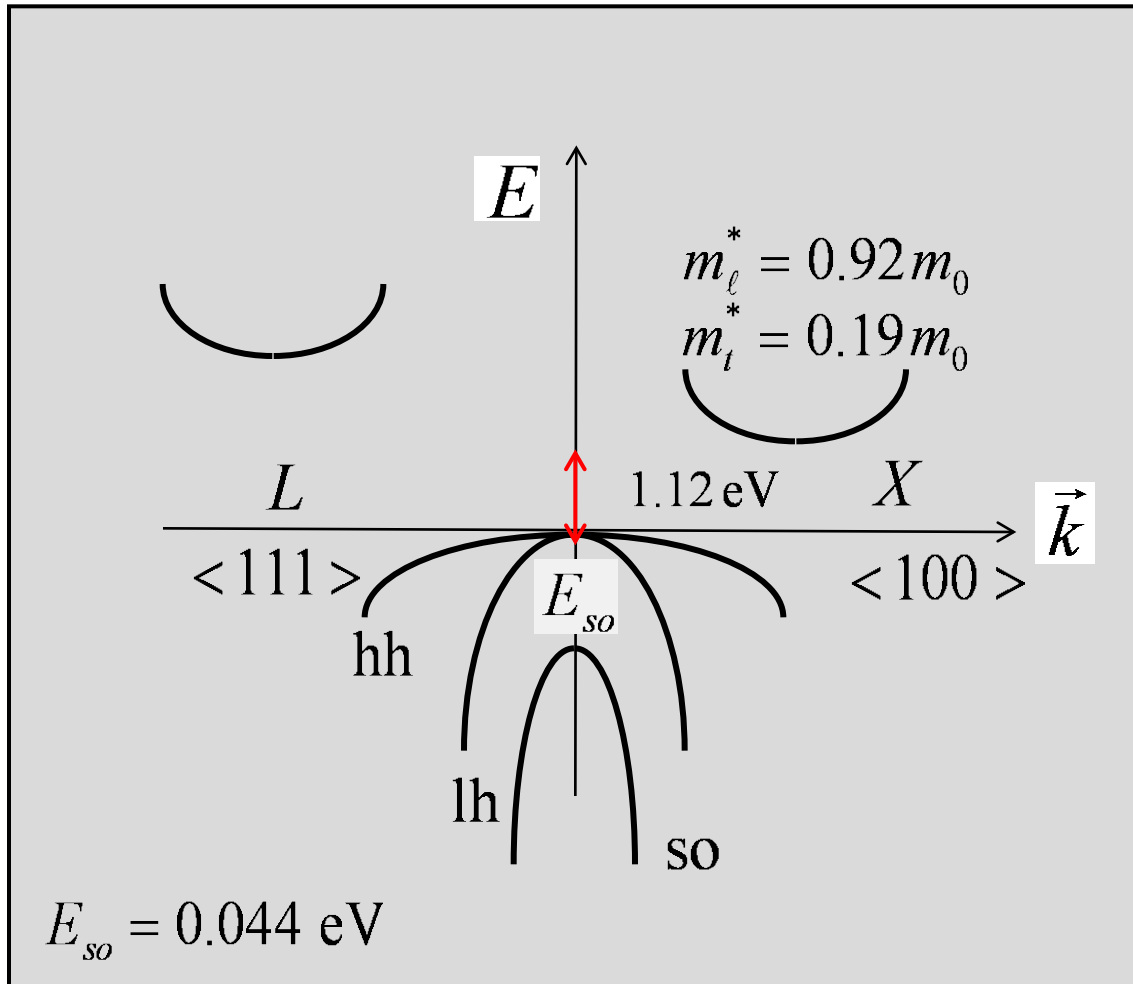
$$m_t^* = 0.19m_0$$



**“valley  
degeneracy”  
of 6**



# Model bandstructure for Si

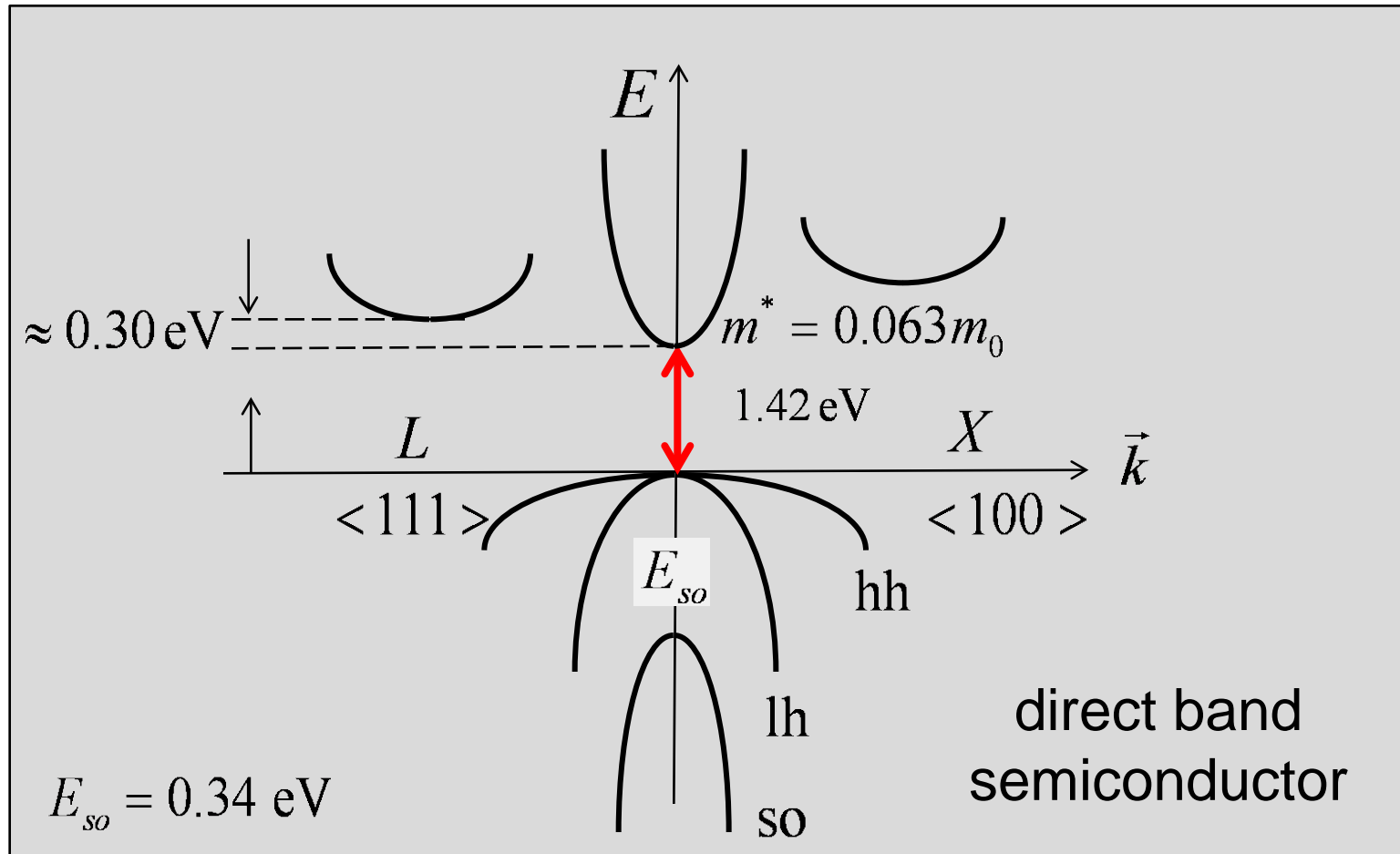


$$E(k) = E_c + \frac{\hbar^2 k^2}{2m_n^*}$$

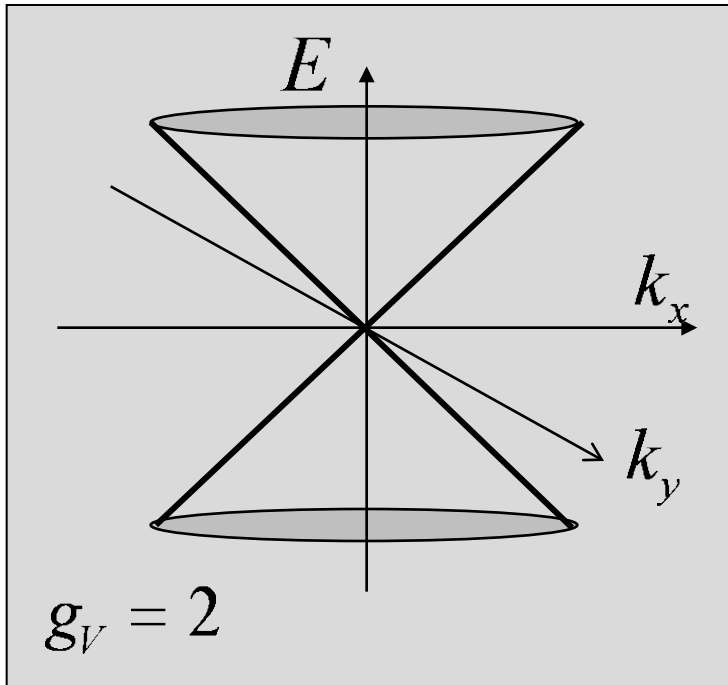
$$E(k) = E_v - \frac{\hbar^2 k^2}{2m_p^*}$$

“indirect” band semiconductor

# Model bandstructure: GaAs



# $E(k)$ for graphene



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

Recall:

$$v_g(\vec{k}) = \frac{1}{\hbar} \frac{dE(k)}{dk}$$

For graphene:

$$v_g(\vec{k}) = v_F \approx 10^8 \text{ cm/s}$$

Also recall:

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

For graphene:

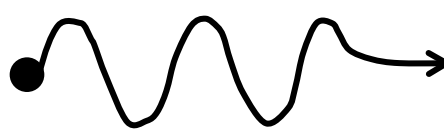
$$m^* = ?$$

## Summary: Band structure

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- 1) Electrons in a solid behave as both particles and as waves.
- 2) Electron waves are described by a band structure,  $E(k)$
- 3) Because the crystal is periodic, the dispersion is periodic in  $k$  (Brillouin zone).
- 4) Since electrons and holes are near the band minima and maxima, we can usually treat the bands as parabolic.
- 5) Electrons and holes can be treated as “semi-classical” particles with an effective mass and a crystal momentum.

# Summary: Mobile electrons in crystals


$$E(k) = \hbar^2 k^2 / 2m^* \qquad p = \hbar k$$
$$v_g = (1/\hbar) dE/dk = \hbar k / m^* \qquad F = dp/dt$$

