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

$$\Psi(x) = A\exp(jkx) + B\exp(-jkx)$$
$$\Psi(x=0) = 0$$
$$\Psi(x) = A[\exp(jkx) - \exp(-jkx)] = 2Aj\sin kx$$

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

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

Solving for E

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

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

- k is similar to wavenumber: ka=nπ 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

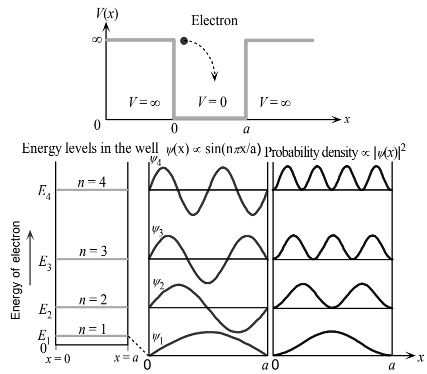

Fig. 3.15: Electron in a one-dimensional infinite PE well. The energy of the electron is quantized. Possible wavefunctions and the probability distributions for the electron are shown.

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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= ___ 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

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

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

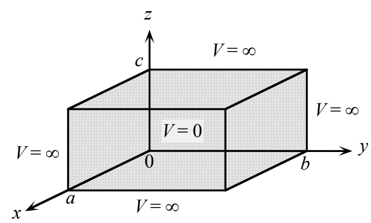

Fig. 3.19: Electron confined in three dimensions by a three dimensional infinite "*PE* box". Everywhere inside the box, $V = 0$, but outside, $V = \infty$. The electron cannot escape from the box. What is the energy and wavefunction of the electron?

26

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Now how do we calculate E?

- Ground state:
- Next state is some permutation of _____ 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,

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

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