ECE-656: Fall 2009

Lecture 1: Bandstructure Review

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outline

1) **Bandstructure in bulk semiconductors**

2) Quantum confinement

3) Summary

electrons in solids

Hydrogen atom:

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

Crystals:

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

$$\psi(\vec{r}) = u_{\vec{k}}(\vec{r})e^{i\vec{k}\cdot\vec{r}} \qquad u_{\vec{k}}(\vec{r}+\vec{a}) = u_{\vec{k}}(\vec{r})$$ "Bloch waves"

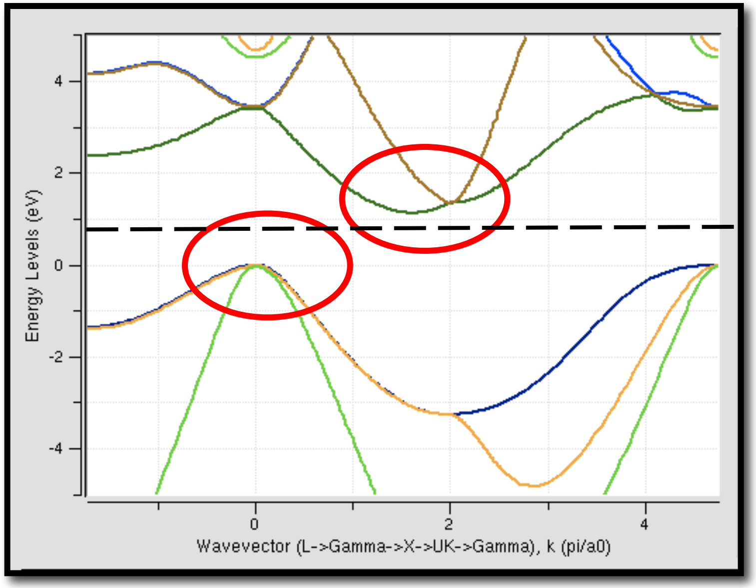
$$H\psi = E_n(\vec{k})\psi \qquad \vec{p} = \hbar\vec{k}$$ "crystal momentum"

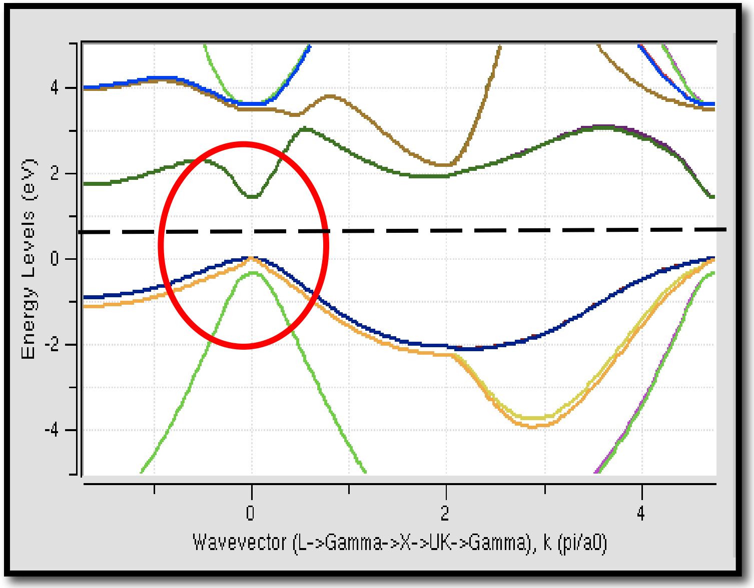
energy bands

For any wavevector, *k*, there is an infinite set of eigenenergies, $E_n(\vec{k})$

'bandstructure'

silicon



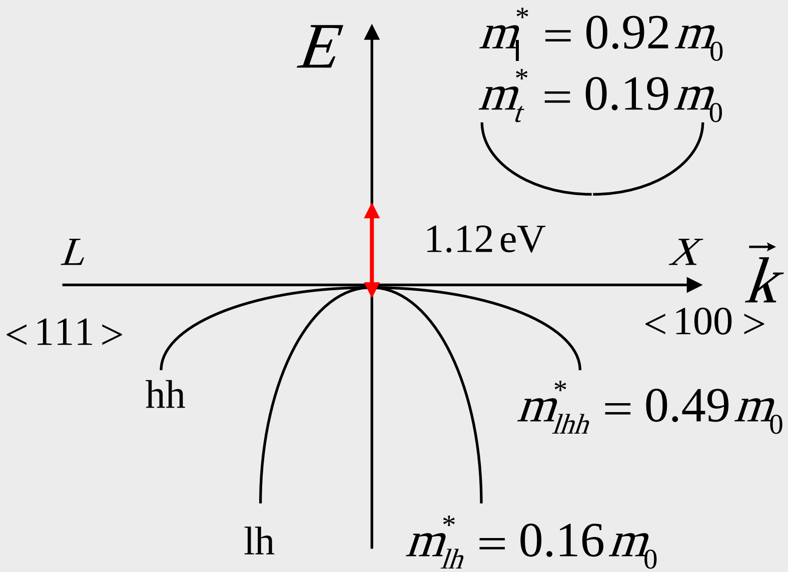


('Bandstructure Lab' at www.nanoHUB.org)

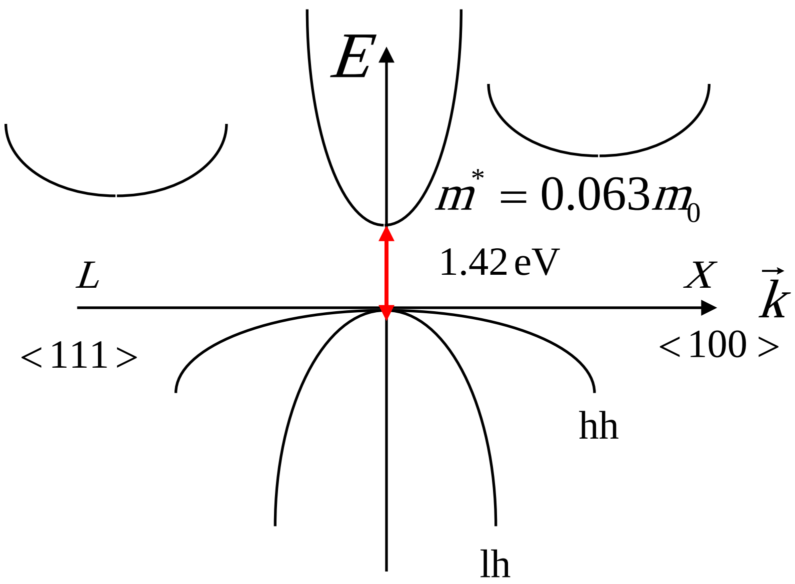
model bandstructure

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

silicon

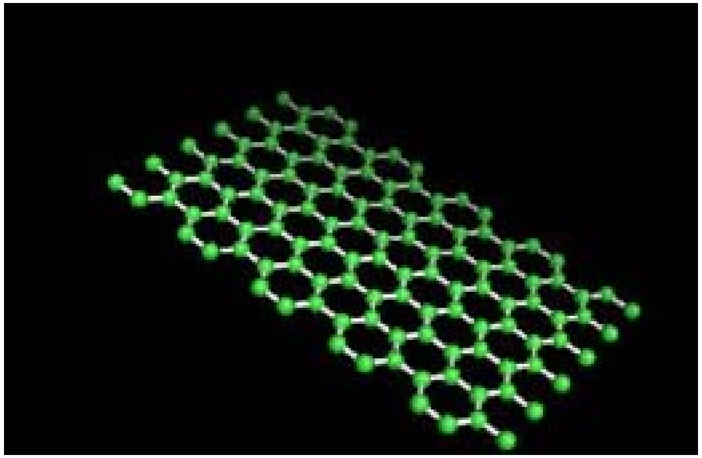


GaAs

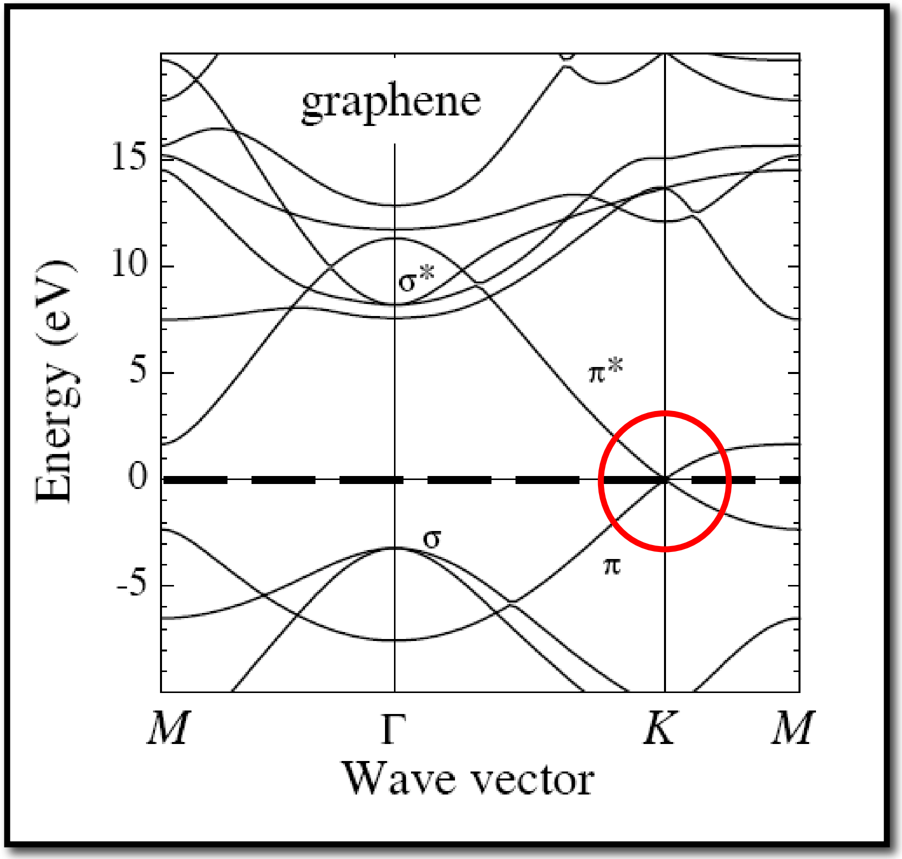


$$E(k) = E_V - \frac{\hbar^2 k^2}{2 m_p^*}$$

bandstructure of graphene



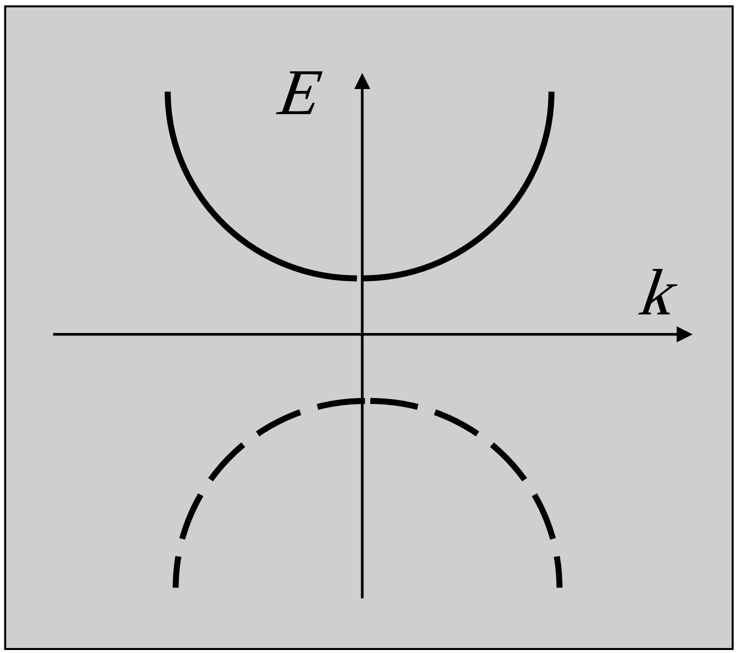
(CNTBands on www.nanoHUB.org)



http://www.szfki.hu/~kamaras/nanoseminar/Reich_Stephanie-85-100.pdf

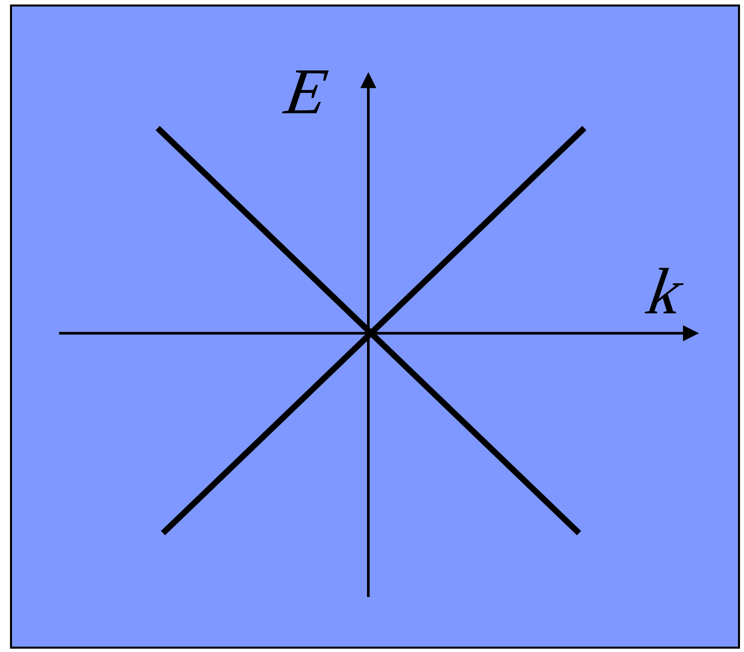
$E(k)$ for these lectures

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

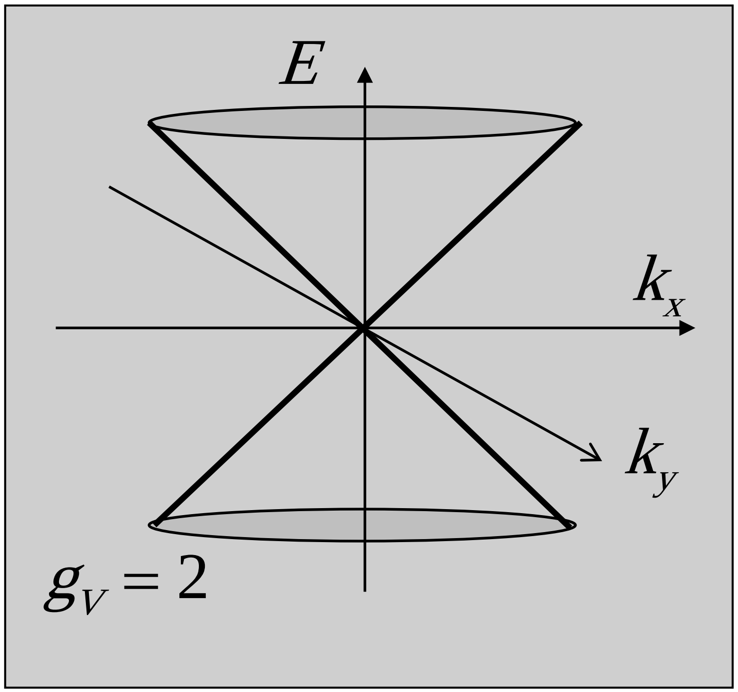


$$E(k) = E_V - \frac{\hbar^2 k^2}{2 m_p^*}$$

$$E(k) = \pm \hbar \upsilon_F k$$



E(*k*) for graphene



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

Recall:

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

For graphene:

$$\upsilon_g(\vec{k}) = \upsilon_F$$

Also recall:

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

For graphene:

$$m^* = ?$$

effective mass for graphene

Mobility:

$$\mu = \frac{q\tau}{m^*}$$

For graphene:

$$\mu = ?$$

As long as we have an *E*(*k*), we have everything we need. There is no need to ask what the effective mass is (but it sometimes can be useful to think in terms of an effective mass).

electronic structure of graphene

For a more thorough, but introductory treatment of bandstructure, see the nanoHUB lectures of Prof. Supriyo Datta:

ECE 495N: Fundamentals of Nanoelectronics
Lecture 18-21: *Bandstructure – I, II, III, and graphene*

http://nanohub.org/courses/fundamentals_of_nanoelectronics

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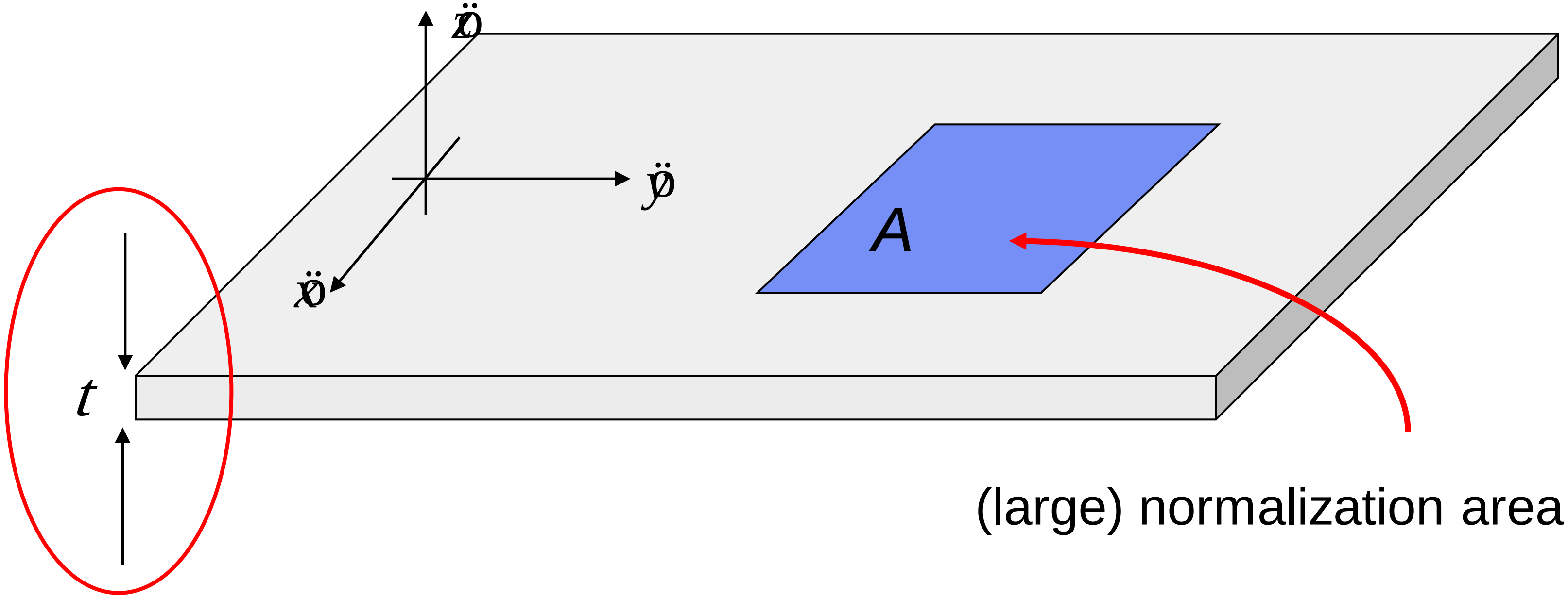
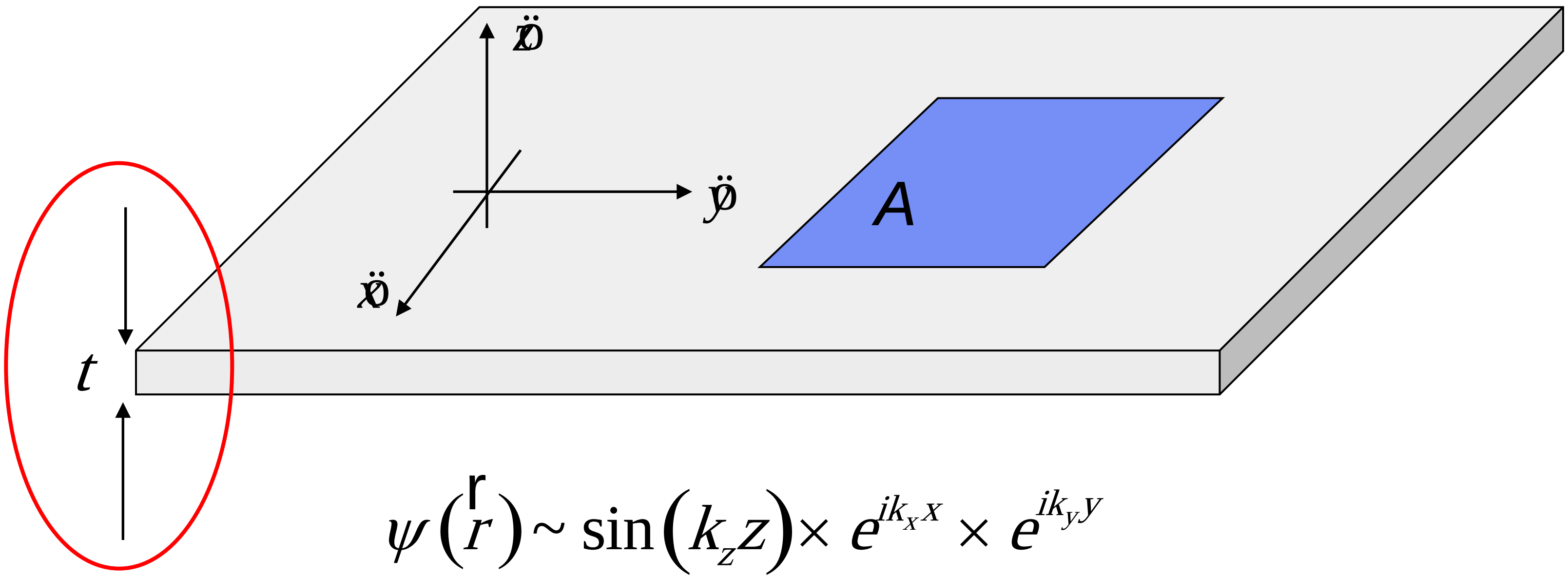
two-dimensional electrons



Semi-infinite in the x-y plane, but very thin in the z-direction.

$$\psi(\vec{r}) \sim e^{i\vec{k}\cdot\vec{r}} \rightarrow \sin(k_z z) \times e^{ik_x x} \times e^{ik_y y}$$

2D electrons: subbands

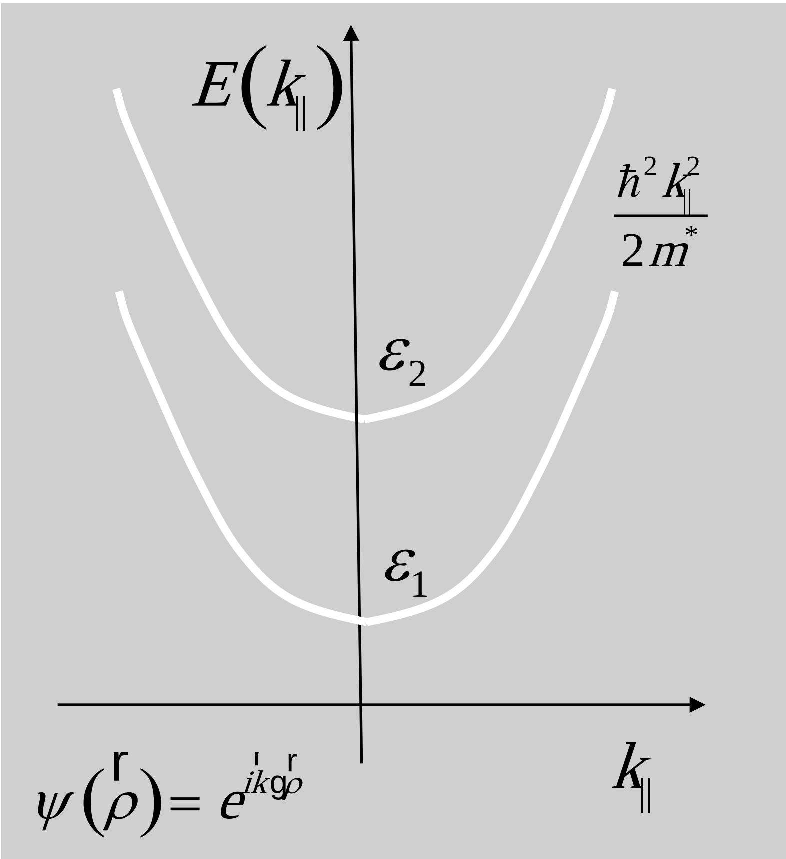


$$\psi(\vec{r}) \sim \sin(k_z z) \times e^{ik_x x} \times e^{ik_y y}$$

$$\psi(z=0) = \psi(z=t) = 0$$

$$k_z t = j\pi \qquad k_z = \frac{j\pi}{t} \qquad \varepsilon_j = \frac{\hbar^2 j^2 \pi^2}{2m^* t^2}$$

subbands

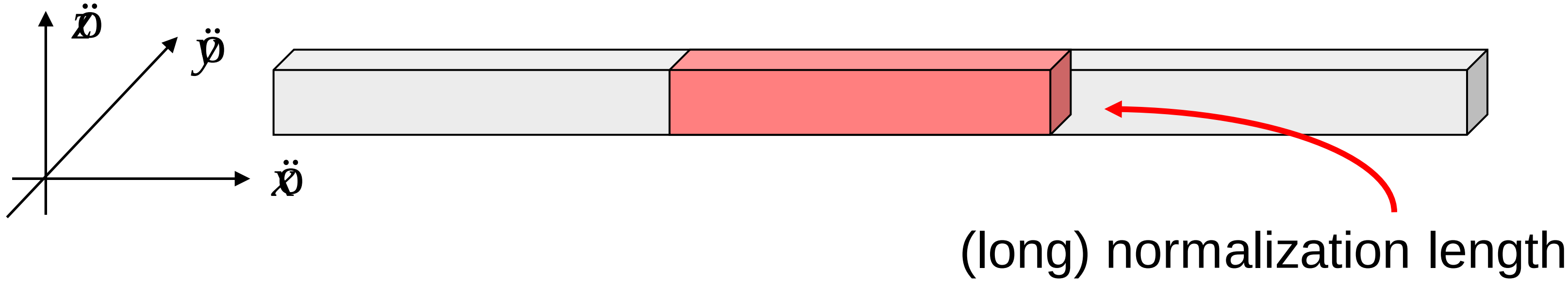


$$\varepsilon_j = \frac{\hbar^2 j^2 \pi^2}{2m^* t^2}$$

$$k_\parallel = \sqrt{k_x^2 + k_y^2}$$

$$E = \varepsilon_j + \frac{\hbar^2 k_\parallel^2}{2m^*}$$

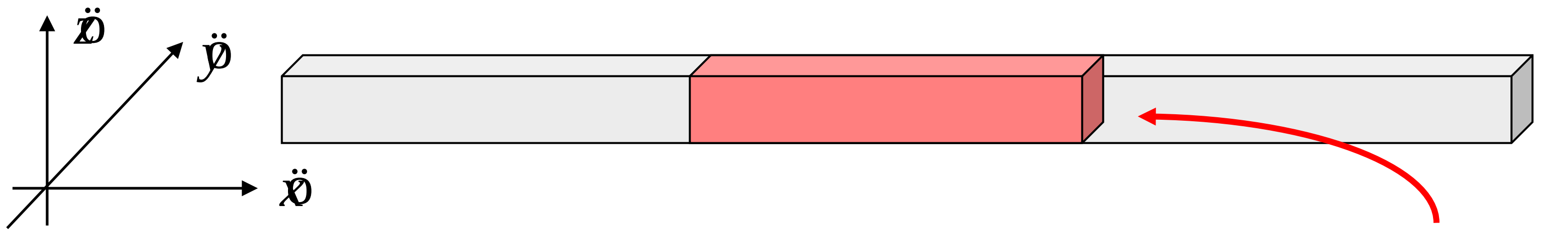
one-dimensional electrons



semi-infinite in along the x-direction, but very small in the y- and z-directions.

$$\psi(\vec{r}) \sim e^{i\vec{k}\cdot\vec{r}} \rightarrow \sin(k_y y)\sin(k_z z)\times e^{ik_x x}$$

one-dimensional electrons



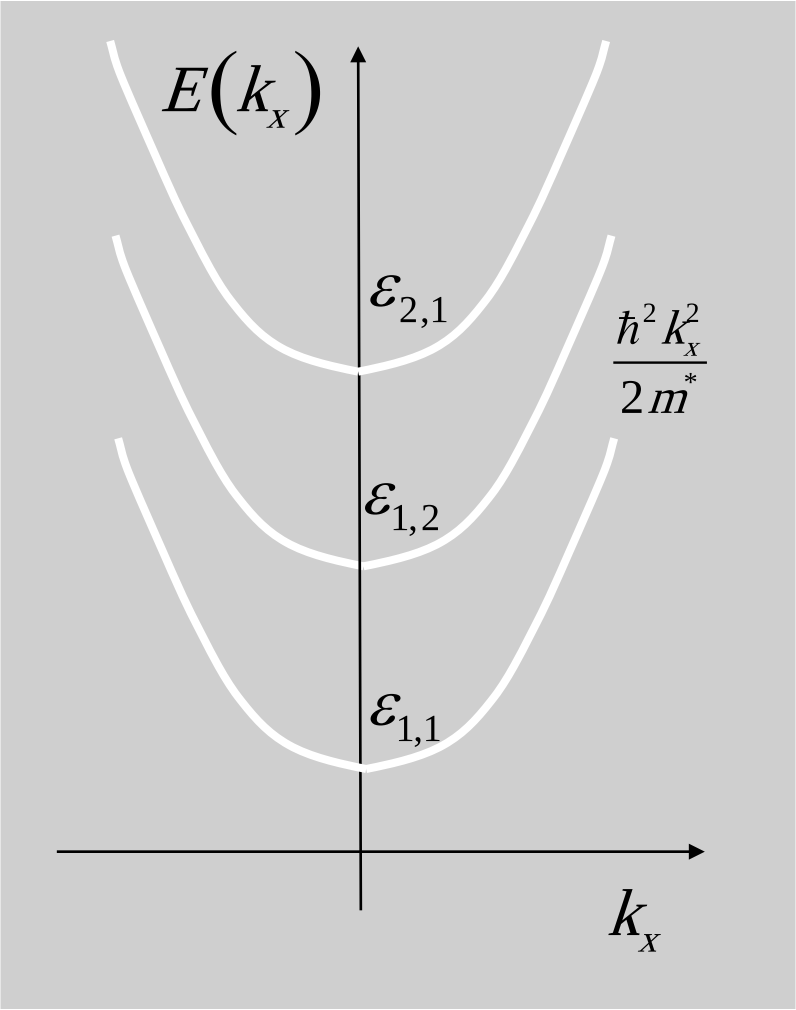
$$\psi(\vec{r}) \sim e^{i\vec{k}\cdot\vec{r}} \rightarrow \sin(k_y y)\sin(k_z z)\times e^{ik_x x}$$

$$\psi(y=0) = \psi(y=t_y) = 0 \qquad \psi(z=0) = \psi(z=t_z) = 0$$

$$k_y t_y = m\pi \qquad k_y = \frac{m\pi}{t} \qquad k_z t_z = n\pi \qquad k_z = \frac{n\pi}{t_z}$$

$$\varepsilon_{m,n} = \frac{\hbar^2 m^2 \pi^2}{2m^* t_y^2} + \frac{\hbar^2 n^2 \pi^2}{2m^* t_z^2}$$

subbands



$$\varepsilon_{m,n} = \frac{\hbar^2 \pi^2}{2m^*}\left(\frac{m^2}{t_y^2} + \frac{n^2}{t_z^2}\right)$$

$$E = \varepsilon_{m,n} + \frac{\hbar^2 k_x^2}{2m^*}$$

outline

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summary

$$E = E_C + E(k)$$

bottom of band or subband

"dispersion"
k in unconfined direction
1D, 2D, 3D

questions

1) Bandstructure in bulk semiconductors

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