

Quantum Confinement

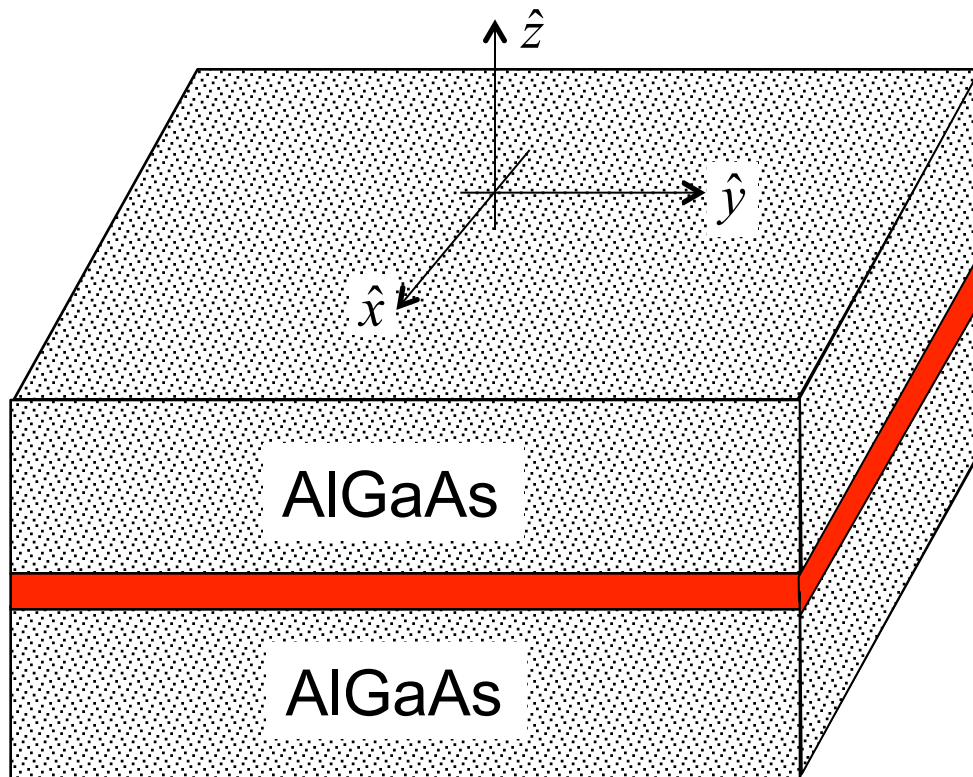
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Outline

- 1) Introduction
- 2) Particle in a box
- 3) 3D wave equation
- 4) 2D electrons
- 5) 1D electrons
- 6) Summary

Quantum confinement with heterostructures



GaAs

Electrons are confined in the z -direction, but free to move in the x - y plane.

“GaAs quantum well”

“Quasi-2D electrons”

Review: 1D particle in a box

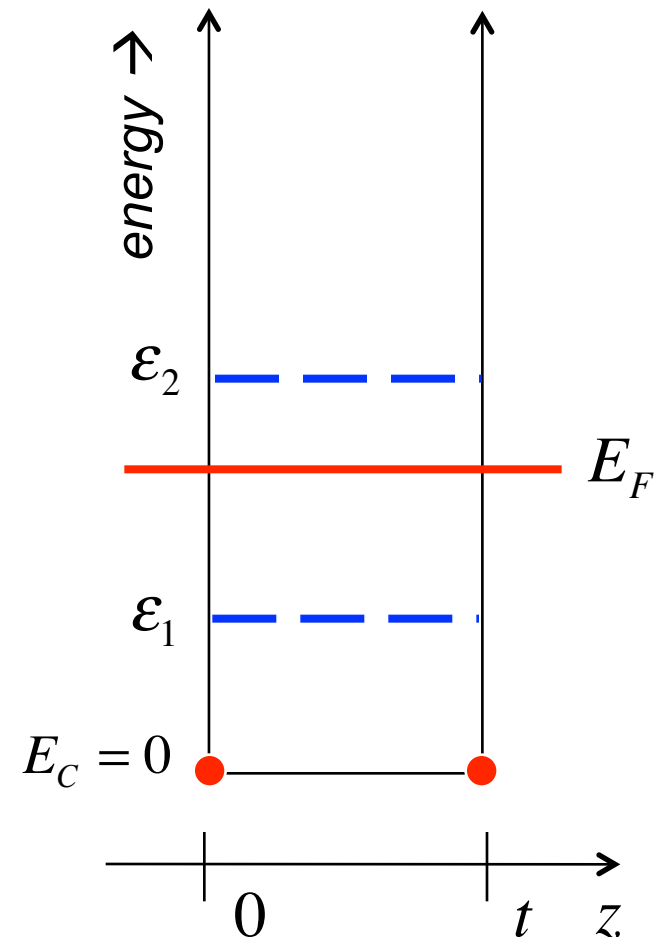
$$\frac{d^2\psi(z)}{dz^2} + k^2\psi = 0 \quad k^2 = \frac{2m^*(E - E_C(z))}{\hbar^2}$$

$$\psi(z) = \sin k_j z$$

$$\psi(0) = \psi(t) = 0 \quad k_j = \frac{\pi}{t} j = 1, 2, 3, \dots$$

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

Light mass or narrow well \rightarrow high subband energy, but specifics depend on the shape of the well.



Note: If electrons are free to move in the x-z plane. **2D electrons.**

3D wave equation

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

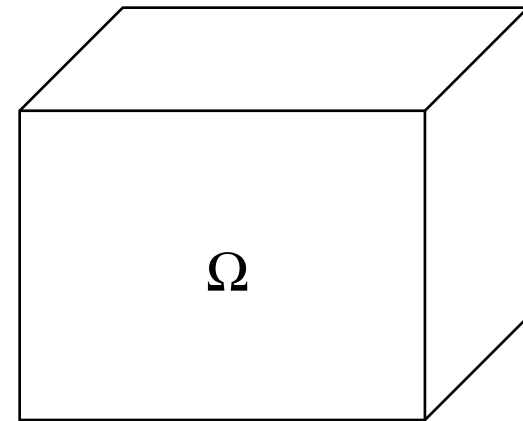
Separation of variables:

$$\psi(\vec{r}) = X(x)Y(y)Z(z)$$

$$U(\vec{r}) = 0$$

$$\psi(\vec{r}) = A e^{ik_x x} \times e^{ik_y y} \times e^{ik_z z}$$

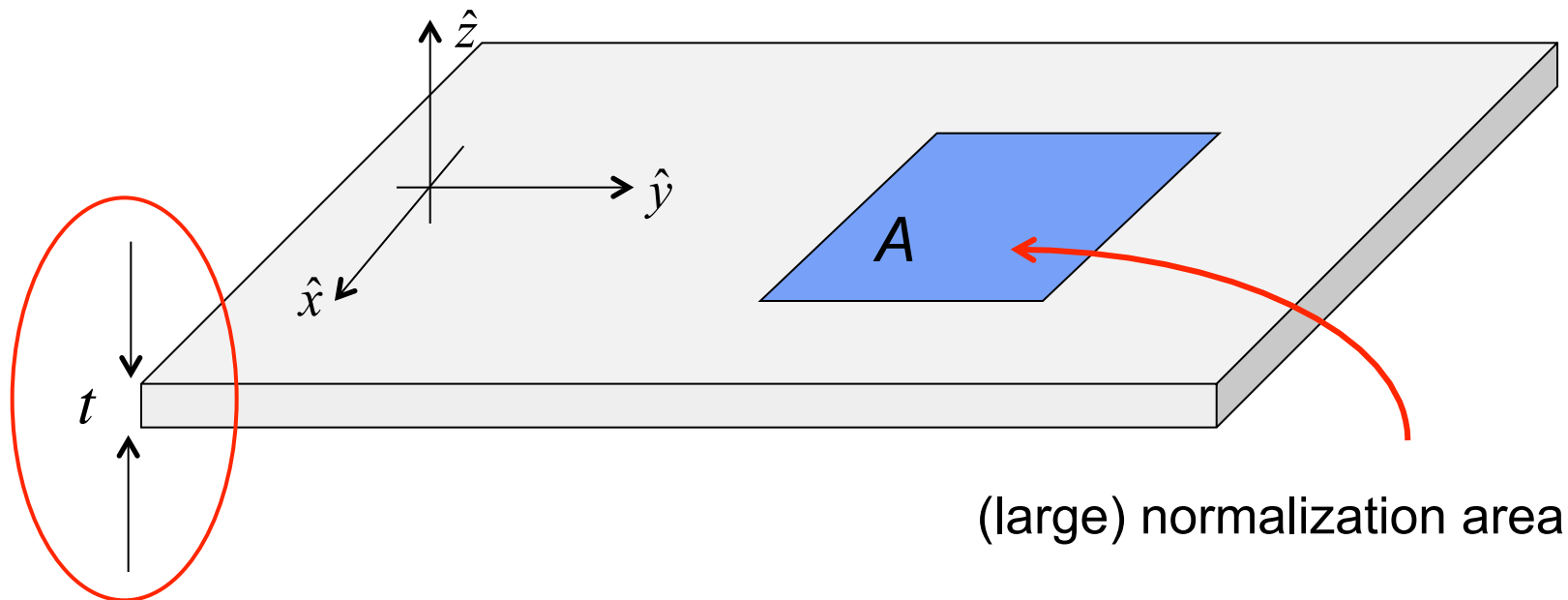
$$E = \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2 k_y^2}{2m^*} + \frac{\hbar^2 k_z^2}{2m^*}$$



$$\int_{\Omega} \psi^*(\vec{r})\psi(\vec{r}) d^3r = 1$$

$$\psi(\vec{r}) = \frac{1}{\sqrt{\Omega}} e^{ik_x x} \times e^{ik_y y} \times e^{ik_z z}$$

Quasi-2D electrons



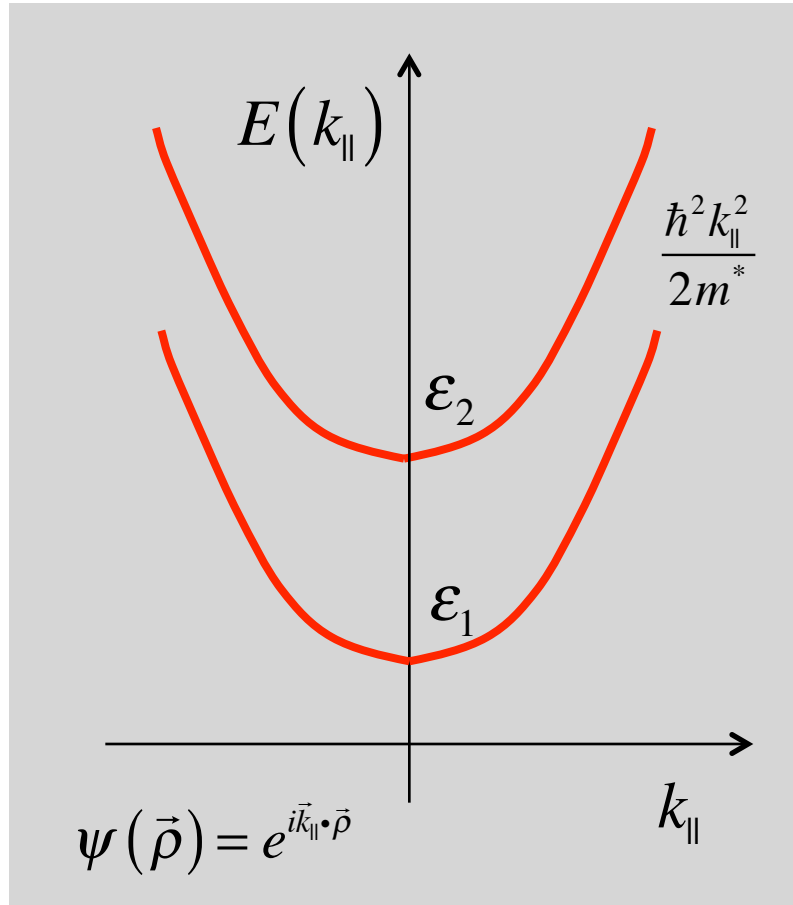
Semi-infinite in the x-y plane, but very thin in the z-direction.

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

$$k_z = k_{zj} = \frac{\pi}{t} j = 1, 2, 3 \dots$$

$$\psi(\vec{r}) = \sqrt{\frac{2}{t}} \sin(k_z z) \times \frac{1}{\sqrt{A}} e^{i(k_x x + k_y y)}$$

“Subbands”



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

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

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

ex. Quantum confinement in Si cond. band.

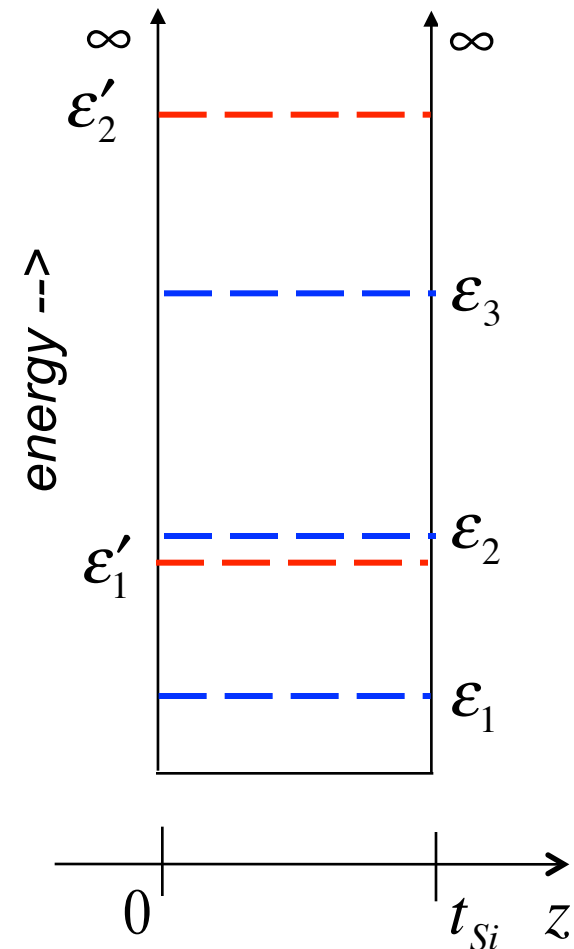
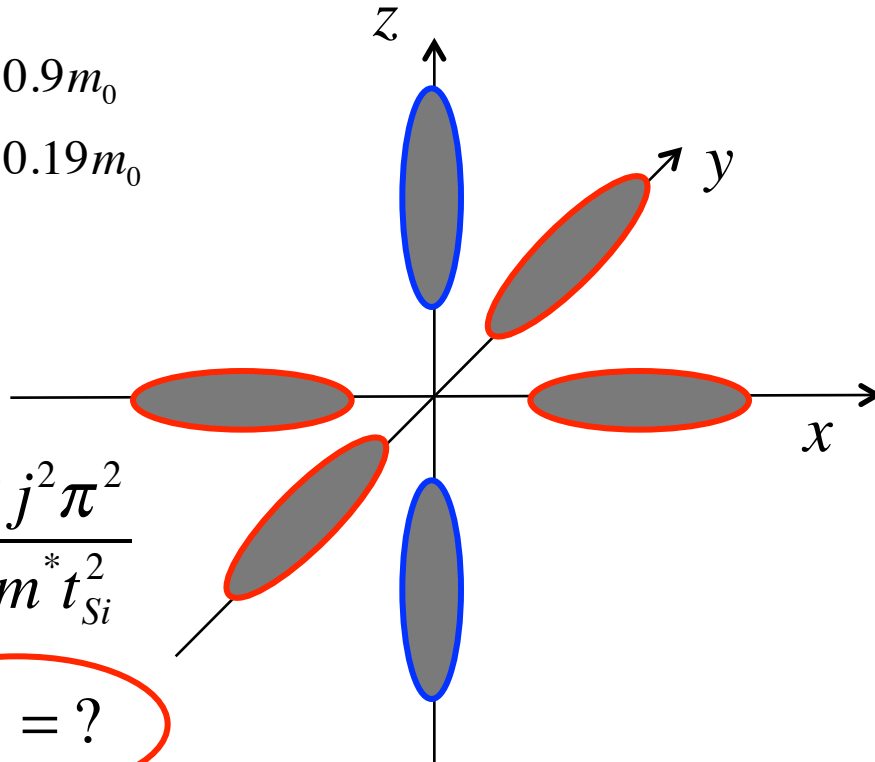
Si conduction band

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

$$m_t^* = 0.19m_0$$

$$\epsilon_j = \frac{\hbar^2 j^2 \pi^2}{2m^* t_{Si}^2}$$

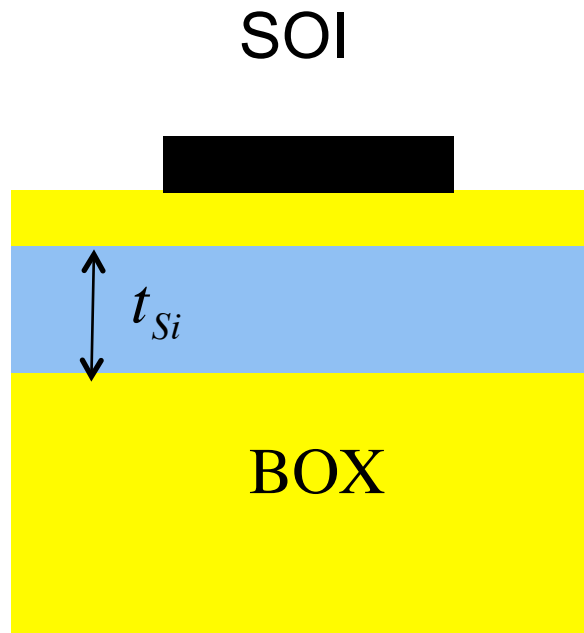
$$m^* = ?$$



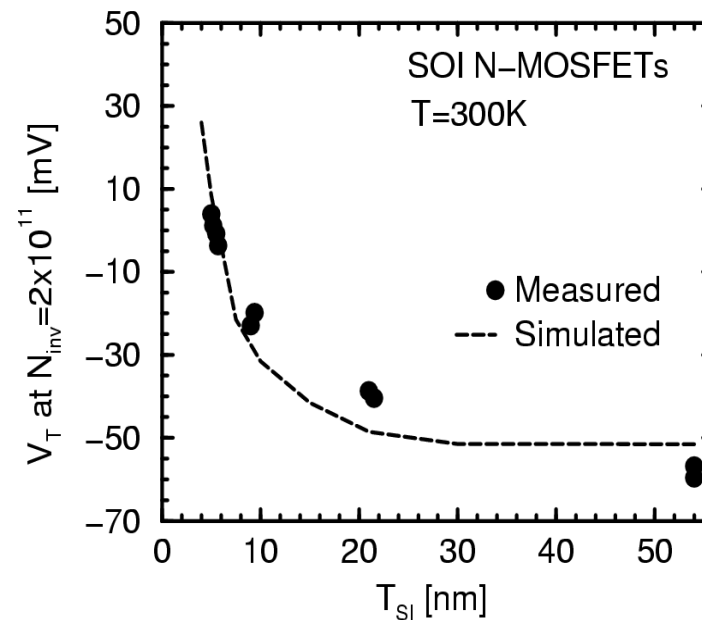
unprimed ladder: $m^* = m_{\ell}^* \quad g_V = 2$

primed ladder: $m^* = m_t^* \quad g_V = 4$

Quantum confinement in SOI

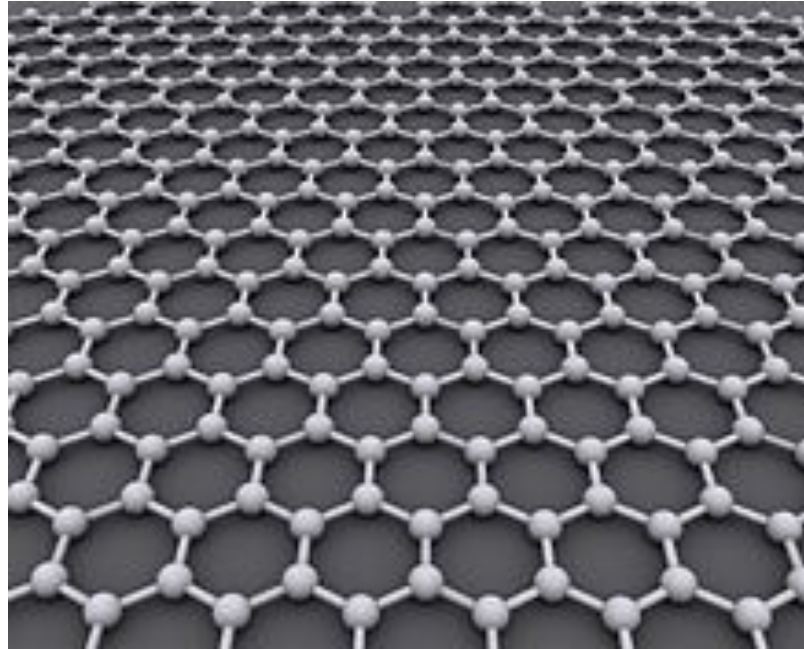


$$\Delta\psi_S^{QM} = \frac{\epsilon_1}{q}$$



(D. Esseni et al. IEDM 2000 and TED 2001)

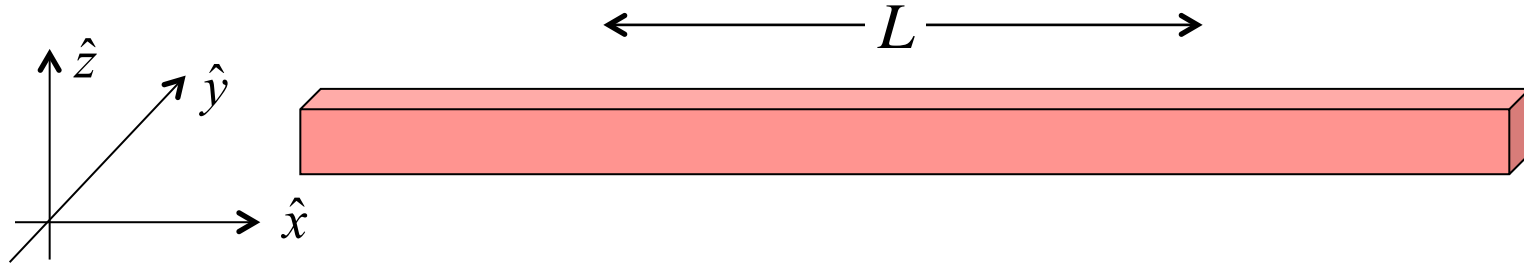
Graphene and 2D materials



A 2D hexagonal lattice of carbon atoms

<https://en.wikipedia.org/wiki/Graphene>

Quantum confinement in 1D



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

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

$$\psi(\vec{r}) = \sqrt{\frac{2}{t_y}} \sin(k_y y) \sqrt{\frac{2}{t_z}} \sin(k_z z) \times \frac{1}{\sqrt{L}} e^{ik_x x}$$

$$\epsilon_{m,n} = \frac{\hbar^2 m^2 \pi^2}{2m^* t_y^2} + \frac{\hbar^2 n^2 \pi^2}{2m^* t_z^2} \quad E = \epsilon_{m,n} + \frac{\hbar^2 k_x^2}{2m^*}$$

Summary

- 1) Quantum confinement introduces subbands.
- 2) The number of subbands that are occupied depends on the location of the Fermi level.
- 3) If one subband is occupied, electrons are “quasi-1D (2D)” electrons.
- 4) If many subbands are occupied, then electrons are 3D-like.

