CHAPTER 4
SCRODINGER'S EQUATION

A. Introduction

The old quantum theory have explained successfully about line spectral in hydrogen atom. This theary also have shown physical phenomena in atomic and subatomic order fulfilled principle and rule which far different from principle and rule which fulfilled in macroscopics physical systems. Nevertheles the old quantum theory still be ad hoc and the fact that it can not be applied in unperiodicaly phenomena in atomic order. Now it is required a new quantum theory which more general and comprehensive.

In 1926 was found a motion equation for physical system in atomic order. The true or false of the quantum mechanics equation depend on the relevance between theorytical result and observatiom result about the physical observables, This is based on the fact that physics is quantitative.

Figure 4.1. Erwin Schrodinger

This presented several essential thing which must be contained in new mechanics theory. Most parts are fundamental thing in old quantum theory as follow:

1. The classical concept about path does not have meaning I quantum physics system, it only can be applied a statistical meaning about the position probability of particle in space (Heisenberg principle).
2. Dualism of wave and particle.
3. If particle is presented as a wave so for the wave fulfilled superposition principle of wave. If ψ_1 and ψ_2 is solution of the wave equation so $\psi=c_1\psi_1+c_2\psi_2$ also the solution of the wave equation (c_1 and c_2 are constant).
4. In the equation is also can be applied de Broglie postulate and Einstein's quantum theory: $\lambda = \dfrac{h}{p}$ and $E = h\upsilon$.

5. The energy conservation law in non relativistic case : $E = \frac{p^2}{2m} + V$, where p linear momentum, m mass of particle, and V potential energy.
6. For constant of V, E and p also must be constant and particle is presented as a monochomatis standing wave (de Broglie).

B. The Difference of Clasiccal Physics and Quantum Physics

Klasik	Kuantum
○ The future of particle can be determined from initial position, initial momentum and force which exert on it. In macroscopics world all quantities can be determined with enough precisition so the classical prediction is according to the observation result.	○ The future of pafrticle does not clear because now era of particle is unknown. Position and momentum of particle can not be determined with enough precision (effect of Heisenberg uncertainty)
○ The approximation version of quantum mechanics.	○ It is more universal.
○ Based on the perception of sense.	○ Based on the behavior of subatomic particle and systems that can not be observed direcly.
○ Describe an individual object in space and its changes in traveling time..	○ Describe the behavior of system statistically.
○ Predict an event.	○ Predict the possibility of event.
○ Assume that objevtive reality was out of there.	○ It does not assume that objective reality is free from our experience.
○ We can observe something without change it.	○ We can not observe something without change it.
○ It claim based on the absolut thruth that real universe was in the back of screen."	○ It claim that can correlate experience correctly.

C. The Meaning of Wave Function

- Wave function usually has a form of complex number: $\psi = A + iB$, which consist of real part and imaginer part.
- Complex conjugate: $\psi^* = A - iB$

- The density of probability:

  $|\psi|^2 = \psi^* \psi = (A - iB)(A + iB) = A^2 + B^2$ always be real.
- $|\psi|^2$ is proportional with probability density for obtaining particle represented by wave function ψ.
- Interpretation of Max Born in 1926 stated that if in time t is made measurement obout position of particle related with wave function of ψ(x,t) so the magnitude of probability P(x,t)dx of particle will be found in interval of x and x+dx is $\psi^*(x,t)\psi(x,t)dx$.

Figure 4.2. Max Born

- Integral of $|\psi|^2$ in all space must be finite.
- $\int_{-\infty}^{+\infty} |\psi|^2 dV = 0$, has meaning is not be found a particle.
- The probability for finding particle in certain time in all space must be equals to 1. So $\int_{-\infty}^{+\infty} |\psi|^2 dV = 1$ atau $\int_{-\infty}^{+\infty} PdV = 1$.
- The normalization of wave function is required : $\int_{-\infty}^{+\infty} |\psi|^2 dV = 1$.
- The *well behaved* of wave fuction are:
  a. ψ has a singe value in a certain position and time.
  b. ψ must be kontinu.
- For particle which move in x axis the probability for finding particle is:

  $P = \int_{-\infty}^{+\infty} |\psi|^2 dx$

D. Wave Equation

The wave equation of y which propagates in x axis with speed of v is:

$$\frac{\delta^2 y}{\delta x^2} = \frac{1}{v^2}\frac{\delta^2 y}{\delta t^2} \tag{4.1}$$

Solution of equation (4.1) is:

$$y = F\left(t \pm \frac{x}{v}\right) \quad (4.2)$$

Where F a function which can be deferentied.

Based on equation (4.2) it means that there are 2 solutions:

1. $y = F\left(t - \frac{x}{v}\right)$ propagates in +x axis direction
2. $y = F\left(t - \frac{x}{v}\right)$ propagates in –x axis direction

General solution for the monochromatic harmonic wave function with a constant angular frequency ω, not be damped (constant amplitude) and propagates in +x axis direction is:

$$y = Ae^{-i\omega\left(t - \frac{x}{v}\right)} \quad (4.3)$$

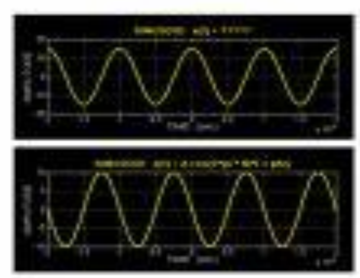

Figure 4.3. Sinusoidal Wave

By remembering : $e^{-i\theta} = \cos\theta - i\sin\theta$ equation (4.3) can be written:

$$y = A\left[\cos\omega\left(t - \frac{x}{v}\right) - i\sin\left(t - \frac{x}{v}\right)\right] \quad (4.4)$$

E. Time Dependent of Schrodinger Equation:

Based on equation of $\psi = Ae^{-i\omega\left(t - \frac{x}{v}\right)}$

By substitute : $\omega = 2\pi\upsilon$ and $v = \upsilon\lambda$ in equation (4.4) it is obtained :

$$\psi = Ae^{-2\pi\upsilon i\left(t - \frac{x}{\upsilon\lambda}\right)}$$

$$\psi = Ae^{-2\pi i\left(\upsilon t - \frac{x}{\lambda}\right)}$$

Because $E = h\upsilon = 2\pi\hbar\omega$ and $\lambda = \frac{h}{p} = \frac{2\pi\hbar}{p}$ it is obtained:

$$\psi = Ae^{-\left(\frac{i}{\hbar}\right)(Et-px)} \tag{4.5}$$

Equation (4.5) is representation of free particle with total energy *E* and momentum *p* moves in +x axis direction.

Then equation (4.5) is deferentiated two times in x, it is obtained:

$$\frac{\delta^2\psi}{\delta x^2} = \frac{\delta^2}{\delta x^2}(Ae^{-\left(\frac{i}{\hbar}\right)(Et-px)})$$

$$= \frac{\delta}{\delta x}\left(-\frac{pi}{\hbar}Ae^{-\left(\frac{i}{\hbar}\right)(Et-px)}\right)$$

$$= -\frac{p^2}{\hbar^2}Ae^{-\left(\frac{i}{\hbar}\right)(Et-px)}$$

$$\frac{\delta^2\psi}{\delta x^2} = -\frac{p^2}{\hbar^2}\psi \tag{4.6}$$

Partial deferential of equation (4.5) in t:

$$\frac{\delta\psi}{\delta t} = \frac{\delta}{\delta t}(Ae^{-\left(\frac{i}{\hbar}\right)(Et-px)})$$

$$= -\frac{iE}{\hbar}Ae^{-\left(\frac{i}{\hbar}\right)(Et-px)}$$

$$\frac{\delta\ \psi}{\delta t} = -\frac{iE}{\hbar}\psi \tag{4.7}$$

Total energy E pada in low speed fulfilled :

$$E = \frac{p^2}{2m} + V$$

Substitute E to ψ it is obtained:

$$E\psi = \frac{p^2}{2m}\psi + V\psi \tag{4.8}$$

From equation (4.7) it is obtained:

$$E\psi = -\frac{\hbar}{i}\frac{\delta\psi}{\delta t} \tag{4.9}$$

From equation (4.6) it is obtained:

$$p^2\psi = -\hbar^2\frac{\delta^2\psi}{\delta x^2} \tag{4.10}$$

By substitute equation (4.9) and (4.10) in (4.8) it is obtained:

$$-\frac{\hbar}{i}\frac{\delta\psi}{\delta t} = -\frac{\hbar^2}{2m}\frac{\delta^2\psi}{\delta x^2} + V\psi$$

$$i\hbar\frac{\delta\psi}{\delta t} = -\frac{\hbar^2}{2m}\frac{\delta^2\psi}{\delta x^2} + V\psi \tag{4.11}$$

Equation (4.11) is a dependent time of Schrodinger equation in one dimensional case. For three dimensional case, the Schrodinger equation is:

$$i\hbar\frac{\delta\psi}{\delta t} = -\frac{\hbar^2}{2m}\left(\frac{\delta^2\psi}{\delta x^2} + \frac{\delta^2\psi}{\delta y^2} + \frac{\delta^2\psi}{\delta z^2}\right) + V\psi \tag{4.12}$$

where operator: $\nabla^2 = \frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2}$

Equation (4.12) can be written in simple term:

$$i\hbar\frac{\delta\psi}{\delta t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \tag{4.13}$$

F. Expectation Value

Definition about probanility density of P give a way to predict the average value of the position of particle in certain time. The average value is called expectation value. The average position of particle fullfilled:

$$\bar{x} = \frac{N_1x_1 + N_2x_2 + N_3x_3 + ...}{N_1 + N_2 + N_3 + ...} = \frac{\sum N_i x_i}{\sum N_i} \tag{4.14}$$

For particle, the number of N_i must be replace with P_i. At position of x_i particle can be found in interval of dx.

$$P_i = |\psi_i|^2 dx$$

Expectation value for finding particle is:

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} x|\psi|^2 dx}{\int_{-\infty}^{+\infty} |\psi|^2 dx} \tag{4.15}$$

If ψ is a normalized wave function so $\int_{-\infty}^{+\infty} |\psi|^2 dx = 1$ that it is obatained an expectation value:

$$\langle x \rangle = \int_{-\infty}^{+\infty} x|\psi|^2 dx \tag{4.16}$$

The same procedure is applied for finding expectation value of <G(x)> as potensial energy of V(x) as follow:

$$\langle G(x) \rangle = \int_{-\infty}^{+\infty} G(x)|\psi|^2 dx \tag{4.17}$$

Expectation value of momentum <*p*> can not obtained by this way, because according to the Heisenberg uncertainty, there is no function of *p(x)*. If we determine of *x* so that Δx=0termine p, because:

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

Similar thing is occurred in expectation value of nergyi <E>.

G. Time Independent of Schrodinger Equation

Based on equation:

$$\Psi = Ae^{-\left(\frac{i}{\hbar}\right)(Et-px)} = Ae^{-\left(\frac{iE}{\hbar}\right)t} e^{\left(\frac{ip}{\hbar}\right)x}$$
$$\Psi = \psi e^{-\left(\frac{iE}{\hbar}\right)t} \tag{4.18}$$

where ψ is a position dependent of wave.

$$\Psi = \psi(t)\psi(x)$$

Substitute equation (4.18) in time dependent of Schrodinger equation (4.11):

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

Is obtained:

$$E\psi e^{-\left(\frac{iE}{\hbar}\right)t}=-\frac{\hbar^2}{2m}e^{-\left(\frac{iE}{\hbar}\right)t}\frac{\partial^2\psi}{\partial x^2}+V\psi e^{-\left(\frac{iE}{\hbar}\right)t}$$

$$\frac{\partial^2\psi}{\partial x^2}+\frac{2m}{\hbar^2}(E-V)\psi=0 \qquad (4.19)$$

Equation (4.19) is *steady state* Schrodinger equation in one dimension.

For three dimensional case:

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\frac{2m}{\hbar^2}(E-V)\psi=0 \qquad (4.20)$$

A steady state Schrodinger equation only can be solved for certai energy E (quantification energy). Kunantification of energy is characteristic of all physical system which is stable.

A near analogy about quantification of energy in solve Schrodinger equation is case of rope with length of L which is strengted with binded of both edge.

H. Particle in One dimensional Box

The analogy of particle in one dimensional box is a standing standing wave of rope with both edge is binded. The wave function in wall equals to zero.

$$\Psi_{dinding}=0$$

The relation between wide of box L and wave length of λ is shown in Figure 4.4.

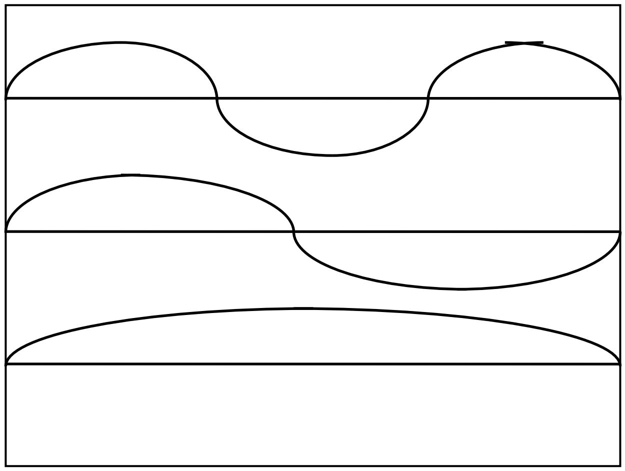

Figure 4.4. The relation between wide of box L and wave length of λ

The de-Broglie wave length of pafrticle in general can be formulated :

$$\lambda_n = \frac{2L}{n} \quad , \ n = 1, 2, 3, \ldots \tag{4.21}$$

Kinetic energy of particle:

$$K = \frac{1}{2}mv^2 = \frac{(mv)^2}{2m} = \frac{p^2}{2m} \tag{4.22}$$

Because $\lambda = \frac{h}{mv} \Leftrightarrow mv = \frac{h}{\lambda}$

Substitute equation (4.21) in equation (4.22), it is obtained kinetic energy of particle *K*:

$$K = \frac{h^2}{2m\lambda^2} \tag{4.23}$$

In this model, potential energy of partile *V*=0, that the energy which belonged to the particle:

$$E_n = K = \frac{h^2}{2m\lambda_n^2} = \frac{h^2}{2m\left(\frac{2L}{n}\right)^2}$$

$$\Leftrightarrow E_n = \frac{n^2h^2}{8mL^2} \tag{4.25}$$

For quantum number n = 1, the energy of particle is:

$$E_1 = \frac{h^2}{8mL^2}$$

The energy of pafrticle with quantum number of n can be written in E_1 as follow:

$$E_n = n^2 E_1 \qquad (4.26)$$

Based on (4.26) it can be concluded that:
- Energy of particle is quatified.
- Quantum number is charactersation of energy state
- Minimum energy of particle $\neq 0$.

The simplest problem in quantum mechanics is problem about particle in one dimensional box which has unfinite hard wall. The motion of particle finited in x axis between x=0 and x=L caused by the unfinite hard wall. A particle does not loose its energy when it collides the wall. It means that the total energy of particle is constant. According to formal view in quantum mechanics, potential energy of particle V to be infinite in both edge of the wall, mean while its potential energy in the box is constant equals to zero.

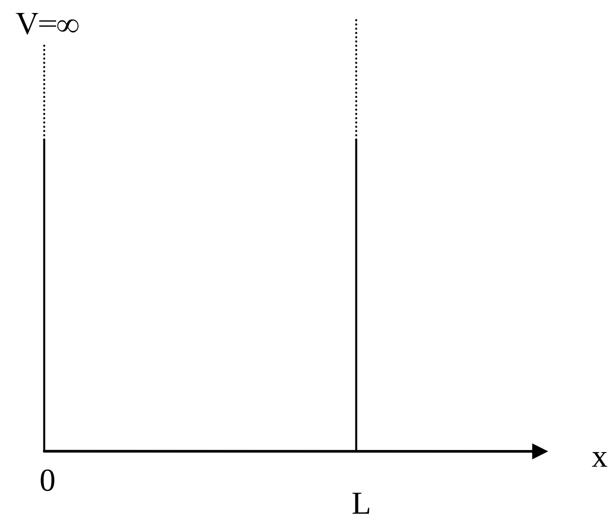

Figure 4.5. Potential Well

Because particle can not has infinite energy, so particle does not probable out of box, so the wave function equals to zero for $x \leq 0$ and $x \geq L$. Our task is determining the wave function in the box.

Schrodinger equation in the box:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0 \qquad (4.27)$$

Equation (4.27) has solution:

$$\psi = A\sin\frac{\sqrt{2mE}}{\hbar}x + B\cos\frac{\sqrt{2mE}}{\hbar}x \qquad (4.28)$$

Which can be proved again in equation (2.27) with A and B are nonstants that must be deremined.

This solving must be limited with boundary requirement $\psi = 0$ for x = 0 and x = L. Because cos 0 =1 the second term does not equal to zero for x = 0, so B must be zero (B=0). Then because sin 0 =0 so the term which consist of sinus always produce $\psi = 0$ for x =0 as which required, but it will be zero at x = L if only:

$$\frac{\sqrt{2mE}}{\hbar}L = n\pi \text{ for } n = 1, 2, 3, \ldots \qquad (4.29)$$

It caused zero value of sinus occurred at the angle of π, 2π, 3π, …

From equation (4.29) it is clear that energy that can belong to the particle has a certain value that called eigen value. The eigen value of energy states fulfilled:

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \text{ where } n = 1, 2, 3, \ldots \qquad (4.30)$$

The wave function of particle in one dimensional box which has energy of E_n is:

$$\psi_n = A\sin\frac{\sqrt{2mE_n}}{\hbar} \qquad (4.31)$$

By substitute equation (4.30) in (3.31) it is obtained:

$$\psi_n = A\sin\frac{n\pi x}{L} \qquad (4.32)$$

Which state eigen function according to value of E_n.

The normalization of the wave function is:

$$\int_0^L |\psi_n|^2 dx = A^2\int_0^L \sin^2\frac{n\pi x}{L}dx = A^2\frac{L}{2}$$

$$A^2 \frac{L}{2} = 1$$

$$A = \sqrt{\frac{2}{L}}$$

So the normalized wave function of particle in one dimensional box is:

$$\psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \text{ ; n = 1, 2, 3, …} \tag{4.33}$$

Probability density of $|\psi_1|^2$, $|\psi_2|^2$, dan $|\psi_3|^2$ is shown in Figure 4.6 as follow:

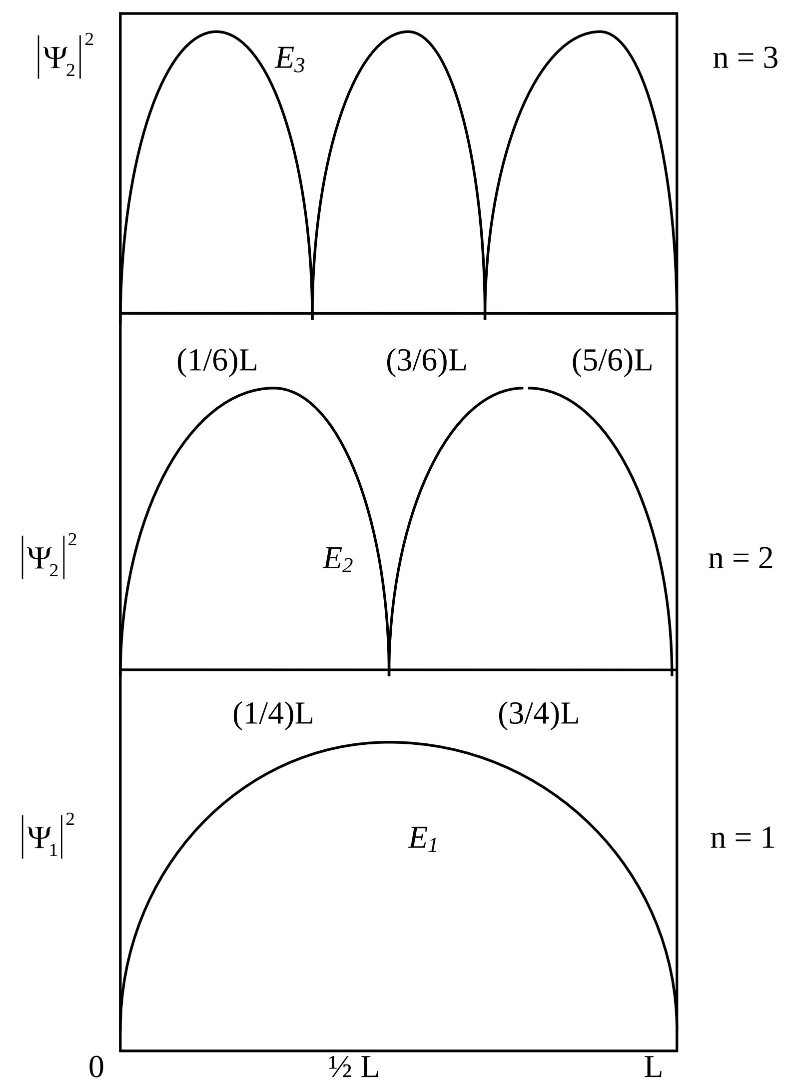

Figure 4.6. Probability Density for Finding Particle in One Dimensional Box

Based on 4.6 it can be described that:

- $|\psi_1|^2, |\psi_2|^2$, dan $|\psi_3|^2$ always positive and because its wave function is normalized so the value of $|\psi_n|^2$ for certain x equals to the probability P for finding particle in that point.

- The biggest probability for finding particle which has energy of E_1 is placed at position of ½L.

- The biggest probability for finding particle which has energy of E_2 is placed at position of ¼ L and ¾ L.

- The biggest probability for finding particle which has energy of E_3 is placed at position of 1/6 L, 3/6 L, and 5/6 L.

- The biggest probability for finding particle is deffretent depend on the wave function of particle, position and its energy state.

- In clasiccal view is stated that it has the same probability for finding particle at each point in one dimensional box.

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