3.012 Fund of Mat Sci: Bonding – Lecture 2

THINK OUT OF THE BOX

Last time: Wave mechanics

1. Classical harmonic oscillator
2. Kinetic and potential energy
3. De Broglie relation $\lambda \cdot p = h$
4. "Plane wave"
5. Time-dependent Schrödinger's equation
6. A free electron satisfies it

Homework for Wed 14

- Study: 15.1, 15.2
- Read: 14.1-14.4

- Office Hours – Monday 4-5 pm

Time-dependent Schrödinger's equation

(Newton's 2nd law for quantum objects)

- An electron is fully described by a wavefunction – all the properties of the electron can be extracted from it
- The wavefunction is determined by the differential equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)+V(\vec{r},t)\Psi(\vec{r},t)=i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$$

Stationary Schrödinger's Equation (I)

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)+V(\vec{r},t)\Psi(\vec{r},t)=i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$$

Stationary Schrödinger's Equation (II)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\varphi(\vec{r}) = E\varphi(\vec{r})$$

Stationary Schrödinger's Equation (III)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\varphi(\vec{r}) = E\varphi(\vec{r})$$

1. It's not proven – it's postulated, and it is confirmed experimentally
2. It's an "eigenvalue" equation: it has a solution only for certain values (discrete, or continuum intervals) of E
3. For those eigenvalues, the solution ("eigenstate", or "eigenfunction") is the complete descriptor of the electron in its equilibrium ground state, in a poteniitial V(r).
4. As with all differential equations, boundary conditions must be specified
5. Square modulus of the wavefunction = probability of finding an electron

From classical mechanics to operators

- Total energy is T+V (Hamiltonian is kinetic + potential)

- classical momentum $\vec{p}$ $\rightarrow$

  $\rightarrow$ gradient operator $-i\hbar\vec{\nabla}$

- classical position $\vec{r}$ $\rightarrow$

  $\rightarrow$ multiplicative operator $\hat{r}$

Operators, eigenvalues, eigenfunctions

Free particle: $\Psi(x,t)=\varphi(x)f(t)$

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(x)=E\varphi(x)$$

$$i\hbar\frac{d}{dt}f(t)=Ef(t)$$

Infinite Square Well (I) (particle in a 1-dim box)

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi(x)}{dx^2} = E\varphi(x)$$

Infinite Square Well (II)

Infinite Square Well (III)

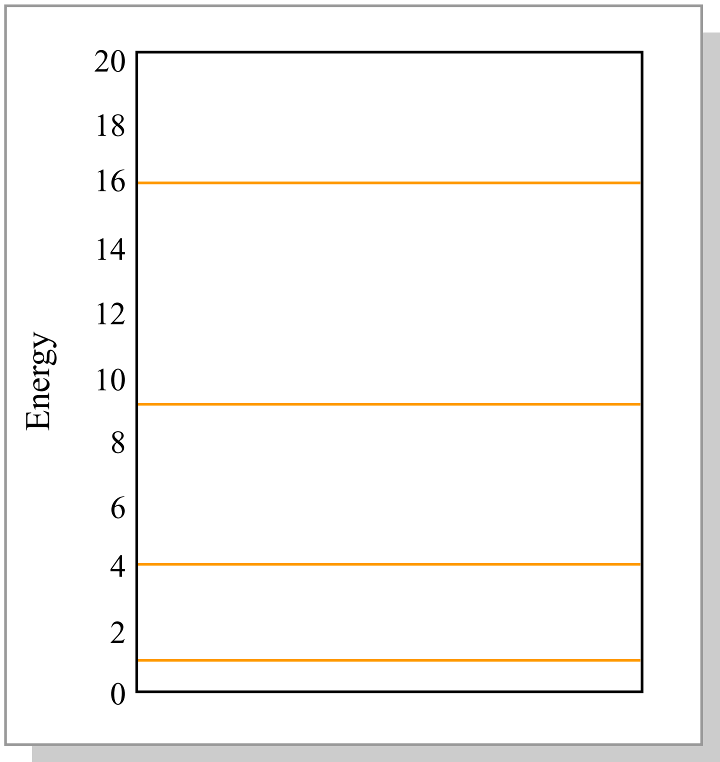

Figure by MIT OCW.

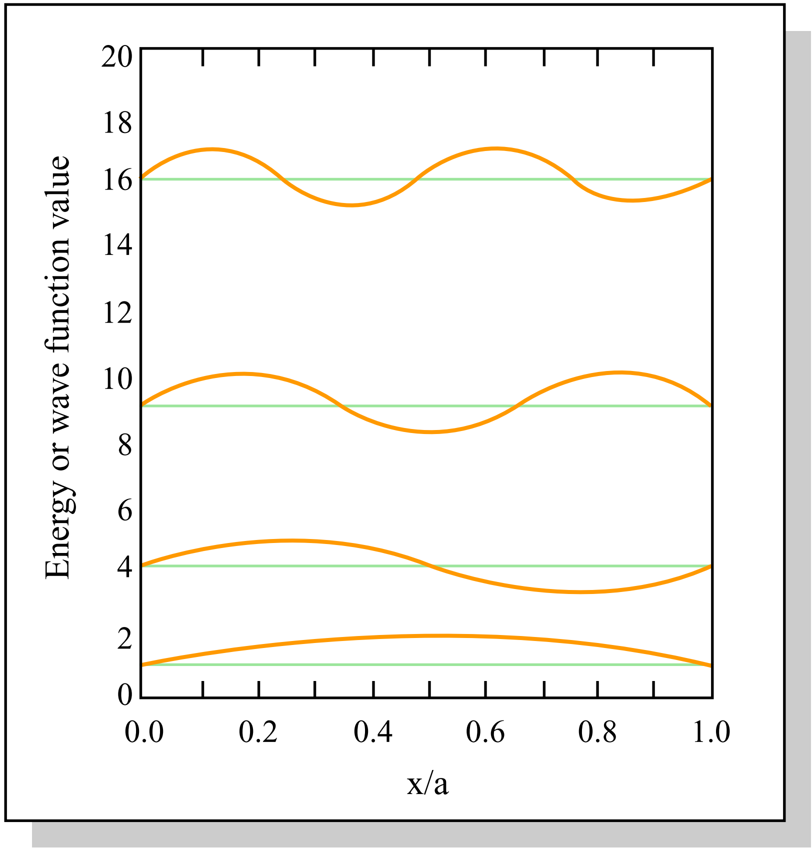

Figure by MIT OCW.