Chapter 2: Quantum Dynamics

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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

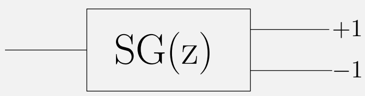
$$\langle x|\psi(t)\rangle = \psi(x,t)$$

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 $\{|u_{\alpha,1}\rangle, |u_{\alpha,2}\rangle, ...\}$ 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 $|\psi(t)\rangle$,

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

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:

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

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

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

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

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

H: Hamiltonian in analog to classical mechanics,

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

and in quantum mechanics, we have

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

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
$$\hat{H} = \frac{\hat{p}_e^2}{2m_e} + \frac{\hat{p}_n^2}{2m_n} - \frac{e^2}{4\pi\varepsilon_0|\vec{r}_e - \vec{r}_n|}$$
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

$$\text{LHS} = \left(\langle p|\frac{\hat{p}^2}{2m}\right)|\psi(t)\rangle = \frac{p^2}{2m}\langle p|\psi(t)\rangle = \frac{p^2}{2m}\psi(p,t) \tag{8}$$
$$\text{RHS} = i\hbar\langle p|\frac{\partial}{\partial t}|\psi(t)\rangle \xlongequal{\frac{\partial}{\partial t}\langle p|=0} i\hbar\frac{\partial}{\partial t}\langle p|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\psi(p,t) \tag{9}$$
$$\Rightarrow \frac{p^2}{2m}\psi(p,t) = i\hbar\frac{\partial}{\partial t}\psi(p,t) \tag{10}$$
$$\Rightarrow \psi(p,t) = \psi(p,0)e^{-i\frac{p^2t}{2m\hbar}} \tag{11}$$

if we let

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

in this case,

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

we have

$$\psi(p,0) = \langle p|x\rangle \text{ momentum representation of } |x\rangle \tag{14}$$
$$\psi(p,t) = \langle p|x + \frac{pt}{m}\rangle \text{ if set } v = \frac{p}{m}\text{, then } x + \frac{pt}{m} = x + vt \tag{15}$$

Box 1.3: Comment

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

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

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

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,

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

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

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

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

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

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

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

$$\psi(x,t) = \Psi(x)\phi(t) \tag{19}$$

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

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

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

$$\begin{aligned} H|\psi(t)\rangle &= i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle \\ \Rightarrow \langle\psi_E|H|\psi(t)\rangle &= i\hbar\frac{\partial}{\partial t}\langle\psi_E|\psi(t)\rangle \quad (21) \\ \Rightarrow E\langle\psi_E|\psi(t)\rangle &= i\hbar\frac{\partial}{\partial t}\langle\psi_E|\psi(t)\rangle \quad (22) \\ \xRightarrow{\xi(t)=\langle\psi_E|\psi(t)\rangle} E\xi(t) &= i\hbar\frac{\partial}{\partial t}\xi(t) \quad (23) \\ \Rightarrow \xi(t) &= e^{-i\frac{Et}{\hbar}}\xi(0) \quad (24) \end{aligned}$$

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

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

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