

Chapter 2: Quantum Dynamics

Yuquan Chen

2019/03/19

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

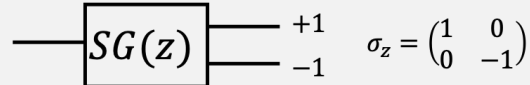
$$\langle x|\psi(t)\rangle = \psi(x, t)$$

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_α is $P(a_\alpha) = |\langle u_\alpha|\psi\rangle|^2$.

Aside: If we have degenerate a_α '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 (1.1) 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 (1.5) 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 $H = \frac{\hat{p}^2}{2m} + V(x)$, $\hat{p} \leftrightarrow -i\hbar \frac{\partial}{\partial x}$,

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

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,

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

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 (2.3), 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

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

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

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

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

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

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 $\{|\psi_E^{(i)}\rangle\}$,

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

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