

Fundamentals of Nanoelectronics

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Lecture 8: Schrödinger Equation

Ref. Chapter 2.1

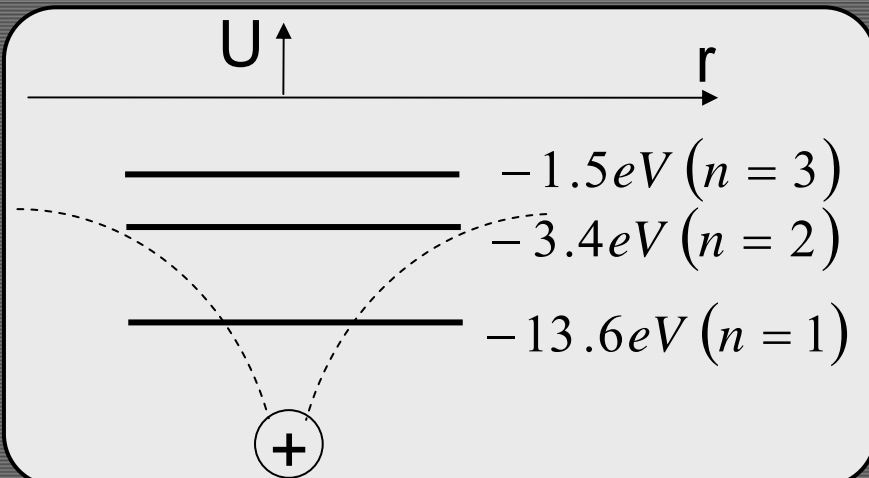


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Schrödinger Equation and Hydrogen Atom

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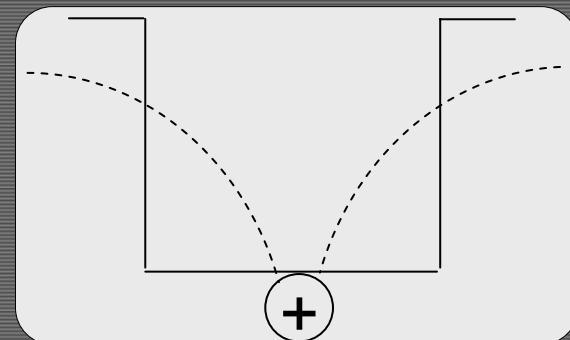
- Schrödinger equation was introduced in 1930's and helped to describe the energy levels of H atom.

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

- This equation provided a conceptual frame work for which wave nature of electrons comes naturally.
- The potential $U(r)$ that appears in the Schrödinger equation, looks like the figure for H atom. The is the Coulomb potential:

$$U(r) = -q^2 / 4\pi\epsilon_0 r$$

- Schrödinger showed that for this potential the equation can be solved analytically and he found solutions, which agreed with the experiments.
- In the next few lectures we want to understand how to solve for the energy levels of a material using Schrödinger equation.
- For H atom, the problem is analytically complicated for the exact shape of potential but if we approximate the potential as a confining box for electron we can get a relatively easy answer that helps us to understand the physics.



1D Solutions

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

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

- This equation in general is a function of time and space (3 dimensions). For the purpose of simplicity we'll solve it in 1 dimension x. This is the same as assuming that nothing varies in y and z dimensions. In 1D:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi + U(x) \Psi$$

- If U is a constant (for instance 0), solutions can be written by inspection. For constant coefficients, exponentials (plane waves) satisfy the equation:

$$\Psi = \Psi_0 e^{ikx} e^{-iEt/\hbar}$$

- To show this, substitute the answer in the equation.

Note:

$$\frac{\partial}{\partial t} e^{\alpha t} = \alpha e^{\alpha t}$$

$$i\hbar \frac{-iE}{\hbar} \Psi = -\frac{\hbar^2}{2m} (ik)^2 \Psi$$

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

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

As long the above equation is satisfied, our guessed solution will satisfy the Schrödinger equation.

Note that for a given value of k, the value of E is fixed but the equation given above.

E-k Relationship

- What if U was a non 0 constant (U_0)? The answer is that the same solution will satisfy the equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi + U_0 \Psi$$

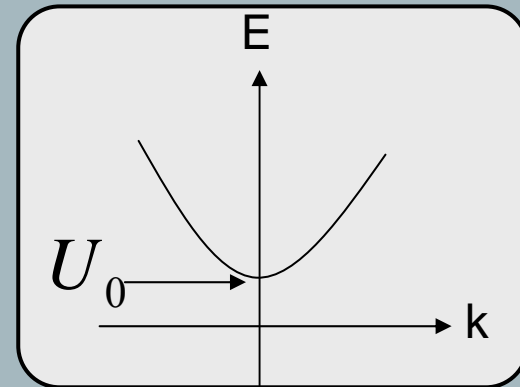
$$E = \frac{\hbar^2 k^2}{2m} + U_0$$

- We have the same solution but a new E-k relationship.
- If U was a function of x , this solution wouldn't work:

$$E = \frac{\hbar^2 k^2}{2m} + U_0(x)$$

- For a given k , both E and k are constants but x can change so E will change and this is a contradiction.

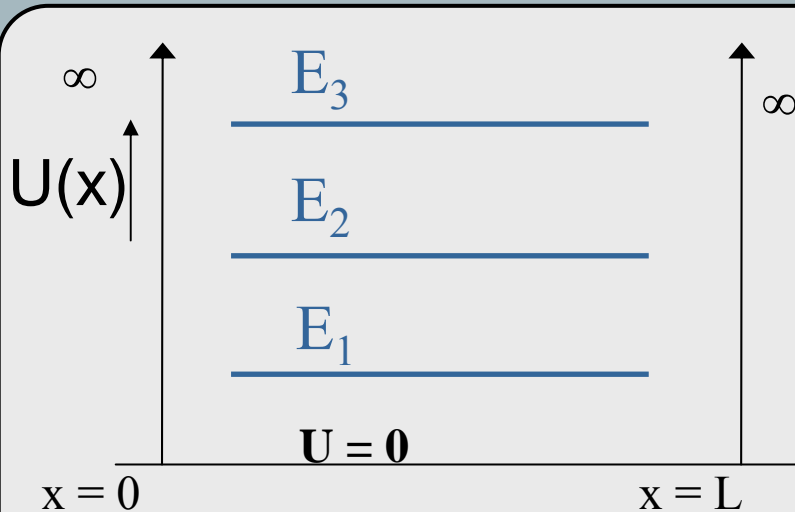
- The general rule is that as long as the coefficients are not function of time, the time portion of the solution is (ϕ is some function of x): $\Psi = \phi(x)e^{-iEt/\hbar}$
- The E-k relationship looks like:



- Notice that there is no quantization involved. All values of energy are allowed. The quantization comes in play when we impose a box.

Particle in a Box

- Consider a $U(x)$ like:



- The question is: what are the allowed energies for this problem?
- Notice that since the potential is infinite at the two sides the wavefunction cannot get out of the box and has to go to 0 at the two sides of the box. We have: $\Psi(x=0) = 0$
B.C. $\Psi(x=L) = 0$

- The solution

$$\Psi = \Psi_0 e^{ikx} e^{-iEt / \hbar}$$

will not work here because it is never 0.

- Since

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi + U_0 \Psi$$

is a linear equation, we can use a superposition solution.

$$e^{ikx} + e^{-ikx} = 2 \cos kx$$

$$e^{ikx} - e^{-ikx} = 2i \sin kx$$

To satisfy the first Boundary Condition (BC), we choose sin function as an answer:

$$\Psi = \Psi_0 \sin(kx) e^{ikx} e^{-iEt / \hbar}$$

To satisfy the second BC: $k_n L = n\pi$

From Confinement to Discreteness

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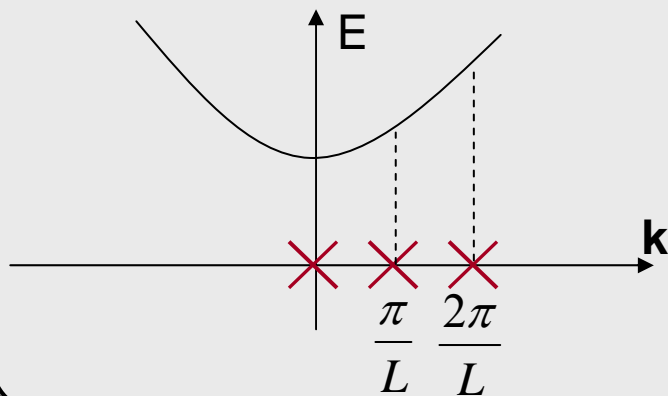
- Only certain values of k are allowed:

$$k_n = n\pi / L$$

- Which if it is put in $E = \frac{\hbar^2 k^2}{2m} + U_0$

- results in discrete allowed values of E :

$$E_n = U_0 + \frac{\hbar^2}{2m} \frac{n^2 \pi^2}{L^2}$$



- The discreteness of energy levels is a consequence of trying to confine the wavefunction in a potential box. If confined in a smaller box, the energy values will be further apart.

- An example for the level spacing:

$$\frac{4\hbar^2}{4 \times 2m} \frac{\pi^2}{L^2} \approx \frac{(6.6 \times 10^{-34} \text{ J} \cdot \text{sec})^2}{8 \times 9.11 \times 10^{-31} \text{ kg} \times (10^{-8} \text{ m})^2} \approx$$

10 meV

- The physical sense is that when an electron is confined in a box of size 100\AA , we'll get discrete levels with the energy spacing of the order few meV.