Time evolution of states in quantum mechanics[1]

The time evolution from time t_0 to t of a quantum mechanical state is described by a linear operator $\hat{U}(t,t_0)$. Thus a ket at time t that started out at t_0 being the ket $|\alpha(t_0)\rangle = |\alpha\rangle$ is

$$|\alpha(t)\rangle = \hat{U}(t,t_0)|\alpha\rangle \tag{1}$$

The time evolution operator $\hat{U}(t,t_0)$, which also is known as a propagator, satisfies three important properties:

1. The time evolution operator should do nothing when $t = t_0$:

$$\lim_{t\to t_0}\hat{U}(t,t_0) = 1 \tag{2}$$

2. The propagator should preserve the normalization of state kets. That is, if $|\alpha\rangle$ is normalized at t_0 it should also be normalized at later times t. This leads to the requirement

$$\begin{aligned}\langle\alpha|\alpha\rangle &= \langle\alpha(t)|\alpha(t)\rangle \\ &= \langle\alpha|\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0)|\alpha\rangle\end{aligned}$$

which implies $\hat{U}^\dagger(t,t_0)\hat{U}(t,t_0) = 1$ or

$$\hat{U}^\dagger(t,t_0) = \hat{U}^{-1}(t,t_0). \tag{3}$$

That is, $\hat{U}(t,t_0)$ is a *unitary* operator. A unitary operator preserves the norm of the states.

3. The propagator should satisfy the composition property

$$\hat{U}(t_2,t_0) = \hat{U}(t_2,t_1)\hat{U}(t_1,t_0) \tag{4}$$

which means that in order to evolve a state from t_0 to t_2 we might as well first evolve the state from t_0 to t_1 and then evolve the state so obtained from t_1 to t_2.

Explicit form of $\hat{U}$

Let us now consider an infinitesimal time evolution step dt, $\hat{U}(t_0+dt,t_0)$. For such a time-evolution the above three properties are satisfied up to order dt by the operator

$$\hat{U}(t_0+dt,t_0) = 1 - i\hat{\Omega}(t_0)dt \tag{5}$$

where $\hat{\Omega}(t_0)$ is a Hermitian operator, $\hat{\Omega}^\dagger(t_0) = \hat{\Omega}(t_0)$.

Let us show that the three above properties are indeed satisfied: Property 1 is obviously fulfilled as the second term in Eq. (5) vanishes when $dt \to 0$. Property 2 holds up to first order in dt as is clear from

$$\hat{U}^\dagger(t_0+dt,t_0)\hat{U}(t_0+dt,t_0) = \left(1 + i\hat{\Omega}(t_0)dt\right)\left(1 - i\hat{\Omega}(t_0)dt\right) = 1 + O(dt^2). \tag{6}$$

[1] Adapted from J.J. Sakurai, Modern Quantum Mechanics, Addison-Wesley 1993

The left hand side of property 3 is

$$\hat{U}(t_0 + 2dt, t_0) = 1 - i2\hat{\Omega}(t_0)dt \tag{7}$$

and the right hand side is

$$\begin{aligned}
\hat{U}(t_0 + 2dt, t_0 + dt)\hat{U}(t_0 + dt, t_0) &= (1 - i\hat{\Omega}(t_0 + dt)dt)(1 - i\hat{\Omega}(t_0)dt) \\
&= (1 - i\hat{\Omega}(t_0)dt + \mathcal{O}(dt^2))(1 - i\hat{\Omega}(t_0)dt) \\
&= 1 - 2i\hat{\Omega}(t_0)dt + \mathcal{O}(dt^2)
\end{aligned}$$

So property 3 holds also to order dt.

Now comes the question of how to identify $\hat{\Omega}$? The answer to this can be guessed from classical mechanics where the generator of time translations is the Hamiltonian of the system. Therefore

$$\hat{\Omega}(t) = \hat{H}(t)/\hbar \tag{8}$$

where $\hat{H}(t)$ is the Hamiltonian. The $\hbar$ is inserted to get the dimensions right. Eq. (8) can in fact be taken as one of the fundamental postulates of quantum mechanics and is, as will be shown below, equivalent to the time-dependent Schrödinger equation. From Eqs. (8) and (5) it follows that

$$\hat{U}(t + dt, t) = 1 - i\frac{\hat{H}(t)}{\hbar}dt \tag{9}$$

Note that in writing this we have kept the possibility of having a Hamiltonian that explicitly has a time dependence. That is, the Hamiltonian *operator* might itself depend on time. We will not encounter many such Hamiltonians in this course, however at this stage it is good to be general. Such time-dependent Hamiltonians are encountered when one considers systems on which there are external time-varying fields imposed.

Schrödinger equation

From the Eq. (9) it is easy to derive the Schrödinger equation.

$$\hat{U}(t + dt, t_0) = \hat{U}(t + dt, t)\hat{U}(t, t_0) = \left(1 - i\frac{\hat{H}(t)}{\hbar}dt\right)\hat{U}(t, t_0) \tag{10}$$

Subtracting $\hat{U}(t, t)\hat{U}(t, t_0) = \hat{U}(t, t_0)$ on both sides one gets

$$\hat{U}(t + dt, t_0) - \hat{U}(t, t_0) = -i\frac{\hat{H}(t)}{\hbar}dt\hat{U}(t, t_0) \tag{11}$$

dividing by dt and multiplying by $i\hbar$ on both sides one gets

$$i\hbar\frac{d}{dt}\hat{U}(t, t_0) = \hat{H}(t)\hat{U}(t, t_0) \tag{12}$$

where we have taken the limit $dt \to 0$. Multiplying both sides by the ket $|\alpha\rangle$ we get

$$i\hbar \frac{d}{dt}\hat{U}(t,t_0)|\alpha\rangle = \hat{H}(t)\hat{U}(t,t_0)|\alpha\rangle \tag{13}$$

$$i\hbar \frac{d}{dt}|\alpha(t)\rangle = \hat{H}(t)|\alpha(t)\rangle \tag{14}$$

which is the Schrödinger equation. The Schrödinger equation is a first order differential equation. Thus the knowledge of $|\alpha(t_0)\rangle$, determines the state at any later time uniquely. Therefore the time-evolution of states in quantum mechanics is deterministic and continuous. In this sense quantum mechanics is as deterministic as classical mechanics. However, there is also another type of (instantaneous) "time"-evolution in quantum mechanics. When a *measurement* is made on the system the state vector changes suddenly. This socalled "collapse of the wave function" is not deterministic nor continuous. In this note we are only concerned about the time evolution of states when no measurements are being made.

Time-independent Hamiltonians

Let us now look at the case where the Hamiltonian is *not* explicitly time dependent. That is, the Hamiltonian operator is not altered when the time parameter t is changed. In this case one can obtain the full expression for $\hat{U}$

$$\hat{U}(t,t_0) = e^{-i\frac{\hat{H}}{\hbar}(t-t_0)} \tag{15}$$

where the exponential of the operator on the right hand side is to be understood as its power series expansion $e^{\hat{x}} = 1 + \hat{X} + \frac{1}{2!}\hat{X}\hat{X} + \cdots$. It is easily checked by differentiation with respect to t that this expression for $\hat{U}$ satisfies eq. (12). With this expression for $\hat{U}$ it is unnecessary to use the Scrödinger equation to obtain the time dependence. Instead one can just multiply the states with the operator $\hat{U}$ in Eq.(15) to obtain the time-dependent result. The result of this multiplication is particularly simple to write down if one expands the initial state in terms of the eigenstates of the Hamiltonian; the energy eigenstates:

Let $|n\rangle$ be the *energy eigenstates* and expand the initial state at $t_0 = 0$ in terms of these

$$|\alpha\rangle = \sum_n \alpha_n |n\rangle \tag{16}$$

then the state at time t is

$$\begin{aligned} |\alpha(t)\rangle &= \hat{U}(t,0)|\alpha\rangle \\ &= \sum_n \alpha_n e^{-i\frac{\hat{H}}{\hbar}t}|n\rangle \\ &= \sum_n \alpha_n e^{-i\frac{E_n}{\hbar}t}|n\rangle \end{aligned}$$

where we have used the series expansion of the exponential to get to the last line:

$$
\begin{aligned}
e^{-i\hat{H}t/\hbar}|n\rangle &= \left(1 + (-it/\hbar)\hat{H} + \frac{(-it/\hbar)^2}{2!}\hat{H}\hat{H} + \dots\right)|n\rangle \\
&= \left(1 - i(t/\hbar)E_n + \frac{(-it/\hbar)^2}{2!}E_n^2 + \dots\right)|n\rangle \\
&= e^{-iE_n t/\hbar}|n\rangle
\end{aligned}
$$

Thus

$$|\alpha(t)\rangle = \sum_n \alpha_n e^{-i\frac{E_n}{\hbar}t}|n\rangle \tag{17}$$

Example: Mixed Harmonic oscillator state

Consider the superposition of two harmonic oscillator energy eigenstates

$$|\beta\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|2\rangle \tag{18}$$

where $|0\rangle$ is the energy eigenket with $E_0 = \hbar\omega/2$ and $|2\rangle$ is the energy eigenket with energy $E_2 = 5\hbar\omega/2$. The harmonic oscillator Hamiltonian is not explicitly dependent on time so we can use eq.(17). The time dependence of this state becomes then

$$
\begin{aligned}
|\beta(t)\rangle &= \frac{1}{\sqrt{2}}e^{-i\omega t/2}|0\rangle + \frac{1}{\sqrt{2}}e^{-i5\omega t/2}|2\rangle \\
&= e^{-i\omega t/2}\left(\frac{1}{\sqrt{2}}|0\rangle + e^{-i2\omega t}\frac{1}{\sqrt{2}}|2\rangle\right)
\end{aligned}
$$

Stationary states

The time dependence of the *expectation value* of an operator is given by

$$\langle\alpha(t)|\hat{O}|\alpha(t)\rangle = \langle\alpha|\hat{U}^\dagger(t,t_0)\hat{O}\hat{U}(t,t_0)|\alpha\rangle \tag{19}$$

For some *states* the expectation value is independent of time:

$$\langle\alpha(t)|\hat{O}|\alpha(t)\rangle = \langle\alpha|\hat{O}|\alpha\rangle. \tag{20}$$

Such states are called **stationary states** if the expectation values of *all* operators $\hat{O}$, all operators that do not explicitly depend on time, are constant in time.

It is clear that when the state is such that the action of $\hat{U}$ is simply to change the state by a global phase

$$\hat{U}(t,t_0)|\alpha\rangle = e^{i\phi(t,t_0)}|\alpha\rangle \tag{21}$$

then the expectation values for all operators will be time-independent and the state is a stationary state. This is because

$$\langle\alpha|\hat{U}^\dagger(t,t_0)\hat{O}\hat{U}(t,t_0)|\alpha\rangle = e^{-i\phi(t,t_0)}e^{i\phi(t,t_0)}\langle\alpha|\hat{O}|\alpha\rangle = \langle\alpha|\hat{O}|\alpha\rangle \tag{22}$$

Note that although the state is stationary the state is still time-dependent as its phase changes with time. Note also that the energy *eigenstates* are such stationary states because the only effect of the time evolution operator is to multiply the state by a time-dependent phase

$$\hat{U}(t,0)|n\rangle = e^{-iE_n/\hbar t}|n\rangle \tag{23}$$

Example of a non-stationary state

Consider again the mixed harmonic oscillator state $|\beta\rangle$ of the previous example and evaluate the expectation value of the position operator squared $\hat{X}^2$.

$$\begin{aligned}\langle\beta(t)|\hat{X}^2|\beta(t)\rangle &= e^{i\omega t/2}\left(\frac{1}{\sqrt{2}}\langle 0| + \frac{e^{2i\omega t}}{\sqrt{2}}\langle 2|\right)\hat{X}^2 e^{-i\omega t/2}\left(\frac{1}{\sqrt{2}}|0\rangle + \frac{e^{-2i\omega t}}{\sqrt{2}}|2\rangle\right)\\ &= \frac{1}{2}\langle 0|\hat{X}^2|0\rangle + \frac{1}{2}\langle 2|\hat{X}^2|2\rangle + \frac{e^{i2\omega t}}{2}\langle 2|\hat{X}^2|0\rangle + \frac{e^{-2i\omega t}}{2}\langle 0|\hat{X}^2|2\rangle\end{aligned}$$

So this state is not stationary. Note that it is the mixed matrix elements $\langle 2|\hat{X}^2|0\rangle$ and $\langle 0|\hat{X}^2|2\rangle$ which cause the time-dependence. If we had considered expectation values of operators where these matrix elements vanish, the expectation values would not depend on time. The state $\beta(t)\rangle$ is not stationary because we can find a (time-independent) operator (here $\hat{X}^2$) which expectation value does depend on time.

Schrödinger and Heisenberg pictures

The discussion above centered on the time evolution of ket states, while there is no time evolution of the operators. This is called the Schrödinger picture. It is however also possible to take another view in which the kets are stationary while the operators evolve in time. This is called the Heisenberg picture. That these pictures are equivalent when calculating matrix elements of operators (which is all one does to calculate outcomes of measurement etc.) follows from the associative equality

$$\begin{aligned}\overbrace{\langle\alpha(t)|\hat{O}|\beta(t)\rangle}^{\text{Schrödinger picture}} &\equiv \left(\langle\alpha|\hat{U}^\dagger(t,t_0)\right)\hat{O}\left(\hat{U}(t,t_0)|\beta\rangle\right)\\ &= \langle\alpha|\left(\hat{U}^\dagger(t,t_0)\hat{O}\hat{U}(t,t_0)\right)|\beta\rangle \equiv \underbrace{\langle\alpha|\hat{O}(t)|\beta\rangle}_{\text{Heisenberg picture}}\end{aligned} \tag{24}$$

where the time evolution of an operator in the Heisenberg picture is defined as

$$\hat{O}(t,t_0) = \hat{U}^\dagger(t,t_0)\hat{O}\hat{U}(t,t_0) \tag{25}$$

Heisenberg equation of motion

Using Eqs. (9) and (25) one can derive an equation analogous to the Schrödinger equation for how an operator in the Heisenberg picture evolves in time. Taking the infinitesimal evolution

$$\begin{aligned}\hat{O}(dt+t,t) &= \left(1+idt\hat{H}(t)/\hbar\right)\hat{O}(t)\left(1-idt\hat{H}(t)/\hbar\right) \\ &= \hat{O}(t)+\frac{i}{\hbar}\left(\hat{H}(t)\hat{O}(t)-\hat{O}(t)\hat{H}(t)\right)dt+\mathcal{O}(dt^2) \qquad (26)\end{aligned}$$

Moving $\hat{O}(t)$ to the left hand side and dividing by dt and taking the limit $dt \to 0$ one gets

$$\frac{d}{dt}\hat{O}(t)=\frac{i}{\hbar}\left[\hat{H}(t),\hat{O}(t)\right] \qquad (27)$$

which is known as the Heisenberg equation of motion which plays the same role in the Heisenberg picture as the Schrödinger equation plays in the Schrödinger picture.