Supplementary (L3)

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Infinite potential well (1)

- A particle in the infinite potential well
  - Schrödinger equation in this example

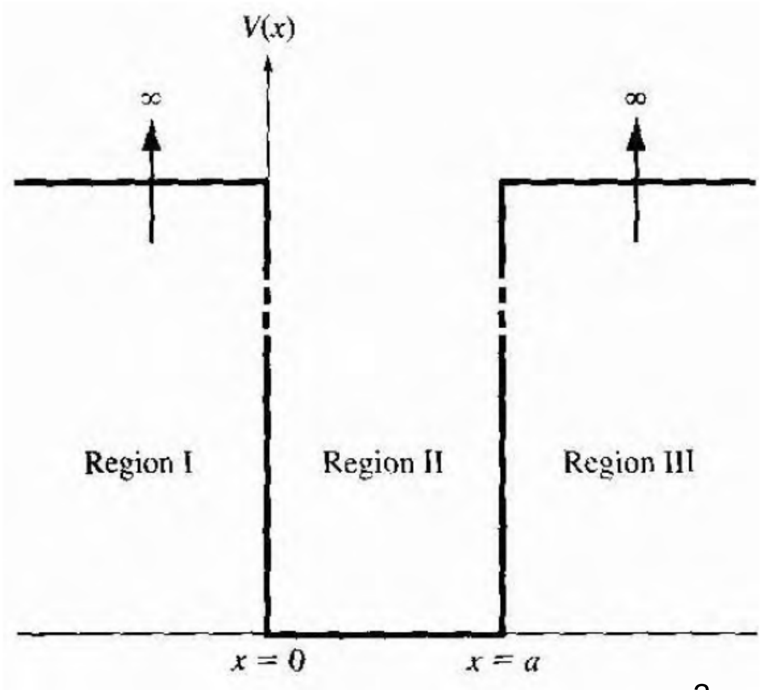
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x), \qquad 0 < x < a$$

  - Boundary conditions:

$$\psi(0) = \psi(a) = 0$$

  - It's an eigenvalue problem.

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x) = -k^2\psi(x)$$



Infinite potential well (2)

- Sine and cosine functions can be solutions.

$$\psi(x) = A_1 \cos kx + A_2 \sin kx$$

  – Cosine term cannot satisfy the boundary condition at $x = 0$.

$$\psi(a) = A_2 \sin ka = 0$$

  – Then, we have

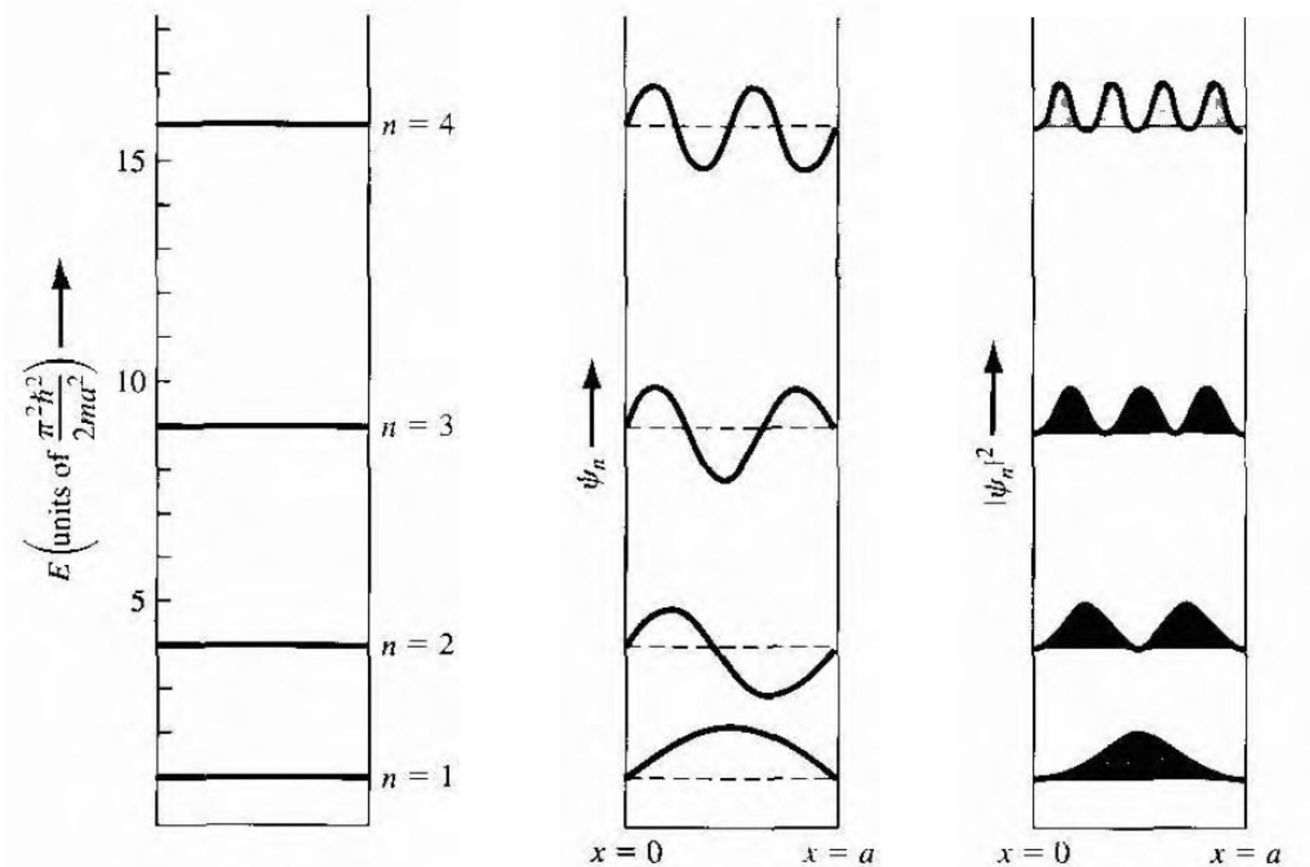
$$ka = \pi n$$

An integer

  – Therefore, allowed values of k are quantized.

Infinite potential well (3)

- Energy levels
  - Total energy is written as $E_n = \frac{\hbar^2}{2m}\left(\frac{\pi n}{a}\right)^2$



Density-of-states (DOS)

- Number of electrons
  - Why is it important? They are charge carriers!
  - Two factors: (number of states) & (probability to occupy them)

(Google images)

- What is the density-of-states?
  - It is related to the "number of states."
  - It is simply the number of states, (E, k) pairs, per unit energy.
  - Unit? [#/cm^3/eV]

An example

- A free electron confined to a 3D infinite potential well (For each direction, the length is a.)
  - Its 3D $E-k$ relation is

$$E = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) = \frac{\hbar^2}{2m}k^2$$

  - Note that k's are NOT continuous.
  - Distance between two neighboring k's is $\frac{\pi}{a}$.
  - Therefore, a volume for a single k point is $\left(\frac{\pi}{a}\right)^3$.
  - For a thin shell between k and $k+\Delta k$, the volume is $4\pi k^2 \Delta k$.
  - The number of states is

$$\frac{4\pi k^2 \Delta k}{\left(\frac{\pi}{a}\right)^3} = \frac{2\pi a^3}{h^3}(2m)^{1.5}\sqrt{E}\, dE \longleftarrow$$

We need an additional factor of 2.

Semiconductor case

- Straightforward extension
  - Assume the parabolic relation,

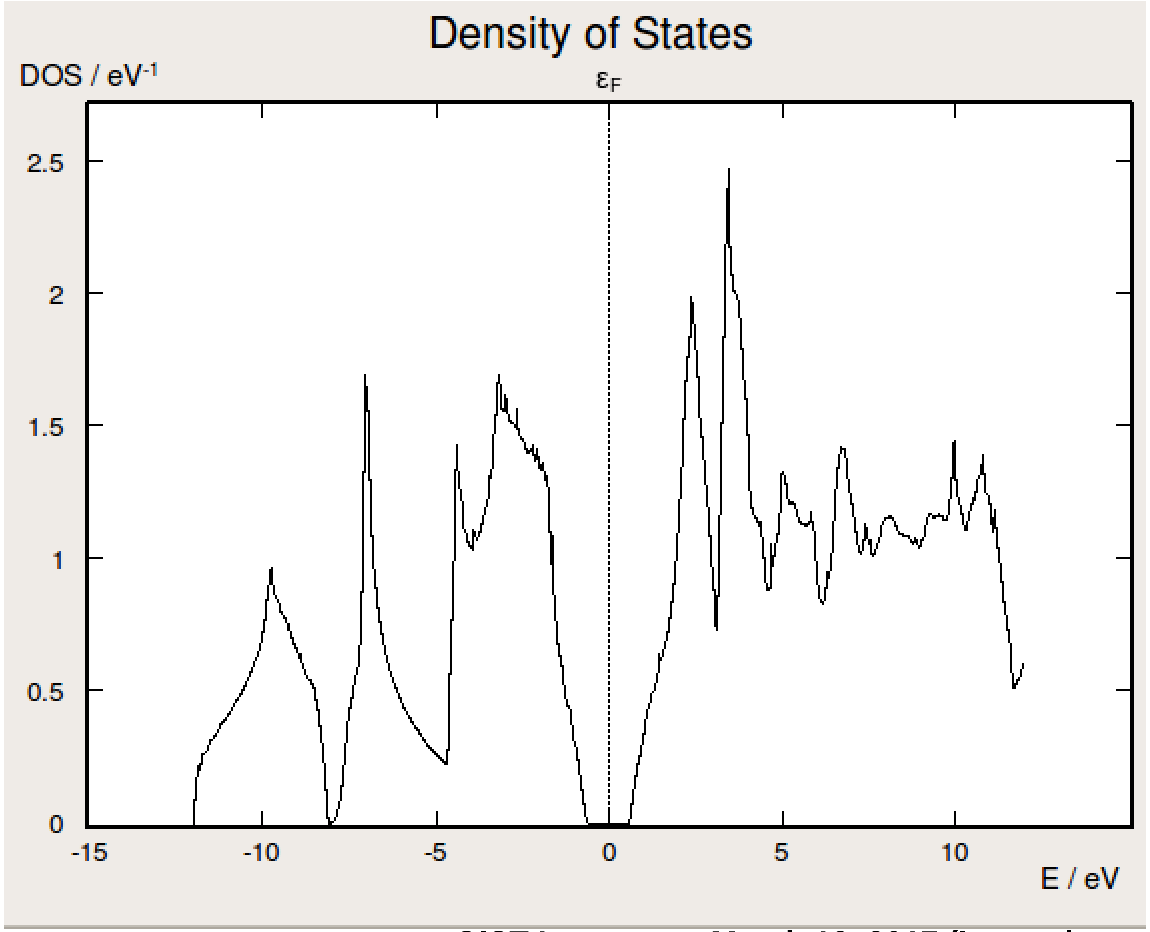
$$E = E_c + \frac{\hbar^2 k^2}{2m_n^*}$$
$$E = E_v - \frac{\hbar^2 k^2}{2m_p^*}$$

  - Then,

$$g_c(E) = \frac{4\,\pi(2m_n^*)^{1.5}}{h^3}\sqrt{E - E_c}$$
$$g_v(E) = \frac{4\,\pi\left(2m_p^*\right)^{1.5}}{h^3}\sqrt{E_v - E}$$

"Real" DOS

- DOS of silicon
  - Where is the square root?



(quantumwise.com)