1952033 侯雅玥 2020.10.7

1 QUANTUM MECHANIC

1.1 Wave Function

- Schrodinger function

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

- Actually, V is called potential function and is independent of time t and it reference to the potential energy of particle

According to the definition of potential function

$$\boldsymbol{E}=-\nabla\varphi(\boldsymbol{r})$$

$\boldsymbol{E}$ is a electrical field function

- hence Schrodinger function can be discribe as

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

$\psi(x)$is the position-dependent portion of wave function and $\phi(t)$ is the time-dependent portion of wave function.

- hence ,we can write the wave function as

$$i\hbar\frac{\partial(\psi(x)\phi(t))}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2(\psi(x)\phi(t))}{\partial x^2}+\psi(x)\phi(t)V(x)$$

$$i\hbar\psi(x)\frac{\partial\phi(t)}{\partial t}=-\frac{\hbar^2}{2m}\phi(t)\frac{\partial^2\psi(x)}{\partial x^2}+\psi(x)\phi(t)V(x)$$

$$i\hbar\frac{\partial\phi(t)}{\phi(t)\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\psi(x)\partial x^2} + V(x)$$

- For the left portion of the function is only related to t and the right portion is only related to x , hence both two parts are constant. Denote this constant by η ,then

$$\eta = i\hbar\frac{\partial\phi(t)}{\phi(t)\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\psi(x)\partial x^2} + V(x)$$

$$\phi(t) = Ce^{-j\frac{\eta t}{\hbar}}$$

And according to eular therom we can get ,

$$\phi(t) = C(cos(\frac{\eta t}{\hbar}) - jsin(\frac{\eta t}{\hbar}))$$

It's a sinusoidal wave, with $\omega = \frac{\eta}{\hbar}$,then we can get ,

$$T = \frac{2\pi}{\omega} = \frac{2\pi\hbar}{\eta} = \frac{h}{\eta}$$

$$\nu = \frac{1}{T} = \frac{\eta}{h}$$

$$\eta = h\nu = E$$

η refrence to the energy of the sinusoidal wave.

- hence ,

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

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

1.2 Physical Meaning of Wave Function

- $|\Psi(x,t)|^2$ refers to the probability density of finding the particle.

$$\phi(t) = Ce^{-j\omega t}$$

$$|\Psi(x,t)|^2 = \Psi\Psi^* = |\psi(x)|^2 Ce^{-j\omega t} Ce^{j\omega t} = C^2|\psi(x)|^2$$

We can incorporate C into $\psi(x)$, then

$$|\Psi(x,t)|^2 = |\psi(x)|^2$$

1.3 Boundry Conditions

- The function need to be normalized , for it is a discription of probability density , hence

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

- If the energy E and the $V(X)$ is both finite ,then there will be two boundry conditons:
  1. $\psi(x)$ must be finite , single-valued , continous
  2. $\frac{\partial\psi(x)}{\partial x}$ must be finite , single-valued , continous

1.4 Application of Wave Function

1.4.1 Electrons in free space

- When there is no force acting on the particle , so $V(x)$ must be a constant .

we have

$$E = h\nu = E_k + V(x)$$

$$E_k = \frac{h^2}{2m}$$

$$E - V(x) = \frac{h^2}{2m}$$

- $E_k \geq 0$ in free space , hence $E \geq V(x)$
  Assume $V(x) = 0$,

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

The solution of linear differential equation with constant coefficients of the second order is as follows :

if the characteristic function has

1. 2 different real root

$$y = C_1 e^{y_1 x} + C_2 e^{y_2 x}$$

2. 2 same real root

$$y = (C_1 + C_2 x) e^{y_1 x}$$

3. 2 conjugate complex root

$$y = e^{\alpha x}(C_1 cos(\beta x) + C_2 sin(\beta x))$$

$$y_1 = e^{\alpha x} cos(\beta x) \qquad y_2 = e^{\alpha x} sin(\beta x)$$

- hence , the solution of the partial differential equation is :

$$\psi(x) = C_1 exp[\frac{\sqrt{2mE}}{\hbar} ix] + C_2 exp[-\frac{\sqrt{2mE}}{\hbar} ix]$$

Assume,

$$k = \frac{\sqrt{2mE}}{\hbar}$$

then ,

$$\psi(x) = C_1 exp[ikx] + C_2 exp[-ikx]$$

- hence , recall the time-dependent function $\phi(t)$, there is

$$\Psi(x,t) = exp[-jwt](C_1 exp[ikx] + C_2 exp[-ikx])$$

We can assume that the particle motion direction is +x then there is $C_2 = 0$
- The relationship between k and λ can be derived as follows :

$$k = \frac{\sqrt{2mE}}{\hbar}$$

And because $V(x) = 0$, hence $E = \frac{1}{2}mv^2$

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

$$k = \frac{p}{\hbar}$$

And according to

$$p = \frac{h}{\lambda}$$

$$k = \frac{2\pi}{\lambda}$$

And ultimately , we get the result of Ψ

$$\Psi(x) = C_1 exp[j(kx - \omega t)]$$

$$\Psi\Psi^* = C_1 C_1^*$$

$\Psi\Psi^*$is independent to positio , when the particle's momentum is well-defined

1.4.2 The Infinite potential well

- In infinite potential well , there is

$$V(\boldsymbol{x}) = \begin{cases} 0 & 0 < r < a \\ \infty & x > a \quad x < 0 \end{cases}$$

When $x > a \qquad x < 0$, if E is finite then , $\psi(x) = 0$
When $0 < x < a$, there is

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

we define :

$$\frac{2mE}{\hbar^2} = k^2 \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

the solution is like :

$$\psi(x) = Asin(kx) + Bcos(kx)$$

- According to boundry condition , when $x = a$ and $x = 0$, $\psi(x) = 0$
hence $B = 0$ and $Asin(ka) = 0$, hence $ka = n\pi$.
For $k \neq 0 \quad a \neq 0$, $kx \neq 0$, hence $n\pi \neq 0 \quad n \neq 0$
And when $n < 0$, for $Asin(-n\pi) = -Asin(n\pi)$ the negative ones can be conbined into A

$$\psi(x) = Asin(kx) = Asin(\frac{n\pi}{a}x) \quad (n = 1, 2, 3, ...)$$

Normalization :

$$|\Psi(x,t)|^2 = |\psi(x)|^2$$

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 = \int_{-\infty}^{+\infty} |\psi(x)|^2 = \int_0^a A^2 sin^2(\frac{n\pi}{a}x) = \frac{aA^2}{2} = 1$$

hence ,

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

$$\psi(x) = \sqrt{\frac{2}{a}} sin(\frac{n\pi}{a}x) \quad (n = 1, 2, 3, ...)$$

1.4.3 The Step potential function

- The potential function is :

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x > 0 \end{cases}$$

- The incident flux and reflected flux are neither 0 ,
- hence in the region $x < 0$

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

the solution is like :

$$\psi_1(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}$$

And $k_1 = \frac{\sqrt{2mE}}{\hbar}$

- The first term is a traveling wave in direction of $+x$
  The second term is a traveling wave in direction of $-x$
  So , the first term refers to incident wave and the second term refers to the reflect wave.
- In th region of $x > 0$, $V(x) \neq 0$, Assume $V(x) > E$, then

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

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

$$k_2=\frac{\sqrt{2m(V(x)-E)}}{\hbar}$$

$$V(x)=V_0 \qquad k_2=\frac{\sqrt{2m(V_0-E)}}{\hbar}$$

Then there will be :

$$\psi_2(x)=A_2e^{k_2x}+B_2e^{-k_2x}$$

According to the boundry condition of finite $A_2=0$

$$\psi_2(x)=B_2e^{-k_2x}$$

According to the boundry condition

$$\psi_1(0)=\psi_2(0)=A_1+B_1=B_2$$

According to my comprehention , the variation of perticle at the two sides of $x=0$ is equal then ,

$$\frac{\partial\psi_1(0)}{\partial x}=\frac{\partial\psi_2(0)}{\partial x}$$

$$ik_1A_1-ik_1B_1=-B_2k_2$$

Then there will be :

$$B_1=\frac{ik_1+k_2}{ik_1-k_2}A_1$$

$$B_2 = \frac{2ik_1}{ik_1 - k_2} A_1$$