Chapter 2

Time - Independent Schrödinger Equation

how to get $\Psi(x,t)$? we need to solve

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi \qquad \text{for a specified potential}$$

Let us assume V independent of t

↳ method of separation of variables $\Big\{$ look for solutions of the form $\Psi(x,t) = \psi(x)\varphi(t)$

$$\underbrace{\frac{\partial \Psi}{\partial t}}_{\text{partial derivative}} = \psi \underbrace{\frac{d\varphi}{dt}}_{\text{ordinary derivative}} \qquad \frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2\psi}{dx^2}\varphi$$

Schröd eq $\quad i\hbar\psi \frac{d\varphi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}\varphi + V\psi\varphi$

Divide by $\psi\varphi$ $\quad \underbrace{\frac{i\hbar}{\varphi}\frac{d\varphi}{dt}}_{\text{function of } t} = \underbrace{-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V}_{\text{function of } x} \Rightarrow$ both sides have to be a constant E

Separation of variables ⇒ partial differential eq. becomes two ordinary differential equations

$$\frac{i\hbar}{\varphi}\frac{d\varphi}{dt} = E \Rightarrow \boxed{\frac{d\varphi}{dt} = -\frac{iE}{\hbar}\varphi} \Rightarrow \varphi(t) = e^{-iEt/\hbar}$$

(const absorbed into normalization of ψ)

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E \Rightarrow \boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi}$$

→ time indep. Schröd. eq.

need V(x) to solve it

Before solving the time <u>indep</u> Schröd eq

let us discuss some properties of the solutions to the time <u>dep</u> Schröd. eq as given by the separation of variables

$$\boxed{\Psi(x,t) = \psi(x)\,\varphi(t)}$$

1.) They are <u>stationary</u> <u>states</u>

$$\Psi(x,t) = \psi(x)\, e^{-iEt/\hbar} \qquad \text{deps on } t$$

but the <u>probability density</u> DOES <u>NOT</u>

$$|\Psi(x,t)|^2 = \Psi^*\Psi = \psi^* e^{-iEt/\hbar}\,\psi\, e^{iEt/\hbar} = |\psi(x)|^2$$

<u>nor</u> does the <u>expectation values</u>

$$\langle Q(x,p)\rangle = \int \Psi^* Q\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi\, dx = \int \psi^*(x)\, Q\left(x, \frac{\hbar}{i}\frac{d}{dx}\right)\psi(x)\, dx$$

↳ $\langle x\rangle$ is CONSTANT $\Rightarrow$ $\boxed{\langle p\rangle = 0}$

2.) They have <u>definite</u> <u>total</u> <u>energy</u> $\left\{\begin{array}{l}\text{the variance of } H \text{ is zero, there is no spread} \\ \text{given a } \Psi(x,t) \text{ we get always the same energy}\end{array}\right.$

class phys: total energy is the <u>Hamiltonian</u>

$$H(x,p) = \frac{p^2}{2m} + V(x)$$

quant mech: $\hat{H}$ is an <u>operator</u> $\quad \hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

time indep Schröd. eq $\Big\}$ $\boxed{\hat{H}\psi(x) = E\,\psi(x)}$ → (energy)

$$\left\{\begin{array}{l}\langle H\rangle = \int \psi(x)\,\underbrace{\hat{H}\psi(x)}_{E\psi(x)}\, dx = E\int|\psi(x)|^2 dx = E \\ \langle H^2\rangle = \int \psi(x)\,\underbrace{\hat{H}\,\underbrace{(\hat{H}\psi)}_{E\hat{\psi}}}_{E^2\hat{\psi}}\, dx = E^2\int|\psi(x)|^2 dx = E^2\end{array}\right.$$

$$\Rightarrow \sigma_H^2 = \langle H^2\rangle - \langle H\rangle^2 = \boxed{0}$$

3) General solution is a linear combination of separable solutions

time indep Schrod eq $\xrightarrow{\text{leads}}$ to various solutions $\psi_1(x),\ \psi_2(x),\ \psi_3(x) \dots$

$$\begin{array}{cccc} \psi_1(x) & \psi_2(x) & \psi_3(x) & \dots \\ \downarrow & \downarrow & \downarrow & \\ E_1 & E_2 & E_3 & \dots \end{array}$$

each associated with a separation const (energy)

For each allowed energy there is a different wave function

$$\Psi_1(x,t) = \psi_1(x)\, e^{-iE_1t/\hbar}$$

$$\Psi_2(x,t) = \psi_2(x)\, e^{-iE_2t/\hbar}$$

$$\vdots$$

Any linear combination is a solution of the time dep Schröd. eq.

General solution:

$$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x)\, e^{-iE_nt/\hbar}}$$

→ the consts c_n are fit according to the initial conditions

RECIPE

STRATEGY

Given $V(x)$ (potential) and $\Psi(x,0)$ (initial condition)

⇒ First: Use time indep. Schröd eq. to find set of solutions $\psi_1(x), \psi_2(x), \dots$ each associated with energies $E_1, E_2, \dots$

⇒ Second: Write down the general linear combination to fit $\Psi(x,0)$

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

⇒ Finally: Solution to time dep Schröd. eq. is simply

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x)\, e^{-iE_nt/\hbar}$$

CAREFUL (!)

Each separable solution $\Psi_n(x,t) = \psi_n(x)\, e^{-iE_n t/\hbar}$ is a stationary state

so probabilities and expectation values are indep. of time

BUT

the GENERAL solution is NOT a stationary state

$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x)\, e^{-iE_n t/\hbar}$ is NOT a stationary state

Example 2.1

$$\Psi(x,0) = c_1 \psi_1(x) + c_2 \psi_2(x)$$

$\Big\{$ assume c_n and $\psi_n(x) \to$ real

$\hookrightarrow \Psi(x,t) = c_1 \psi_1(x)\, e^{-iE_1 t/\hbar} + c_2 \psi_2(x)\, e^{-iE_2 t/\hbar}$

while $|\Psi_1(x,t)|^2 = |\psi_1(x)|^2$ and $|\Psi_2(x,t)|^2 = |\psi_2(x)|^2$ do not dep on time

we see that

$$|\Psi(x,t)|^2 = \left(c_1 \psi_1(x)\, e^{iE_1 t/\hbar} + c_2 \psi_2(x)\, e^{iE_2 t/\hbar}\right)\left(c_1 \psi_1(x)\, e^{-iE_1 t/\hbar} + c_2 \psi_2(x)\, e^{-iE_2 t/\hbar}\right) =$$

$$= c_1^2 \psi_1^2 + c_1 c_2 \psi_1 \psi_2\, e^{-i(E_2-E_1)t/\hbar} + c_1 c_2 \psi_1 \psi_2\, e^{i(E_2-E_1)t/\hbar} + c_2^2 \psi_2^2$$

$$\boxed{= c_1^2 \psi_1^2 + c_2^2 \psi_2^2 + 2 c_1 c_2 \psi_1 \psi_2 \cos\left[(E_2-E_1)t/\hbar\right]}$$

- prob. density oscillates sinusoidally at an angular frequency $(E_2-E_1)/\hbar$
- it is NOT a stationary state