Fundamentals of Nanoelectronics

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Lecture 9: Schrödinger Equation
Ref. Chapter 2.1

Network for Computational Nanotechnology

nanoHUB
online simulations and more
NCN

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

• We've been talking about solutions to 1D Schrödinger equation. A simple example is the case of constant potential. For harder cases, we we'll learn a numerical method that would help us to solve for the energy levels of a material with arbitrary potential. First we'll consider the 1D case and then we'll get into 3D.
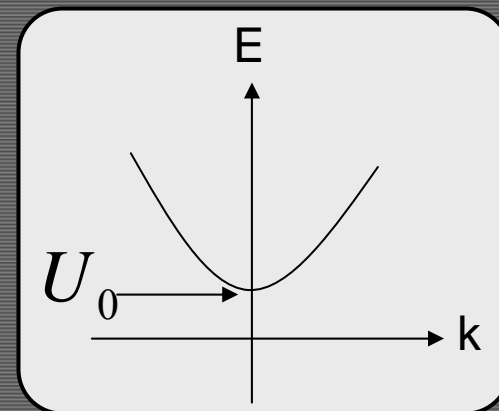
• The simplest case is:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi + U_0 \Psi \quad (1)$$

• The solutions to a differential equation with constant coefficients (like above) can be solved by plane waves:

$$\Psi(x,t) = Ae^{ikx}e^{-iEt/\hbar} \quad (2)$$

• Substitution of this solution into the equation leads to an E-k relationship.
• (2) in (1) =>
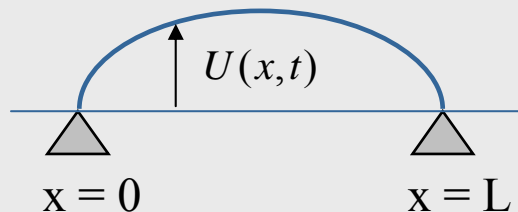
$$i\hbar \cdot \frac{-iE}{\hbar}\Psi = -\frac{\hbar^2}{2m}(ik)^2\Psi + U_0\Psi$$

$$E_n = U_0 + \frac{\hbar^2 k_n^2}{2m} \quad \text{Dispersion Relation}$$

• Schrödinger equation is a wave equation. A common example of a wave equation is the acoustic waves on a string. There the quantity that is used to describe the wave is the displacement of each point on a string from an equilibrium point at a particular time.

Harmonically oscillating string

$U(x,t)$

x = 0   x = L

• The equation describing such waves is:

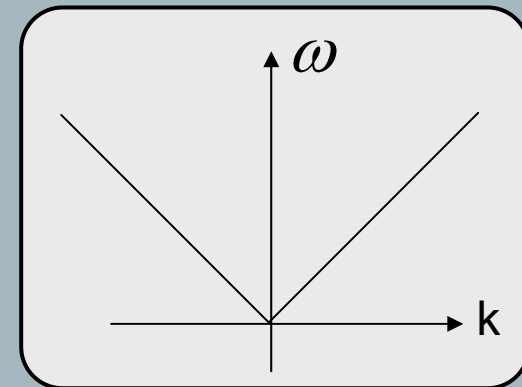$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial u^2} \quad (1)$$

• Solutions can be written as:

$$U(x,t) \propto e^{ikx} e^{-i\omega t} \quad (2)$$

• Again by substituting the solution in the wave equation we can get the dispersion relation. (1) in (2) =>

$$(-i\omega)^2 u = v^2 (ik)^2$$

$$\omega^2 = v^2 k^2 \quad \text{Dispersion Relation}$$

ω

k

• You can see the analogy between the two wave equations.
• One point is in order and that is: there are times where people start from a dispersion relation and deduce form it a differential equation; reveres of what we've done here.
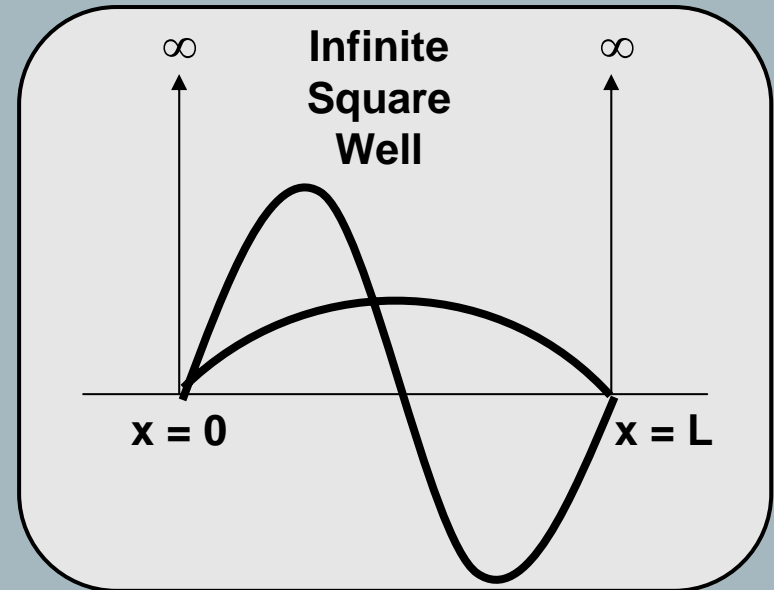
• The next thing to understand is solving for the energy levels having more complicated potential functions. The first example that was presented was that of a particle in a box.
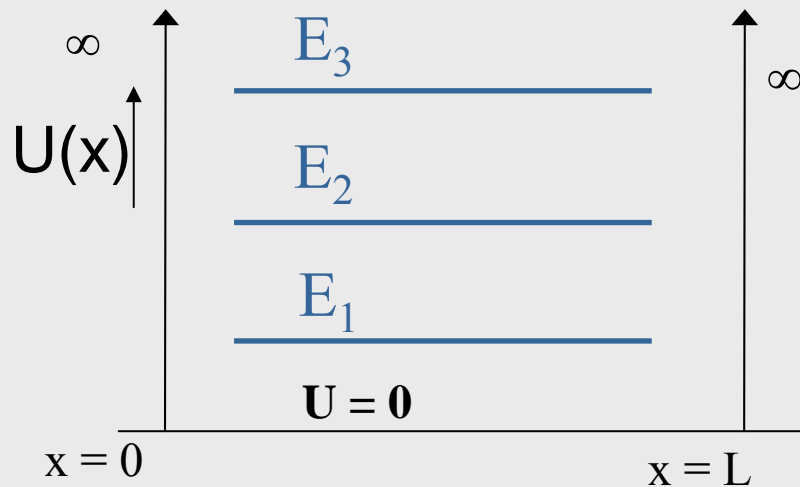
• Assuming that the potential is very high at the two ends, one can show that the wave function has to go to 0 at the two ends: $\Psi(x=0)=0$ & $\Psi(x=L)=0$

• This way we can have solutions like:

Infinite Square Well

• This allows only certain values of k which leads to discreteness in the energy levels shown in the left figure. The reason is that the wavelength must be such that the wave could fit inside the box. (k is related to the wavelength by $k=2\pi/\lambda$)

• What we saw last day was that for the wave that goes to 0 at the two ends we cannot use:

$$\Psi(x,t) = A e^{ikx} e^{-iEt/\hbar}$$

because this is never 0. Notice that there are two values of k for a given energy. We can use a superposition of solutions with k and –k to write the proper solution.
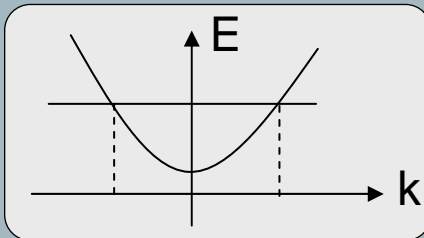
• We have:
$$e^{ikx} + e^{-ikx} = 2\cos kx$$
$$e^{ikx} - e^{-ikx} = 2i\sin kx$$

• Since in this problem the wave has to go to 0 at x=0, we choose the "sinkx". Further, the boundary condition at x=L requires: $k_n L = n\pi$

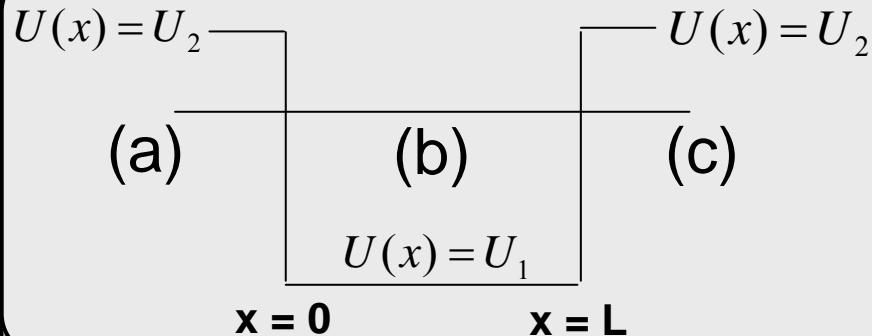• The corresponding energy also becomes quantized:

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

• This shows that whenever an electron is confined in a certain region, the allowed energy values become quantized.

• Suppose we have potential box like:

$$U(x) = U_2 \quad\rule{} \quad \rule{} \quad U(x) = U_2$$

(a)   (b)   (c)

$$U(x) = U_1$$

x = 0   **x = L**

• We are trying to find a solution with a given E. A solution like

$$\Psi(x,t) = A e^{ikx} e^{-iEt/\hbar}$$

will not satisfy the equation because we have two different values for the potential; hence two different values for k. To see this consider:

$$E = U + \frac{\hbar^2 k^2}{2m} \Rightarrow \hbar k = \sqrt{2m(E-U)} \quad (1)$$

• In region b we can write the solution as:

$$\Psi_1 = A e^{ik_1 x} + B e^{-ik_1 x}$$

• This is because we get two possible values of k for a given U from equation (1) so we can use a linear combination as a general solution.

• In regions b & c we can write the solution as:

$$\Psi_2 = A e^{ik_2 x} + B e^{-ik_2 x}$$

• If E<U2, then $\hbar k_2 = \sqrt{2m(E - U_2)}$ Gives an imaginary value for k2 and we get a decaying exponential in region a & c:

$$\Psi_a = D e^{+\gamma x} \qquad \Psi_c = C e^{-\gamma x}$$

• For region (c), exp(γx) is not allowed because the wavefunction cannot go to infinity for large x.

• For region (a), exp(-γx) is not allowed because the wavefunction cannot go to infinity for large negative x.

• The solutions in the regions a, b and c need to match at the boundaries x=o and x=L. Taking this requirement into account puts a restriction on the allowed values of constants A,B,C and D. We can use this restrictions to find the constants. These restrictions are called Boundary Conditions (BC's).

$De^{+\gamma x}$ (a)

$Ae^{ik_1 x} +$
$Be^{-ik_1 x}$ (b)

$Ce^{-\gamma x}$ (c)

x = 0   x = L

• The first BC is that the wavefunction has to be continuous across the boundaries.
• The second BC is that the derivative of wavefunction has to be continuous across the boundaries.

• What we mean is that discontinuities…

Discontinuous $\psi(x)$ or $d\psi/dx$

(x)
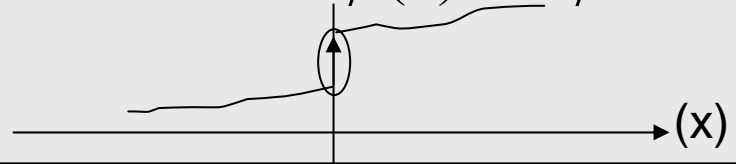
are not allowed because then the Schrödinger equation will not be satisfied at the point of discontinuity. Same is true for the derivative of the wavefunction. The reason is that in each case there will be an unmatched delta function (infinite height) in the Schrödinger equation where all other entities are finite:

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

Note: if Ψ is discontinuous, then dΨ/dx is a delta function. If dΨ/dx is discontinuous, then d^2Ψ/dx^2 is discontinuous.

$$De^{+\gamma x}$$

$$Ae^{ik_1 x} +$$

$$Be^{-ik_1 x}$$

$$Ce^{-\gamma x}$$

(a)　　　　(b)　　　　(c)

x = 0　　　　**x = L**

• We will not get into the details of this problem. Instead we'll use a more convenient method of solving and that is the numerical method.

• We can utilize BC's as follows:
• Continuity of Ψacross x=0 gives us one equation that relates A, B and D:

$$D = A + B$$

• Continuity of Ψacross x=L gives us one equation that relates A, B and C. Similarly, continuity if dΨ/dx gives us two equations at the two boundaries. One gets a set of equations that could be used to eliminate the unknown constants.

• In electronic devices we are interested in two things the most: electron density inside a device and current flow.
• If an electron has a wavefunction , the associated electron density is: $n = \Psi^* \Psi$
• For example take the potential well:

Infinite Square Well

∞   ∞

x = 0   x = L
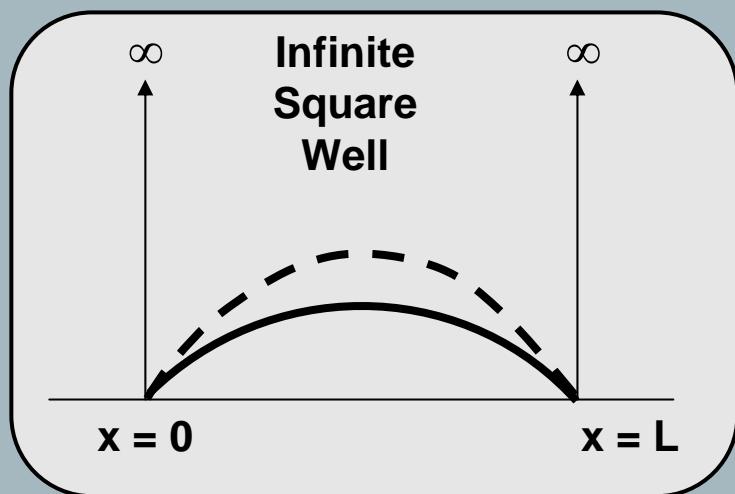
•The associated electron density would come from squaring the sin wave inside the box. (solid:Ψ & dashed :n)

• Notice that for 1 electron inn the box, the shape of electron density n may indicate that there is a fraction of electron at each point. This is not right. The correct view is that to look at these fractional values as probabilistic values of finding the electron at each point.
• Notice for adding electrons in different states we have two ways to come up with n:

$$\Psi_1^* \Psi_1 + \Psi_2^* \Psi_2 \text{ or } \left(\Psi_1 + \Psi_2\right)^* \left(\Psi_1 + \Psi_2\right)$$

• The correct answer is the first one. With electrons what we have to add are the electron densities not the wavefunctions.

- For an electron that has the wavefunction: $\Psi(x,t) = Ae^{ikx}e^{-iEt/\hbar}$ (1)

- Electron density is: $n = \Psi^*\Psi$ (2)

- Current can be written as (the reason comes later):
$$I = (-q)\frac{i\hbar}{2m}\left(\psi\frac{d\psi^*}{dx} - \psi^*\frac{d\psi}{dx}\right) (3)$$

- (1) in (2) => $n = A^2$

- (1) in (3) => $I = (-q)\frac{i\hbar}{2m}\left(-ikA^2 - ikA^2\right) = -q\frac{\hbar k}{m}A^2$

- Where did equation (3) come from? If one accepts (2), then (3) is the only consistent expression for current "I" considering the fact that Ψ has to satisfy the Schrödinger equation. Accepting (2) and (3) will satisfy the continuity equation and since the equation of continuity is general true argument (3) must be the right choice for "I".

Continuity Equation: $\frac{\partial(-qn)}{\partial t} = -\frac{\partial I}{\partial x}$

This is a general argument and states that the electron density in a region cannot change over time unless the gradient of current is non-0 in the region. Moreover, the amount of current leaving the region has to be equal to the rate of change of electron density.