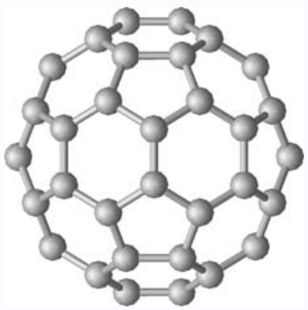
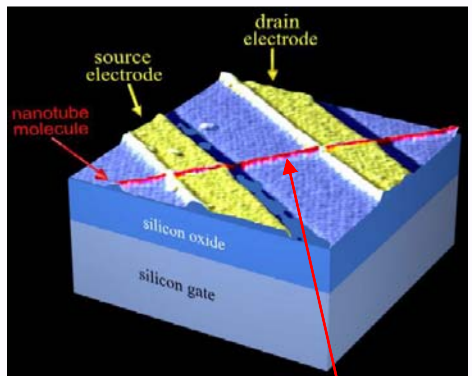
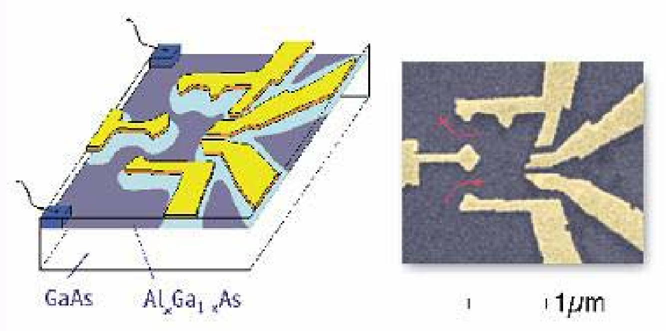
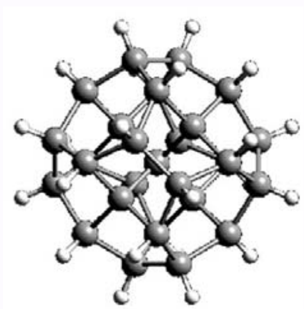
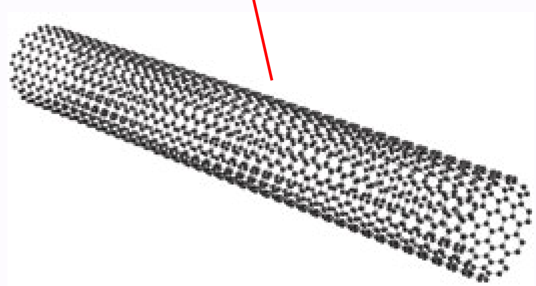
Lecture 21: Nanostructures
Kittel Ch 18
+ extra material in the class notes

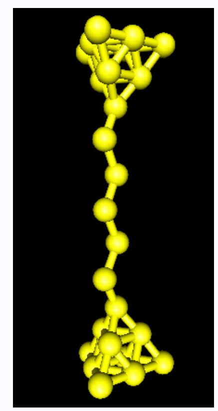












Outline

- **Electron in a box (again)**
- **Examples of nanostructures**
- **Created by Applied Voltages**
  Patterned metal gates on semiconductors
  Create "dots" that confine electrons
- **Created by material structures**
  Clusters of atoms, e.g., $Si_{29}H_{36}$, CdSe clusters
  Clusters of atoms embedded in an insulator
  e,g., Si clusters in SiO_2
  Buckyballs, nanotubes, . . .
- **How does one study nanosystems?**
- **What are novel properties?**
- **See Kittel Ch 18 and added material in the lecture notes**

Probes to determine stuctures

- Transmission electron microscope (TEM)
- Scanning electron microscope (SEM)
- Scannng tunneling microscope (STM) – more later

Figures in Kittel Ch 18

How small – How large?

- “Nano” means size ~ nm
- Is this the relevant scale for “nano effects” ?
  - Important changes in chemistry, mechanical properties
  - Electronic and optical properties
  - Magnetism (later)
  - Superconductivity (later)
- Changes in chemistry, mechanical properties
  - Expect large changes if a large fraction of the atoms are on the surface
- Electronic and optical properties
  - Changes due to the importance of surface atoms
  - Quantum “size effects” – can be very large and significant \

“Surface” vs “Bulk” in Nanosystems

- Consider atomic “clusters” with ~ 1 nm
- Between molecules (well-defined numbers and types of atoms – well-defined structures) and condensed matter (“bulk” properties are characteristic of the “bulk” independent of the size – surface effects separate)
- Expect large changes if a large fraction of the atoms are on the surface
- Typical atomic size ~ 0.3 nm
- Consider a sphere – volume $4\pi R^3/3$, surface area $4\pi R^2$ --- Rough estimates
  - R = 3 nm $\Rightarrow$ ~ 10^3 atoms - 10^2 on the surface – 10%
  - R = 1.2 nm $\Rightarrow$ ~ 64 atoms - 16 on the surface – 25%
  - R = 0.9 nm $\Rightarrow$ ~ 27 atoms - 9 on the surface – 33%

Quantum Size Effects

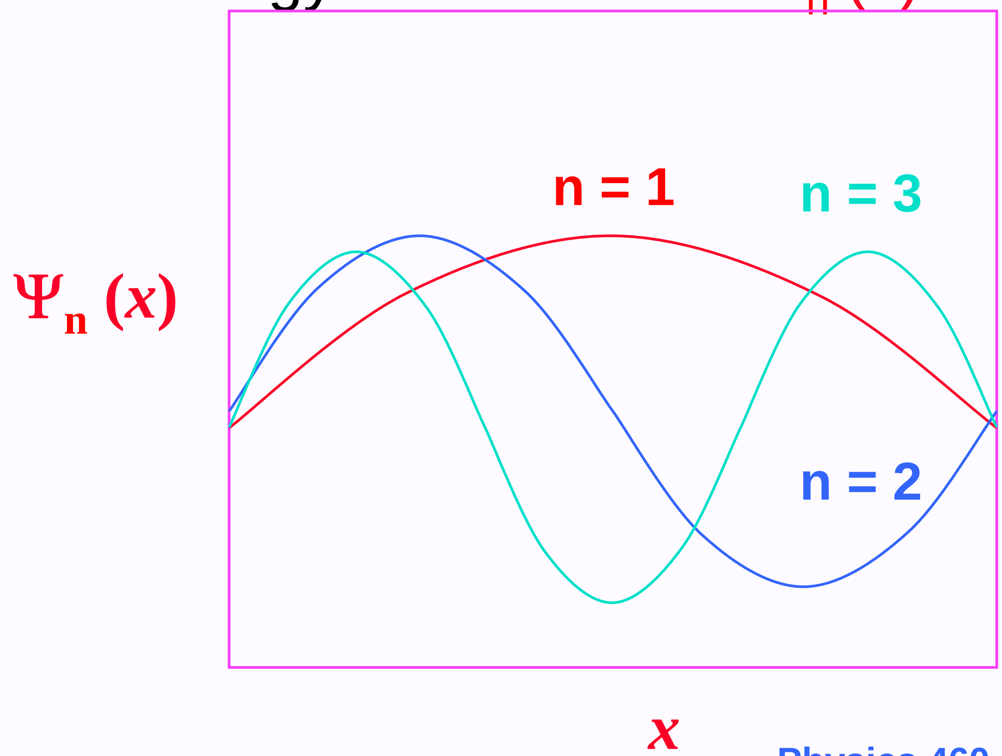
- We can make estimates using the "electron in a box" model of the previous lecture
- The key quantity that determines the quantum effects is the mass
- When can we use $m = m_{electron}$?
  In typical materials (metals like Na, Cu, ..
  the intrinsic electrons in semiconductors,…
- When do we use the effective mass m*
  For the added electrons or holes in a semiconductor

Quantization for electrons in a box in one dimension

- $E_n = (\hbar^2/2m)\, k_z^{\ 2}$, $k_z = n\,\pi/L$, n = 1,2, ...
  $= (h^2/4mL^2)\, n^2$, n = 1,2, ...

m = m_e
or m = m*

- Lowest energy solutions with $\Psi_n\,(x) = 0$ at x = 0,L

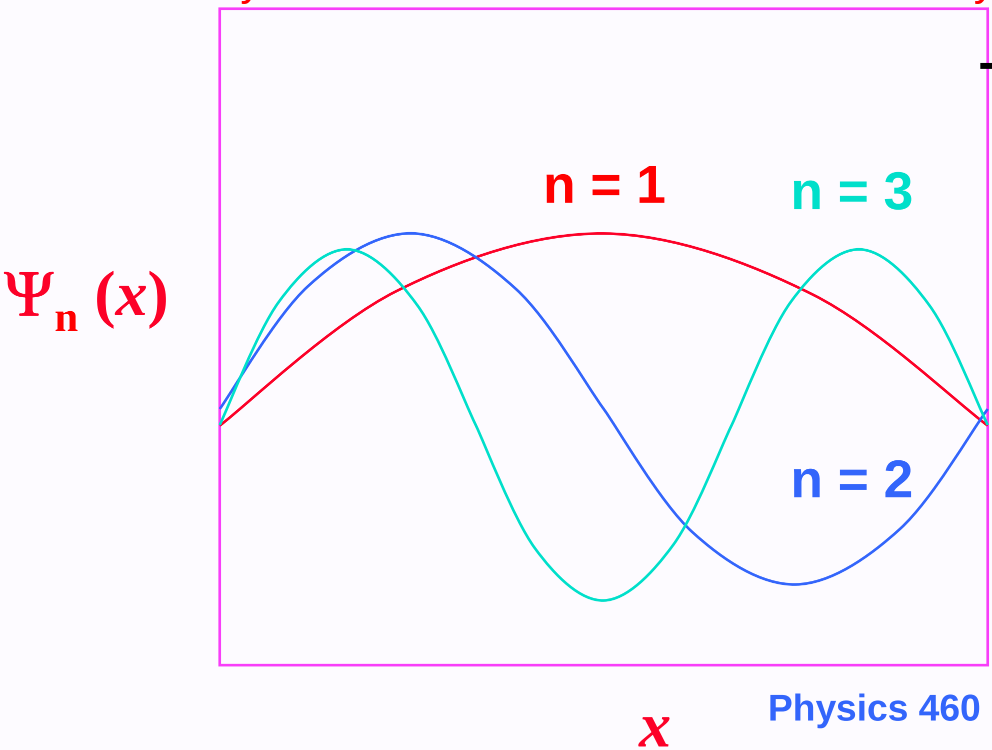


Here we emphasize the case where the box is very small

Electron in a box

- If the electrons are confined in a cubic box of size L in all three dimensions then the total energy for the electrons:

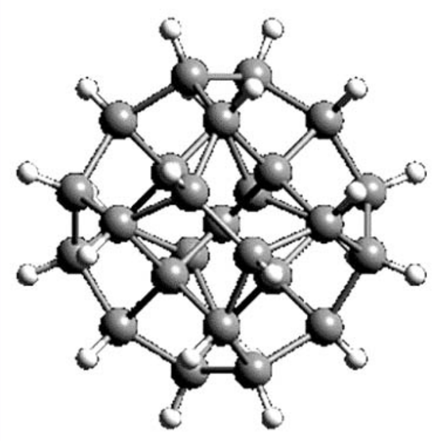
$$E\,(n_x, n_y, n_z) = (h^2/4m\,L^2)\,(n_x^2 + n_y^2 + n_z^2)$$



The wavefunction has this form in each direction

Nanoscale clusters

- Estimate the quantum size effects using the electron in a box model
- The discrete energies for electrons are given by
  $E = (h^2/4m L^2) (n_x^2 + n_y^2 + n_z^2)$

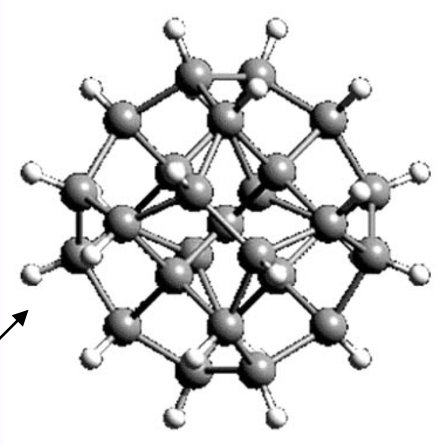


- The typical energy scale is
  $h^2/(4m L^2) = 3.7$ eV/ L^2
  where L is in nm

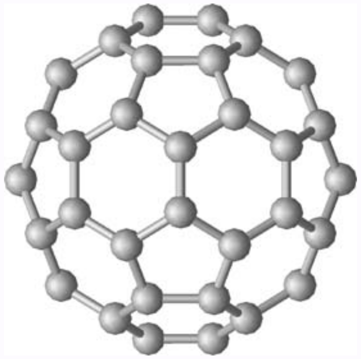
- Thus for 3 nm, the confinement energy is
  ~ 3 x 3.7 eV/9 ~ 1 eV
  As large as the gap in Si!

Nanoscale clusters - II

- Example: Silicon clusters
  - Must have other atoms to “passivate” the “dangling bonds” at the surface – is ideal
  - $Si_{29}H_{36}$ – bulk-like cluster with 18 surface atoms, each with 2 H attached
  - $Si_{29}H_{24}$ – 5 bulk-like atoms at the center and 24 rebonded surface atoms, each with one H attached – shown in the figure



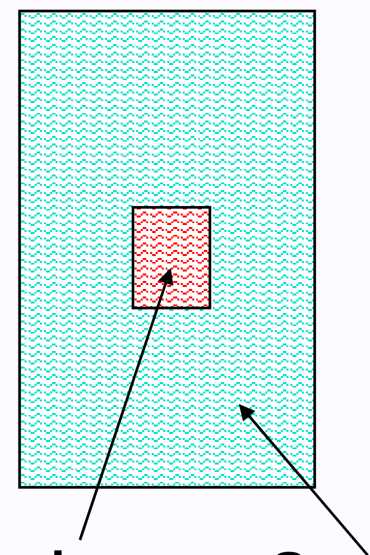
- Carbon “Buckyballs”
  - Sheet of graphite (graphene) rolled into a ball (C_{60} forms a soccer ball with diameter ~ 1nm)
  - Graphene is a zero gap material, and the size effect causes C_{60} to have a gap of ~ 2eV



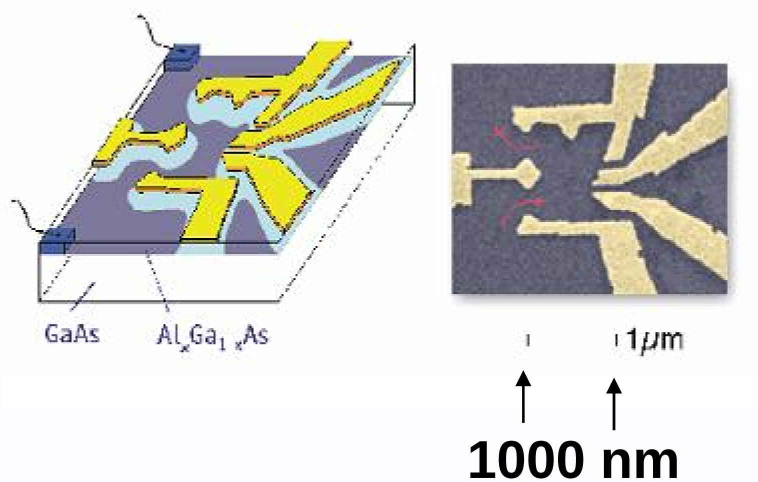
Special Presentation
Prof. Munir Nayfeh

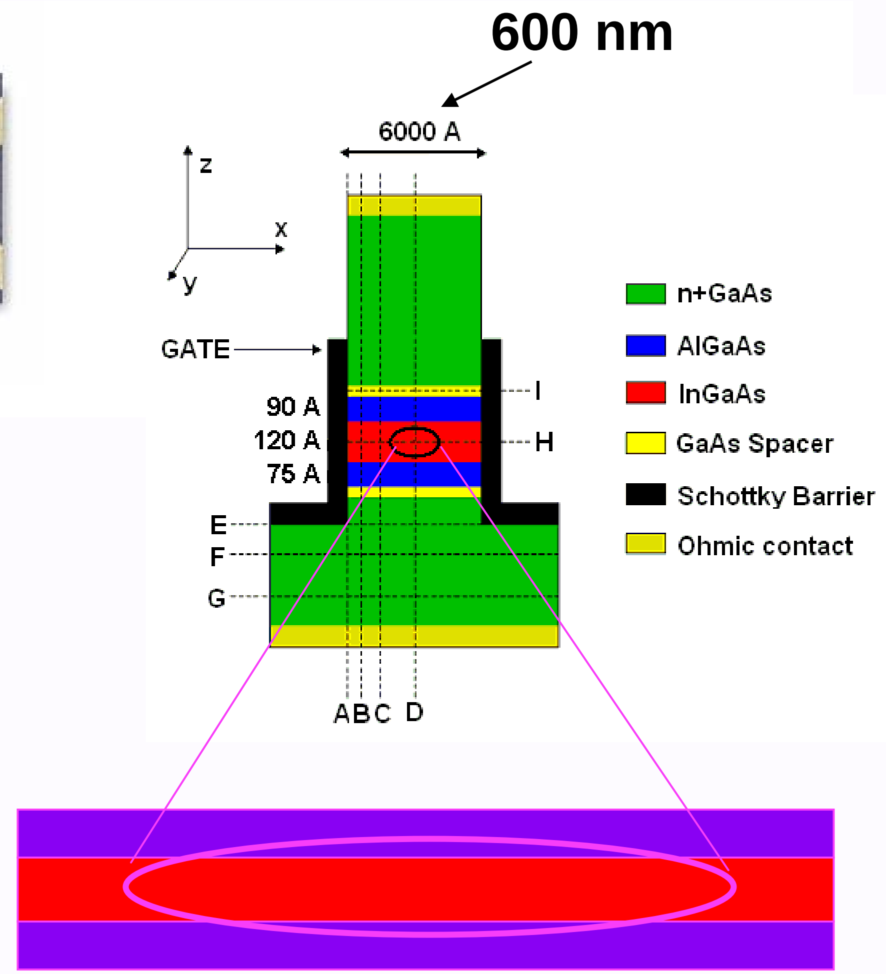
Semiconductor Quantum Dots

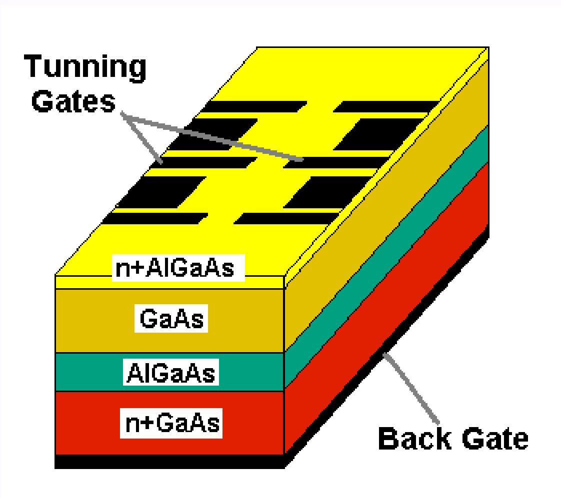
- Structures with electrons (holes) confined in all three directions
- The discrete energies for electrons are given by
  $E = (\hbar^2/2m L^2)(n_x^2 + n_y^2 + n_z^2)$
- The energy scale factor is
  $\hbar^2/(2m L^2) = 3.7\ \text{eV}(m_e/m^* L^2)$
  where L is in nm
- If $m^* = 0.01\ m_e$, then the confinement energy is
  ~ 1eV for L ~ 30nm
  ~ 0.04 eV for L ~ 150nm
  (note 300K ~ .025 eV)



Semiconductor Structures







One dimensional nanowires

- The motion of the electrons is exactly like the "electron in a box" problems discussed in Kittel, ch. 6
- Except the electrons have an effective mass m*
- And in this case, the box has length L in two directions (the y and z directions) and large in the x direction (L_x very large)

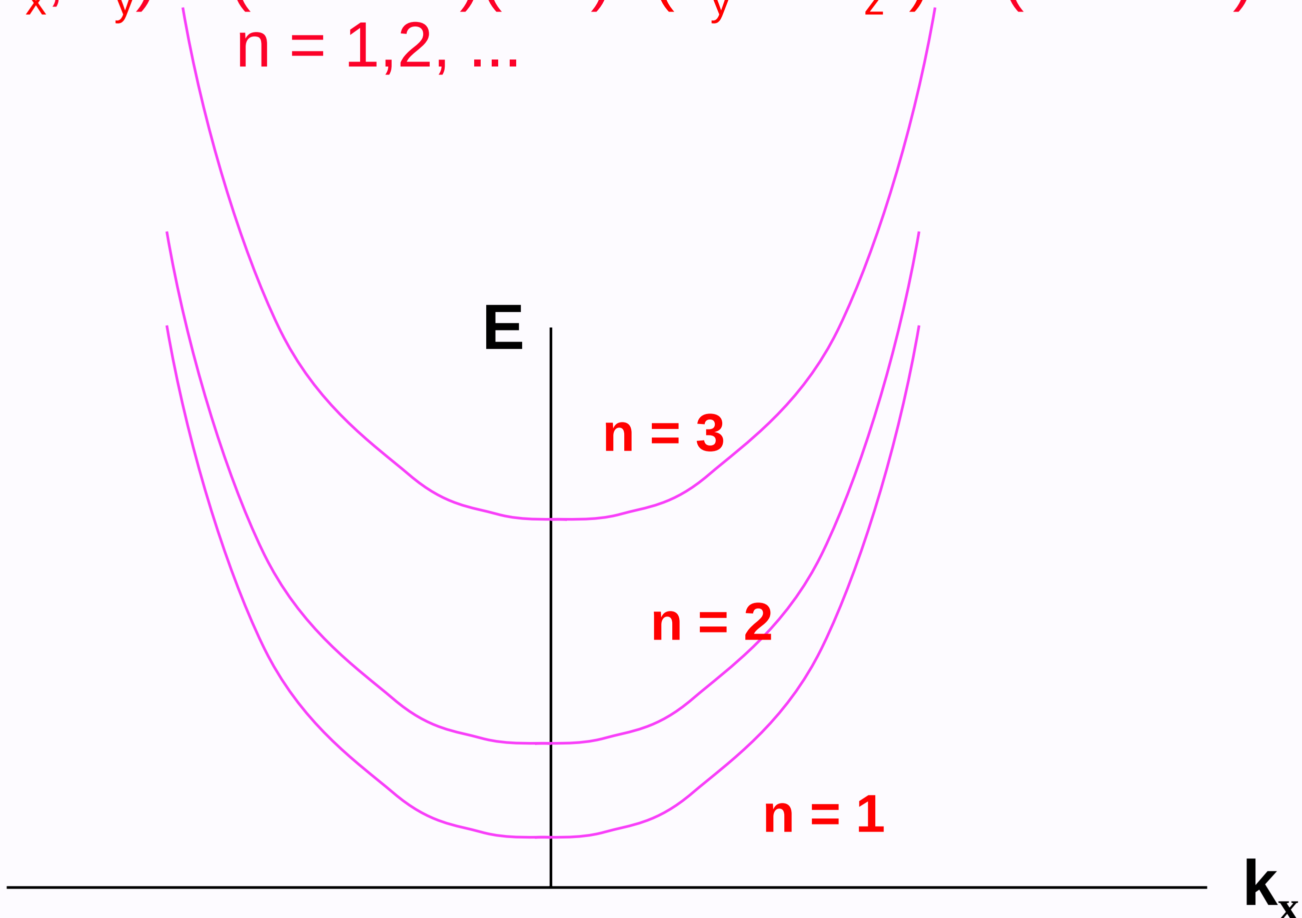
- Key Point: For ALL "electron in a box" problems, the energy is given by

$$E(\underline{\mathbf{k}}) = (\hbar^2/2m)(k_x^2 + k_y^2 + k_z^2)$$

For this case $m = m^*$ and $k_y = (\pi/L)\, n_y$, $k_z = (\pi/L)\, n_z$

Quantized one-dimensional bands

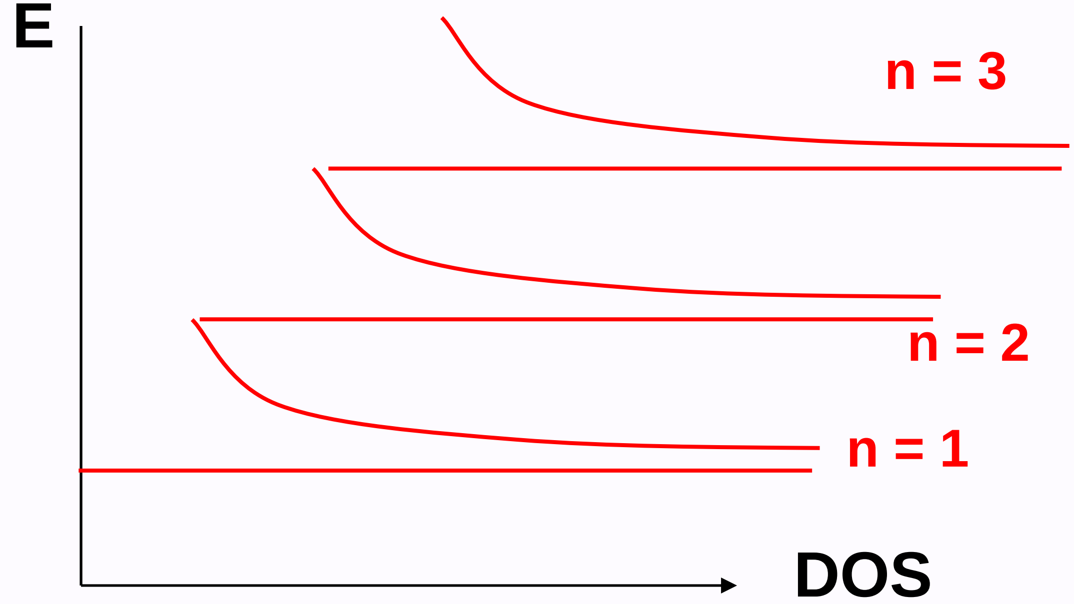
- $$E_n\,(k_x, k_y) = (\hbar^2/2m^*)(\pi/L)^2\,(n_y^2 + n_z^2) + (\hbar^2/2m^*)\,k_x^2$$
  $n = 1,2, \ldots$



Density of States in two-dimensions

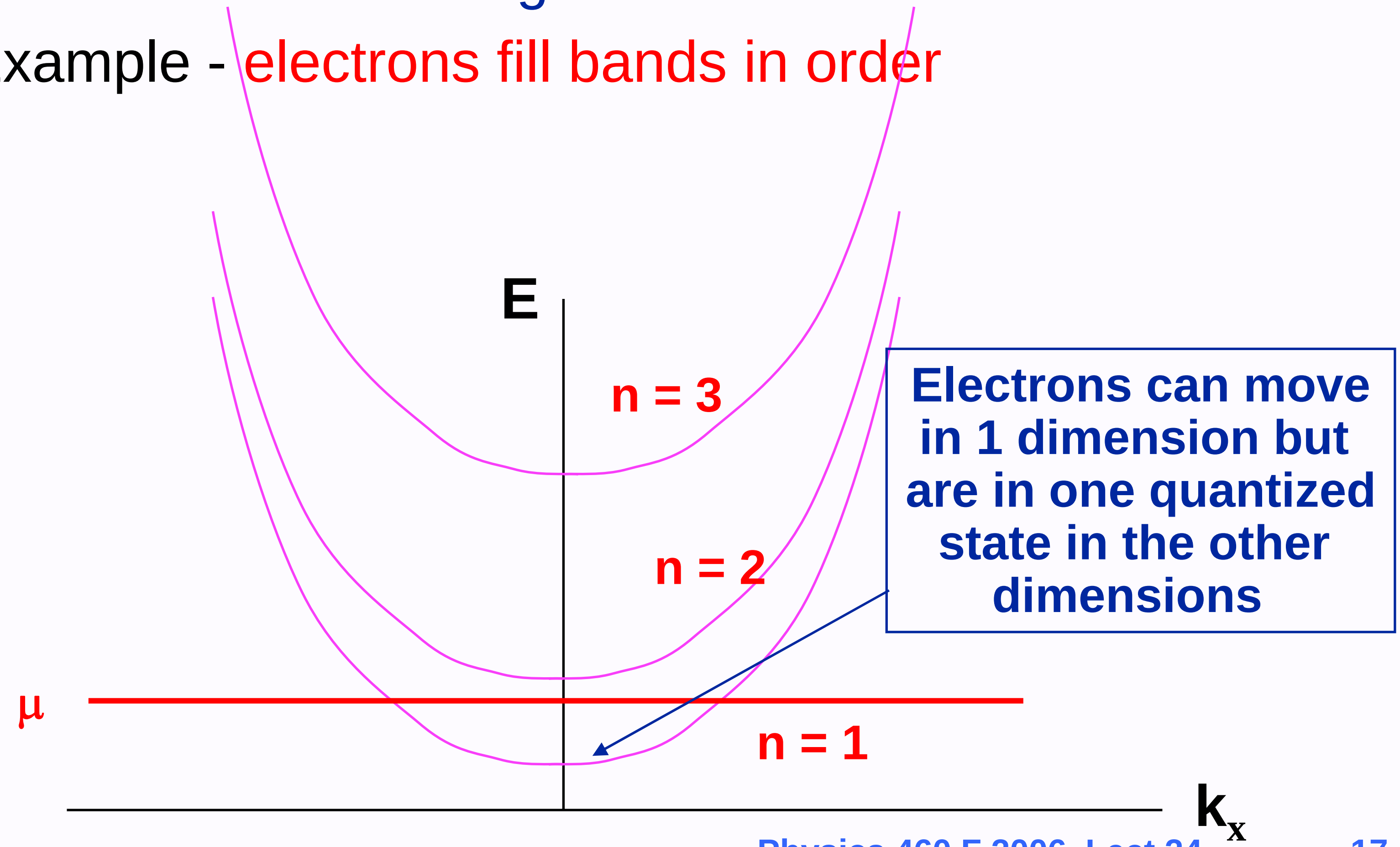
- Density of states (DOS) for each band is constant
- Example - electrons fill bands in order

- The density of states in a nanotube have this form
  – See Kittel, Ch 18

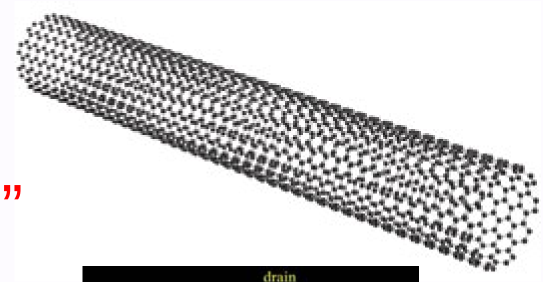


Quantized one-dimensional bands

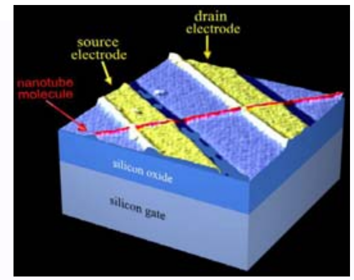
- What does this mean? One can make one-dimensional electron gas in a semiconductor!
- Example - electrons fill bands in order

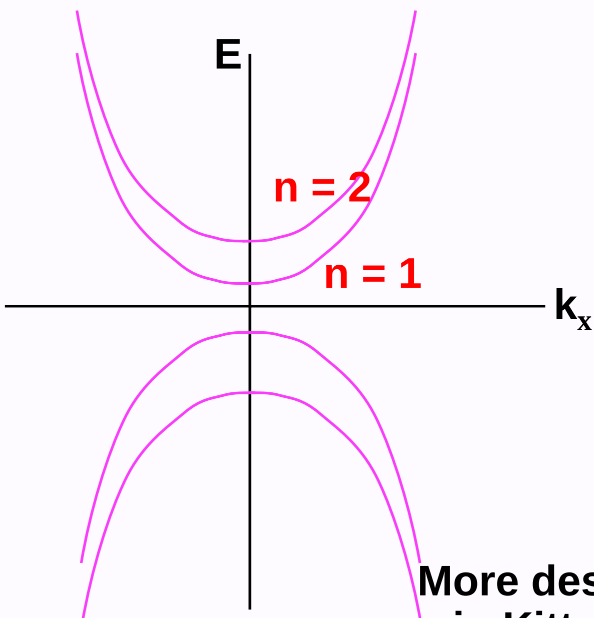


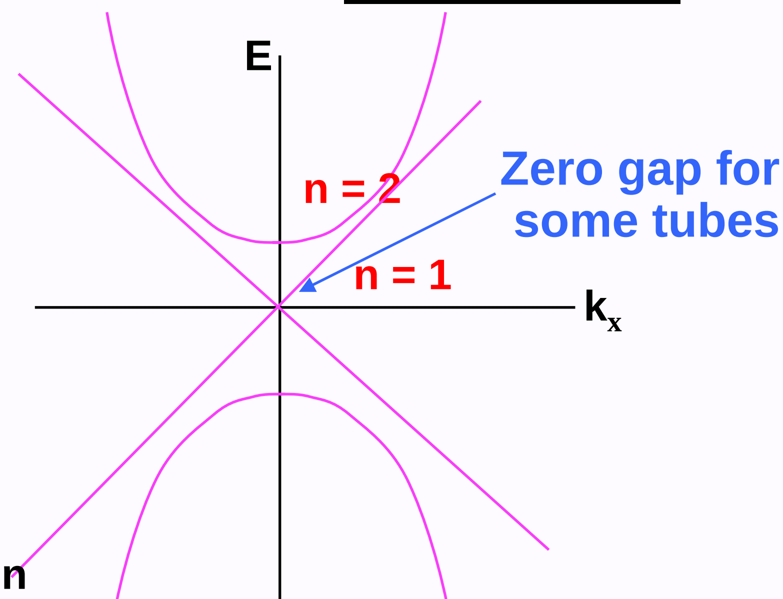
Nanotubes



- Carbon nanotubes are similar except there is a special “zero gap” feature in some cases
- Electrons can be added using a FET







More description in Kittel Ch 18

Summary

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  Patterned metal gates on semiconductors
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Next time

- **Metals – start superconductivity**