Recitation #2

ENEE 313: Introduction to Device Physics

Fall, 2018

1 summary

To understand the scope of the chapter s, you need to ask yourself that what findings in photoelectric effect and atomic spectra puzzled us at that time and what's the drawback of the Bohr model. All these motivate scientists to develop Quantum mechanics to model the world downsizing to small particles. Also, you need to learn how to use the Schrodinger equation to real problems, solve the boundary conditions, and understand the physical interpretation under the equation.

Chapter 2 starts from photoelectic effect and atomic spectra. The effect indicates that electrons can be emitted from a metal surface if you shined light of high enough frequency.

1. electric current could be emitted from the metal surface if you shined light of high enough frequency

2. increasing intensity of light results in the increase of photocurrent

3. the energy of the individual electrons wouldnt change with the intensity of light, only frequency. If you shined light of higher frequency, then the energy of the emitted electrons would be greater.

4. low frequency light cannot make the emission of photoelectrons no matter what the intensity of the incident light was.

Atomic spectra tells you that when electric current ran through the tube, the emitted light/energy has discrete set of frequencies. The discrete frequencies obeyed certain relationships which were governed by reciprocals of integers squared. The Bohr model explains the spectra. However, the frequency-dependent intensity of electrons puzzle and the incompetence of describing more complicated atomic model than hydrogen by the Bohr model make us realize classical theories like mechanics and electrodynamics are not enough to do it. This lead to the development of Quantum mechanics. The hear of Quantum mechanics include the uncertainty principle and the Schrodinger wave equation, which involving probability theory and solving partial differential equation. Please find time to review probability, ODE, and PDE.

The Schrodinger wave equation, $\Psi(x, y, z, t)$. The probability density function of finding a particle at (x,y,z,t) is

$$\text{probability density function} = |\Psi^{*}\Psi|^{2}$$

The probability of finding the particle in small volume element dxdydz around the point (x, y, z) at time t is

$$\text{probability} = |\Psi(x,y,z,t)|^2 dxdydz$$

Since the magnitude of the Schrodinger equation is probability density function, it satisfies

$$\int_{-\infty}^{\infty} |\Psi^* \Psi|^2 dxdydz = 1$$

An usually approach to solve the Schrodinger equation is separation of variables and it results in two equations. Let's assume $\Psi(x,y,z,t) = \psi(x,y,z)\phi(t)$

1. Time-independent Schrodinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z) + V(x,y,z)\psi(x,y,z) = E\psi(x,y,z)$$

2. Time-dependent part

$$\frac{d\phi(t)}{dt} + \frac{jE}{\hbar} = 0$$

What interests us is use the potential function V to describe the state of electrons. For example, $V = 0$ means electrons are free to flow in a medium. The infinity potential well problem in the textbook describe that electrons are bounded in the well and cannot escaped.

To make sure feasibility of the solution to the Schrodinger equation corresponds to physically realistic situations, the wave function must satisfy the following set of boundary conditions:

1. $\Psi = 0$ at $+\infty$ and $-\infty$
2. Ψ is continuous across all boundaries
3. $\frac{\partial \Psi}{\partial x}$ is also continuous
4. In regions where $V(x)$ is infinite, Ψ must be zero.

Exercise The Particle in finite potential well. Let's use an finite potential well problem for exercising. Figure 1 shows a 1D finite potential energy well. The potential energy barriers outside the well are not infinity, but have a finite height which is equal to V_0. We need to divide the space into three regions solve the Schrodinger equation.

1. Region I,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_I(x)}{\partial x^2} + V_0\psi_I(x) = E\psi_I(x)$$

   The solution is simply,

$$\psi_I(x) = Aexp(K_I x) + Bexp(K_I x),$$
$$K_I = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

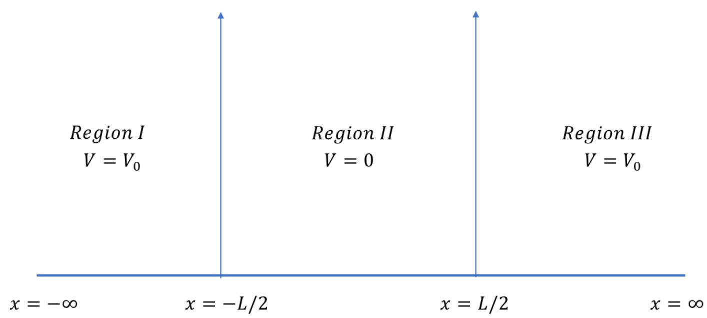

Figure 1: Finite potential well

2. Region II,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_{II}(x)}{\partial x^2} = E\psi_{II}(x)$$

The solution is,

$$\psi_{II}(x) = Ccos(K_{II}x) + Dsin(K_{II}x),$$
$$K_{II} = \sqrt{\frac{2m}{\hbar^2}E}$$

3. Region III, the PDE is similar with the one in the region I. The solution is

$$\psi_{III}(x) = Fexp(K_{III}x) + Gexp(K_{III}x),$$
$$K_{III} = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

To get the six coefficients, we need to apply the boundary conditions discussed above.

1. $\psi(x) = 0$ at $+\infty$ and ∞.
2. $\psi(x)$ is continuous at the boundary between the region I and region II and the boundary between the region II and the region III
3. $\frac{\partial\psi}{\partial x}$ is continuous at the boundary between the region I and region II and the boundary between the region II and the region III

Therefore, $\psi_I(-\infty) = 0$ gives $B = 0$ and $\psi_{III}(+\infty) = 0$ gives $F = 0$.

$$\psi_{II}(\frac{L}{2}) = \psi_{III}(\frac{L}{2}),$$
$$\psi_I(-\frac{L}{2}) = \psi_{II}(-\frac{L}{2}),$$
$$\frac{\partial\psi_{II}}{\partial x}|_{\frac{L}{2}} = \frac{\partial\psi_{III}}{\partial x}|_{\frac{L}{2}},$$
$$\frac{\partial\psi_{II}}{\partial x}|_{-\frac{L}{2}} = \frac{\partial\psi_{III}}{\partial x}|_{-\frac{L}{2}},$$

Additional condition is that the Ψ function satisfies

$$\int_{-\infty}^{\infty} |\Psi^* \Psi|^2 dxdydz = 1$$

Solving these equations is not trivial. The physical interpretation of the wave function in this example is that since $|\psi_I|^2$ and $|\psi_{III}|^2$ are not zero, this means the particles can be found outside the well even they don't have enough energy to jump out of the barrier formed by the well.

In the next recitation, I'll give you an exercise for the tunneling phenomena.