

# Chapter 2

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## 1 Time evolution operator and Hamiltonian

Here, we talk about non-relativistic situation, and we think about time as a parameter, not an operator. The position representation  $\langle x|\psi\rangle = \psi(x)$ , adding the time evolution, we have

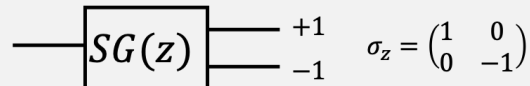
$$\langle x|\psi(t)\rangle = \psi(x, t)$$

First, we talk about 6 postulates of quantum mechanics.

### Box 1.1: Postulates of Quantum Mechanics

**Postulate 1.** At any time  $t$ , the state of a physical system is defined by a ket  $|\psi\rangle$ , or *state* in a relevant Hilbert space  $H$ .

**Postulate 2.** The only possible result of measuring observable  $A$  is one of the eigenvalues of  $A$


$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Aside:

1. If  $A$  is Hermitian, then the measurement gives a real number.
2. If  $A$ 's spectrum is discrete, then we only see quantized result.

**Postulate 3.** Every measurable physical quantity  $A$  is described by a Hermitian operator.

**Postulate 4.** If  $A|u_\alpha\rangle = a_\alpha|u_\alpha\rangle$ , then for a system in  $|\psi\rangle$ , when we measure  $A$ , then the probability of getting  $a_\alpha$  is  $P(a_\alpha) = |\langle u_\alpha|\psi\rangle|^2$ .

Aside: If we have degenerate  $a_\alpha$ 's  $\{|u_{\alpha,1}\rangle, |u_{\alpha,2}\rangle, \dots\}$  share the same eigenvalue, then  $P(a_\alpha) = \sum_i |\langle u_{\alpha,i}|\psi\rangle|^2$

Example:  $A = I$ , all  $a_\alpha = 1$

**Postulate 5.** If a measurement projects  $|\psi\rangle$  into a new state  $|u_\alpha\rangle$ , then a physical new state should be  $|u'_\alpha\rangle = \frac{|u_\alpha\rangle}{\sqrt{\langle u_\alpha|u_\alpha\rangle}}$ , so that  $\langle u'_\alpha|u'_\alpha\rangle = 1$ .

**Postulate 6.** Between measurement the state vector  $|\psi(t)\rangle$  evolves in time with time dependent Shrödinger's equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle$$

here  $\hat{H}$  is a Hamiltonian.

We let a displacement  $dt'$  on state  $|\psi(t)\rangle$ ,

$$\Rightarrow U(dt') |\psi(t)\rangle = |\psi(t + dt')\rangle, \text{ where } UU^\dagger = 1 \quad (1)$$

It's similar to momentum, in that case, we have

$$\begin{cases} U(dt') = I - i\frac{\hat{H}}{\hbar} dt' \\ \hat{H} \text{ is Hermitian, called Hamiltonian} \end{cases}$$

so (1) could be evaluated as:

$$\text{LHS} = \left( I - i\frac{\hat{H}}{\hbar} dt' \right) \psi(x, t) = \psi(x, t) - i\frac{\hat{H}}{\hbar} dt' \psi(x, t) \quad (2)$$

$$\text{RHS} = \psi(x, t + dt') = \psi(x, t) + \left( \frac{\partial}{\partial t} \psi(x, t) \right) dt' \quad (3)$$

$$\Rightarrow \boxed{i\hbar \frac{\partial}{\partial t} \psi(x, t) = H \psi(x, t)} \quad (4)$$

which is Shrödinger's equation in position representation. In general, we have

$$\boxed{i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle} \quad (5)$$

$H$ : Hamiltonian in analog to classical mechanics,

$$H = T + V, \quad \begin{cases} T = \frac{p^2}{2m} \text{ is kinetic energy} \\ V \text{ is potential energy} \end{cases} \quad (6)$$

and in quantum mechanics, we have

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + \hat{V}(x) \quad (7)$$

Here are some examples of Hamiltonians in different systems.

### Box 1.2: Examples of Hamiltonians in different systems

1. A free particle  $V = 0$

$$\hat{H} = \frac{\hat{p}^2}{2m}$$

2. Hydrogen atom

$$\hat{H} = \frac{\hat{p}_e^2}{2m_e} + \frac{\hat{p}_n^2}{2m_n} - \frac{e^2}{4\pi\epsilon_0|\vec{r}_e - \vec{r}_n|}$$

3. A particle with magnetic momentum  $\vec{\mu}$ , in external magnetic field  $\vec{B}$

$$\hat{H} = -\vec{\mu} \cdot \vec{B}$$

As  $\hat{H} = \frac{\hat{p}^2}{2m}$ , it's convenient to work in momentum representation  $\{|p\rangle\}$  as our basis. We apply  $\langle p|$  on the left of equation  $H|\psi(t)\rangle = i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle$ , we get

$$\text{LHS} = \left( \langle p| \frac{\hat{p}^2}{2m} \right) |\psi(t)\rangle = \frac{p^2}{2m} \langle p|\psi(t)\rangle = \frac{p^2}{2m} \psi(p, t) \quad (8)$$

$$\text{RHS} = i\hbar \langle p| \frac{\partial}{\partial t} |\psi(t)\rangle \stackrel{\frac{\partial}{\partial t} \langle p|=0}{=} i\hbar \frac{\partial}{\partial t} \langle p|\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} \psi(p, t) \quad (9)$$

$$\Rightarrow \frac{p^2}{2m} \psi(p, t) = i\hbar \frac{\partial}{\partial t} \psi(p, t) \quad (10)$$

$$\Rightarrow \psi(p, t) = \psi(p, 0) e^{-i \frac{p^2 t}{2m\hbar}} \quad (11)$$

if we let

$$\psi(p, 0) = \frac{1}{\sqrt{2\pi\hbar}} e^{-i \frac{px}{\hbar}} \sim \langle x|p\rangle \quad (12)$$

in this case,

$$\psi(p, t) = \frac{1}{\sqrt{2\pi\hbar}} e^{-i \frac{px}{\hbar}} e^{-i \frac{p^2 t}{2m\hbar}} = \frac{1}{\sqrt{2\pi\hbar}} e^{-i \frac{p}{\hbar} \left( x + \frac{pt}{m} \right)} \quad (13)$$

we have

$$\psi(p, 0) = \langle p|x\rangle \text{ momentum representation of } |x\rangle \quad (14)$$

$$\psi(p, t) = \langle p|x + \frac{pt}{m}\rangle \text{ if set } v = \frac{p}{m}, \text{ then } x + \frac{pt}{m} = x + vt \quad (15)$$

### Box 1.3: Comment

We should observe structure of  $H$ , and choose the right representations. We have

$$\psi(x, 0) \xrightarrow[\text{rewrite in p-repres}]{\text{Fourier transform}} \psi(p, 0)$$

$$\psi(p, t) \stackrel{H=\frac{p^2}{2m}}{=} \psi(p, 0) e^{-i \frac{p^2 t}{2m\hbar}}$$

if we need  $\psi(x, t)$ , we can get it from another Fourier transformation from  $\psi(p, t)$ .

## 2 Static Shrödinger's equation

Recall equation (5) that

$$\hat{H}|\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle$$

in position representation,

$$\langle x | \hat{H} | \psi(t) \rangle = i\hbar \frac{\partial}{\partial t} \langle x | \psi(t) \rangle \quad (16)$$

$$\Rightarrow H\psi(x, t) = i\hbar \frac{\partial}{\partial t} \psi(x, t) \quad (17)$$

where  $H = \frac{\hat{p}^2}{2m} + V(x)$ ,  $\hat{p} \leftrightarrow -i\hbar \frac{\partial}{\partial x}$ ,

$$\Rightarrow \boxed{-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) + V(x)\psi(x, t) = i\hbar \frac{\partial}{\partial t} \psi(x, t)} \quad (18)$$

### Box 2.1: A common mistake

We know that in  $x$  representation,  $\hat{p} \leftrightarrow -i\hbar \frac{\partial}{\partial x}$ , but

$$\langle x | \hat{p}^2 | \psi \rangle \neq -\hbar^2 \left( \frac{\partial}{\partial x} \psi(x) \right)^2$$

instead,

$$\boxed{\langle x | \hat{p}^2 | \psi \rangle = -\hbar^2 \frac{\partial^2}{\partial x^2} \psi(x)}$$

because we have

$$\langle x | \hat{p} | \psi \rangle = -i\hbar \frac{\partial}{\partial x} \langle x | \psi \rangle = -i\hbar \frac{\partial}{\partial x} \psi(x)$$

then

$$\begin{aligned} \langle x | \hat{p}^2 | \psi \rangle &\stackrel{|\phi\rangle=\hat{p}|\psi\rangle}{=} \langle x | \hat{p} | \phi \rangle = -i\hbar \frac{\partial}{\partial x} \langle x | \phi \rangle = (-i\hbar) \frac{\partial}{\partial x} \langle x | \hat{p} | \psi \rangle \\ &= (-i\hbar) \frac{\partial}{\partial x} \left( -i\hbar \frac{\partial}{\partial x} \langle x | \psi \rangle \right) = -\hbar^2 \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} \psi(x) \right) \\ &= -\hbar^2 \frac{\partial^2}{\partial x^2} \psi(x) \end{aligned}$$

To solve equation (18), it's best to separate the variables. Suppose we set

$$\psi(x, t) = \Psi(x)\phi(t) \quad (19)$$

where  $\hat{H}$  is Hermitian, and the eigenfunction is

$$H|\psi_E\rangle = E|\psi_E\rangle, \quad \begin{cases} E \text{ is eigen energy} \\ |\psi_E\rangle \text{ is eigenstate} \end{cases} \quad (20)$$

if we assume  $|\psi(t=0)\rangle = |\psi_E\rangle$ , then

$$\begin{aligned} H|\psi(t)\rangle &= i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle \\ \Rightarrow \langle \psi_E | H | \psi(t) \rangle &= i\hbar \frac{\partial}{\partial t} \langle \psi_E | \psi(t) \rangle \end{aligned} \quad (21)$$

$$\Rightarrow E \langle \psi_E | \psi(t) \rangle = i\hbar \frac{\partial}{\partial t} \langle \psi_E | \psi(t) \rangle \quad (22)$$

$$\xrightarrow{\xi(t) = \langle \psi_E | \psi(t) \rangle} E \xi(t) = i\hbar \frac{\partial}{\partial t} \xi(t) \quad (23)$$

$$\Rightarrow \xi(t) = e^{-i \frac{Et}{\hbar}} \xi(0) \quad (24)$$

### Theorem 2.1

We know a inner product of a state  $|\psi(t)\rangle$  with eigenstate  $|\psi_E\rangle$  is getting a phase  $e^{-i \frac{Et}{\hbar}}$  over time.

Probability of measuring with  $H$  after time  $t$  of evolution, is the same as any other time.

$$P_E(t) = |\langle \psi_E | \psi(t) \rangle|^2 = |e^{-i \frac{Et}{\hbar}} \langle \psi_E | \psi(0) \rangle|^2 = |\langle \psi_E | \psi(0) \rangle|^2 = P_E(t=0)$$

### Corollary 2.1

In the basis of energy  $\{|\psi_E^{(i)}\rangle\}$ ,

$$|\psi(0)\rangle \xrightarrow{\text{discrete}} \sum_i c_i |\psi_E^{(i)}\rangle \quad (25)$$

$$|\psi(t)\rangle \xrightarrow{H \neq H(t)} \sum_j c_j e^{-i \frac{E_j t}{\hbar}} |\psi_E^{(j)}\rangle \quad (26)$$