Quantum Dynamics (part 2)

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Quantum Dynamics

Time Evolution Operator:

$$|\Psi(t)\rangle = \hat{T}|\Psi(0)\rangle.$$

Schrödinger's Picture

$$|\Psi(t)\rangle \to \hat{T}|\Psi(0)\rangle,$$

with operators unchanged.

Heisenberg's Picture

$$\hat{X} \to \hat{T}^\dagger X \hat{T},$$

with state kets unchanged.

Schrödinger and Heisenberg

Schrödinger and Heisenberg

Schrödinger Equation of Motion

The Schrödinger equation of Motion is given by

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

Substituting $|\Psi(t)\rangle = \hat{T}|\Psi(0)\rangle$,

$$i\hbar \frac{d|\hat{T}\Psi(0)\rangle}{dt} = \hat{H}|\hat{T}\Psi(0)\rangle.$$

It yields, $i\hbar \frac{d\hat{T}}{dt} = \hat{H}\hat{T}$ When $\hat{H}$ is time-independent,

$$\hat{T} = e^{-i\hat{H}t/\hbar}.$$

Heisenberg Equation of Motion

The expectation value of an observable X at time t is given by

$$\begin{aligned} \langle X \rangle &= \langle \Psi(t)|X|\Psi(t)\rangle \\ &= \langle T\Psi(0)|X|T\Psi(0)\rangle \\ &= \langle \Psi(0)|T^\dagger XT|\Psi(0)\rangle \end{aligned}$$

In the Heisenberg's picture, all state kets remains constant in time $\Psi(0)$, but operators evolve with time as

$$X(t) = T^\dagger XT. \tag{1}$$

Heisenberg Equation of Motion

Considering an operator $X(t) = T^\dagger X T$ and a Hamiltonian $H(t) = T^\dagger H T$,

$$\frac{dX(t)}{dt} = \frac{d}{dt}[T^\dagger X T] = \frac{dT^\dagger}{dt}(XT) + T^\dagger X \frac{dT}{dt}.$$

Since the Schrödinger equation for the time evolution operator is

$$\frac{dT}{dt} = \frac{1}{i\hbar}\hat{H}T,$$

the time evolution of the operator is given by

$$\begin{aligned}
\frac{dX(t)}{dt} &= -\frac{1}{i\hbar}(T^\dagger \hat{H} X T) + T^\dagger X \frac{1}{i\hbar}\hat{H}T \\
&= \frac{1}{i\hbar}\left[T^\dagger X \hat{H} T - (T^\dagger \hat{H} X T)\right] \\
&= \frac{1}{i\hbar}\left[T^\dagger X T T^\dagger \hat{H} T - (T^\dagger \hat{H} T T^\dagger X T)\right] \\
&= \frac{1}{i\hbar}[X(t), H(t)]. \qquad (2)
\end{aligned}$$

Heisenberg Equation of Motion

Note that $[T^\dagger HT, H)] = [H, T^\dagger HT] = 0$, because $\hat{T} = e^{-i\hat{H}t/\hbar}$. It looks obvious but we have to check [see Assignment].

Therefore,

$$\frac{dH(t)}{dt} = \frac{1}{i\hbar}[H, H] = 0, \tag{3}$$

meaning that the Hamiltonian in Schrödinger and Heisenberg pictures are the same and a constant in time.

In general, an observable is a constant of the motion if an observable X satisfies the condition $[X, H] = 0$

Decomposition

We introduce a set of orthonormal bases $|i\rangle$ (or simply orthogonal bases of eigenstates)

$$|A\rangle = \sum_i \alpha_i |i\rangle.$$

Then, we can derive some useful relations

$$\langle j|A\rangle = \langle j| \sum_i \alpha_i |i\rangle = \sum_i \alpha_i \langle j|i\rangle$$

$$= \sum_i \alpha_i \delta_{ij} = \alpha_j.$$

$$|j\rangle\langle j|A\rangle = \alpha_j |j\rangle$$

$$|j\rangle\langle j| : \quad \text{projection operator}$$

$$|A\rangle = \sum_i \langle i|A\rangle |i\rangle = \sum_i |i\rangle\langle i|A\rangle.$$

$$\mathbb{1} = \sum_i |i\rangle\langle i| : \quad \text{identity operator}$$

Continuous Spectra

For continuous spectra, the identity relation is given by

$$\int_{-\infty}^{\infty} |x\rangle\langle x| dx = 1.$$

Then, a state ket $|A\rangle$ can be represented with an eigenket $|x\rangle$ corresponding to the eigenvalue x as

$$\begin{aligned} |A\rangle &= \int_{-\infty}^{\infty} dx |x\rangle\langle x|A\rangle \\ &= \int_{-\infty}^{\infty} dx \langle x|A\rangle|x\rangle. \end{aligned}$$

The quantity $\langle x|A\rangle$ is a complex function of the position eigenvalue x and the famous *wavefunction* in quantum mechanics.

Schrödinger Wave Equation

Suppose that $|x\rangle$ represents a simultaneous eigenket of the position operators, $\hat{x}|x\rangle = x|x\rangle$ (Note the orthogonality $\langle x|x'\rangle = \delta(x - x')$). Then, the wavefunction of the system corresponding the a state $|A\rangle$ is

$$\Psi_A = \langle x|A\rangle. \tag{4}$$

The inner product is

$$\begin{aligned}
\langle B|A\rangle &= \langle B| \int_{-\infty}^{\infty} dx|x\rangle\langle x|A\rangle \\
&= \int_{-\infty}^{\infty} dx\langle B|x\rangle\langle x|A\rangle \\
&= \int_{-\infty}^{\infty} \Psi_B^* \Psi_A dx.
\end{aligned}$$

Schrödinger Wave Equation in the Position Space

The Schrödinger equation of a state S is given by

$$\begin{aligned}
i\hbar\frac{d\Psi}{dt} &= i\hbar\frac{d\langle x|S\rangle}{dt} \\
&= \langle x|\hat{H}|S\rangle \\
&= \langle x|\frac{\hat{p}^2}{2m} + \hat{V}|S\rangle \\
&= \langle x| - \frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \hat{V}|S\rangle \\
&= \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \hat{V}\right]\langle x|S\rangle \\
&= -\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + \hat{V}\Psi
\end{aligned}$$

Schrödinger Wave Equation in the Momentum Space

The wavefunction in the momentum space is

$$\Phi = \langle p|S\rangle, \tag{5}$$

where $|A\rangle$ is a state ket, $|p\rangle$ is a eigenket of the momentum operators.

The Schrödinger equation of a state A is given by

$$\begin{aligned} i\hbar\frac{d\Phi}{dt} &= i\hbar\frac{d\langle p|S\rangle}{dt} \\ &= \langle p|\hat{H}|S\rangle \\ &= \langle p|\frac{\hat{p}^2}{2m} + \hat{V}(p)|S\rangle \\ &= \left[\frac{\hat{p}^2}{2m} + \hat{V}(p)\right]\langle p|S\rangle \\ &= \left[\frac{\hat{p}^2}{2m} + \hat{V}(p)\right]\Phi \end{aligned}$$

with $\hat{x} = i\hbar\frac{d}{dp}$.

Commutation Relation

$$[x,p] = i\hbar. \tag{6}$$

$$\begin{aligned}
[x,p]f(x) &= x\left(-i\hbar\frac{d}{dx}\right)f(x) - \left(-i\hbar\frac{d}{dx}\right)[xf(x)] \\
&= x\left(-i\hbar\frac{df(x)}{dx}\right) + i\hbar f(x) + i\hbar x\frac{df(x)}{dx} \\
&= i\hbar f(x).
\end{aligned}$$

$$\begin{aligned}
[x,p]f(p) &= \left(i\hbar\frac{d}{dp}\right)[pf(p)] - p\left(i\hbar\frac{d}{dp}\right)f(p) \\
&= i\hbar f(p).
\end{aligned}$$

Fourier Transformation: Position and Momentum Space

Let us consider the momentum eigenkets $|p_x\rangle$ in the coordinate space. Then, $\langle x|p_x\rangle$ must satisfy

$$\begin{aligned}\langle x|\hat{p}_x|p_x\rangle &= p_x\langle x|p_x\rangle \\ &= -i\hbar\frac{d}{dx}\langle x|p_x.\rangle\end{aligned}$$

Solving the equation, we find

$$\langle x|p_x\rangle \sim e^{ipx/\hbar} = e^{ikx},$$

where $p = \hbar k$.

Fourier Transformation: Position and Momentum Space

With the proper normalization, we find

$$\langle x|p_x\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}.$$

Then, it is easily shown that

$$\begin{aligned} \Psi(x) &= \langle x|S\rangle \\ &= \int_{-\infty}^{\infty} dp \langle x|p\rangle\langle p|S\rangle \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp e^{ipx/\hbar} \langle p|S\rangle \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp e^{ipx/\hbar} \Phi(p). \\ \Phi(p) &= \langle p|S\rangle \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx e^{-ipx/\hbar} \Psi(x). \end{aligned}$$

Where to go next...

Measurements and the Uncertainty Relation