

Week 5: Electron in a Box Announcements

Electron in a Well/Box (Solution 2)

- New solution to Schrodinger's Equation

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\Psi = 0$$

- This uses the boundary conditions

Solving for E

- At boundary of well ($x=0$ and $x=a$) Ψ must be 0

$$\Psi(x) = A \exp(jkx) + B \exp(-jkx)$$

$$\Psi(x=0) = 0$$

$$\Psi(x) = A[\exp(jkx) - \exp(-jkx)] = 2A_j \sin kx$$

$$-2A_j k^2 \sin kx + \left(\frac{2m}{\hbar^2}\right)E(2A_j \sin kx) = 0$$

$$E = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m}$$

Solving for E

- Satisfy the boundary conditions ($\sin=0$ at $x=0$ and $x=a$)
To get $\sin ka = 0$

$$E = \frac{\hbar^2 (\pi n)^2}{2ma^2} = \frac{\hbar^2 n^2}{8ma^2}$$

- k is similar to wavenumber: $ka=n\pi$ where a is the size of the well
- n is an _____, an integer
- _____ are value of Ψ_n when n is an integer number: 1,2,3...
- These represent the only possible wave functions (states) for electrons!

Electron in a Well

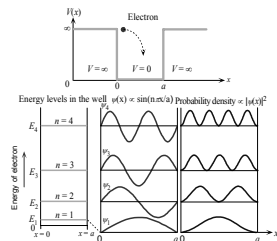


Fig. 3.15: Electron in a one-dimensional infinite PE well. The energy of the electron is quantized. Possible wavefunctions and the probability distributions for the electron are shown.

From: Principles of Electronic Materials and Devices, Second Edition, S.O. Kasap (© McGraw-Hill, 2002) <http://www.mhhe.com/engbook>

How does this differ from free electron model?

- Electron in a box puts boundary conditions at $x=0$ and $x=a$ that further constrain the allowed energies
- In the free electron model, any k is allowed
- In the electron in a box model, k must be integer values of π

Ground state

- $n=1$ is the lowest energy an electron can possess
 - ground state
- If an electron gets increments of energy exactly equal to the difference in levels- it can be excited: raised to a higher energy level

$$\Delta E = E_{\text{final}} - E_{\text{initial}} = \frac{h^2}{8ma^2} (n_{\text{final}}^2 - n_{\text{initial}}^2)$$

In 3-D: Electron in a Box

- The equation for E in 3-D becomes:

$$E = \frac{h^2}{8m} \left[\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2} \right]$$

- If it is a cube (with sides all equal to a):

Electron in a Box

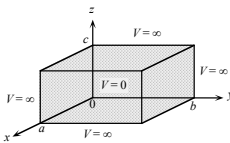


Fig. 3.19: Electron confined in three dimensions by a three dimensional infinite "PE box". Everywhere inside the box, $V = 0$, but outside, $V = \infty$. The electron cannot escape from the box. What is the energy and wavefunction of the electron?

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*Used with permission from Kasap

Now how do we calculate E?

- Ground state:
- Next state is some permutation of $(1,1,1)$ but will depend on how a,b,and c relate
 - Lowest energy will be permutation that gives lowest value of:

$$E \propto \left[\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2} \right]$$

- Must define series of energy levels based on specifics of the set-up

Degeneracy

- If $a=b=c$,

$$E \propto \frac{(n_1^2 + n_2^2 + n_3^2)}{a^2}$$

- So _____
 - These are degenerate (have the same energy levels)
 - The degeneracy of the level is 3 (three states have the same level)